



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:09 pm BST

PDB ID : 5J88
Title : Structure of the E coli 70S ribosome with the U1060A mutation in 16S rRNA
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-04-07
Resolution : 3.32 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

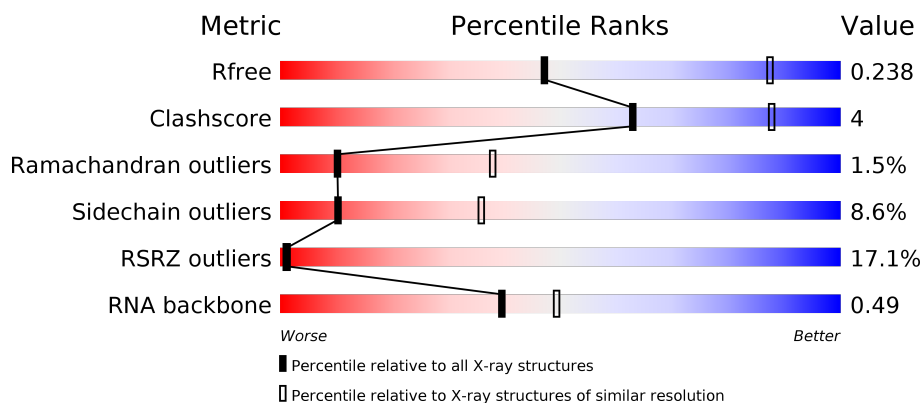
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)
RNA backbone	3102	1125 (3.74-2.90)

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

Mol	Chain	Length	Quality of chain
1	AA	1534	<div> <div>7%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
1	BA	1534	<div> <div>17%</div> <div>66%</div> <div>29%</div> <div>.</div> </div>
2	AB	224	<div> <div>25%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
2	BB	224	<div> <div>20%</div> <div>81%</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	129	
11	BK	129	
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	272	
29	DC	272	
30	CD	209	
31	CA	2904	
32	DD	209	
33	CE	201	
33	DE	201	
34	CF	178	
34	DF	178	
35	CG	176	
35	DG	176	
36	CH	149	
36	DH	149	
37	CJ	135	
37	DJ	135	
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	127	
42	DO	127	
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	100	
48	DU	100	
49	CV	103	
49	DV	103	
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
1	2MG	BA	966	-	-	-	X
1	5MC	BA	967	-	-	-	X
56	MG	AA	1603	-	-	-	X
56	MG	AA	1604	-	-	-	X
56	MG	AA	1605	-	-	-	X
56	MG	AA	1615	-	-	-	X
56	MG	AA	1616	-	-	-	X
56	MG	AA	1621	-	-	-	X
56	MG	AA	1622	-	-	-	X
56	MG	AA	1623	-	-	-	X
56	MG	AA	1625	-	-	-	X
56	MG	AA	1626	-	-	-	X
56	MG	AA	1627	-	-	-	X
56	MG	AA	1660	-	-	-	X
56	MG	AA	1665	-	-	-	X
56	MG	BA	1623	-	-	-	X
56	MG	BA	1624	-	-	-	X
56	MG	BA	1625	-	-	-	X
56	MG	BA	1626	-	-	-	X
56	MG	BA	1637	-	-	-	X
56	MG	CA	3007	-	-	-	X
56	MG	CA	3022	-	-	-	X
56	MG	CA	3026	-	-	-	X
56	MG	CA	3056	-	-	-	X
56	MG	CA	3075	-	-	-	X
56	MG	CA	3077	-	-	-	X
56	MG	CA	3104	-	-	-	X
56	MG	CA	3113	-	-	-	X
56	MG	CA	3116	-	-	-	X
56	MG	CA	3123	-	-	-	X
56	MG	CA	3132	-	-	-	X
56	MG	CA	3135	-	-	-	X
56	MG	CA	3139	-	-	-	X
56	MG	CA	3140	-	-	-	X
56	MG	CA	3145	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	CA	3154	-	-	-	X
56	MG	DA	3130	-	-	-	X
56	MG	DA	3156	-	-	-	X
56	MG	DA	3163	-	-	-	X
56	MG	DA	3168	-	-	-	X
56	MG	DA	3182	-	-	-	X
58	MPD	DE	301	-	-	-	X
59	PUT	AA	1673	-	-	-	X
59	PUT	AA	1674	-	-	-	X
59	PUT	AA	1675	-	-	-	X
59	PUT	DA	3195	-	-	-	X
61	PEG	D3	102	-	-	-	X
61	PEG	DP	201	-	-	-	X
61	PEG	DQ	201	-	-	-	X
62	EDO	DA	3002	-	-	-	X
62	EDO	DA	3198	-	-	-	X
66	ACY	DA	3202	-	-	X	-
68	TRS	DA	3220	-	-	-	X

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295119 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
			32932	14695	6044	10659	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32910	14685	6039	10653	1533			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1060	A	U	conflict	GB 675819282
BA	1060	A	U	conflict	GB 675819282

- 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
			2082	1288	423	364	7			
29	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	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
			1410	899	249	256	6			
34	DF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	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
			738	466	139	131	2			
48	DU	93	Total	C	N	O	S	0	0	0
			738	466	139	131	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
			779	492	146	141				
49	DV	102	Total	C	N	O	S	0	0	0
			779	492	146	141				

- 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).

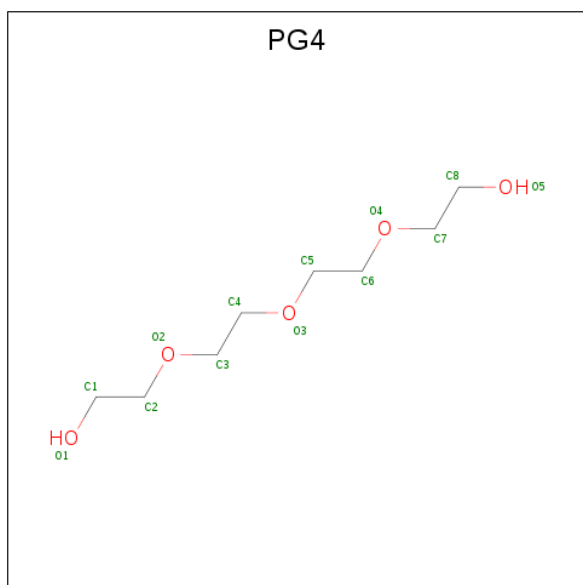
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	41	Total	Mg	0	0
			41	41		
56	CA	156	Total	Mg	0	0
			156	156		
56	CB	3	Total	Mg	0	0
			3	3		
56	DM	1	Total	Mg	0	0
			1	1		
56	DR	1	Total	Mg	0	0
			1	1		
56	AA	70	Total	Mg	0	0
			70	70		
56	DA	184	Total	Mg	0	0
			184	184		

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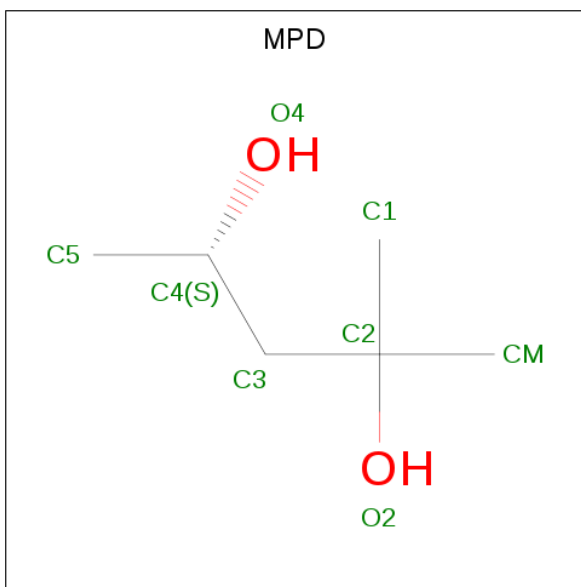
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DB	9	Total	Mg	0	0
			9	9		
56	DD	1	Total	Mg	0	0
			1	1		

- Molecule 57 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



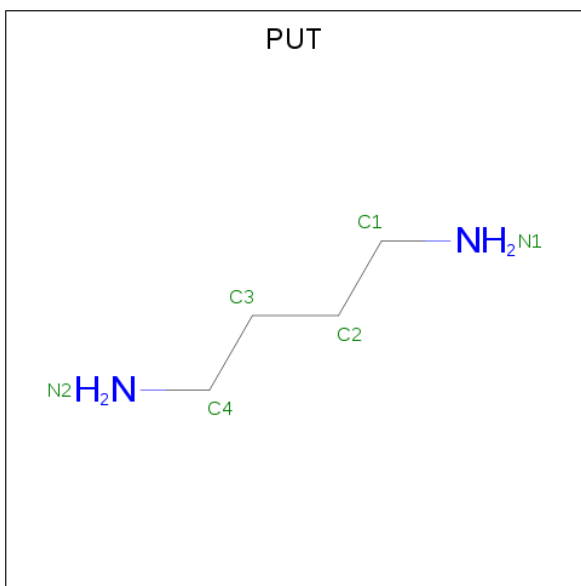
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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	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		

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



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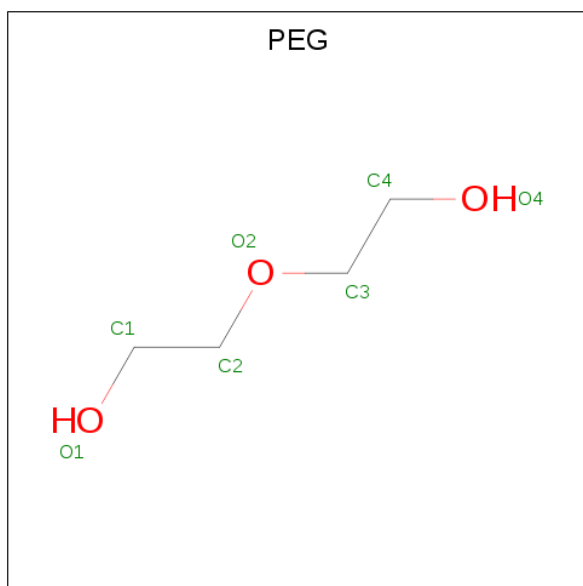
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		

- 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: C₄H₁₀O₃).



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

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

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



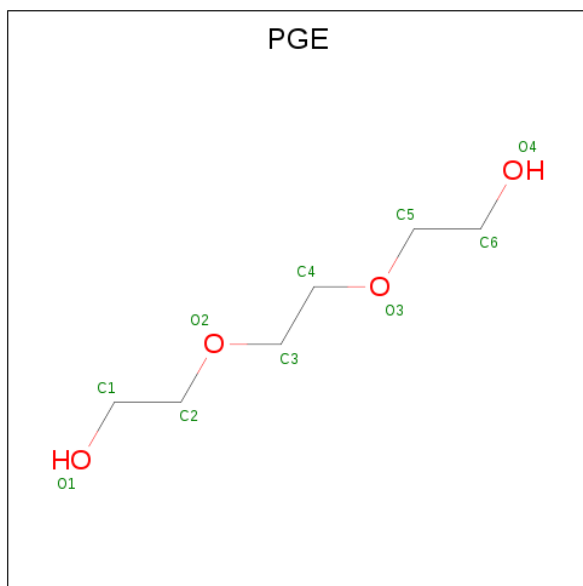
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	D1	1	Total	C	O	0	0
			4	2	2		
62	D0	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		

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

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



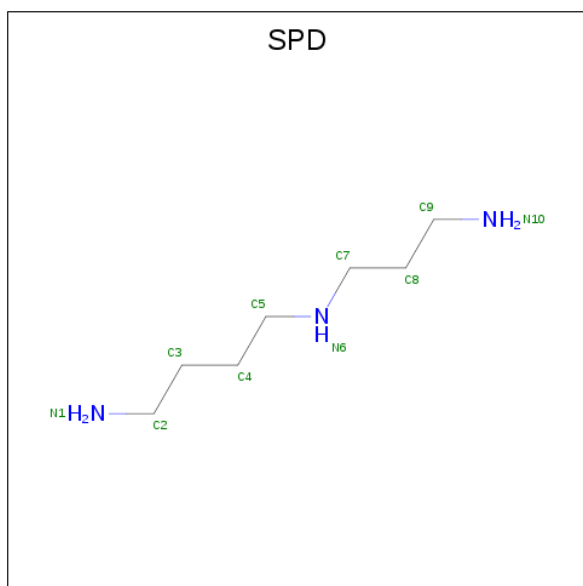
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			10	6	4		
63	D3	1	Total	C	O	0	0
			10	6	4		

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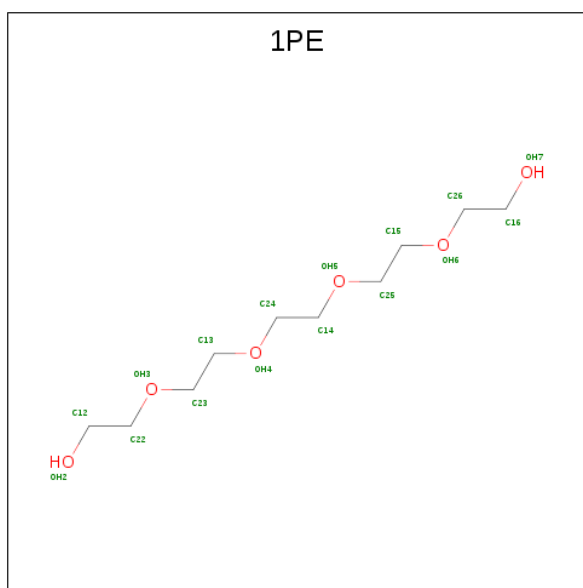
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	DD	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		

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



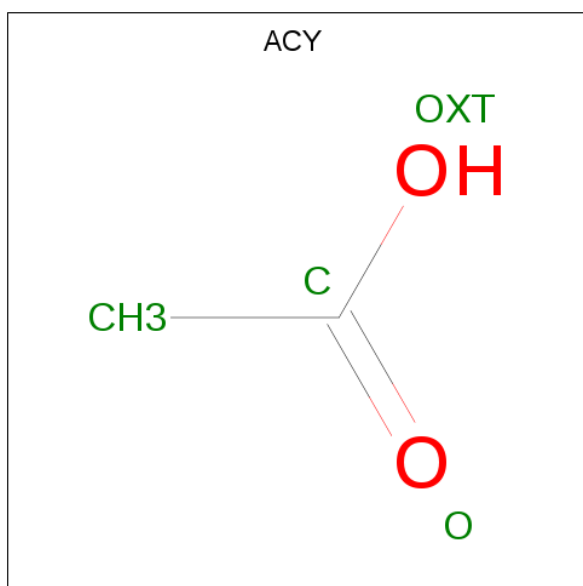
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

- 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: $C_2H_4O_2$).



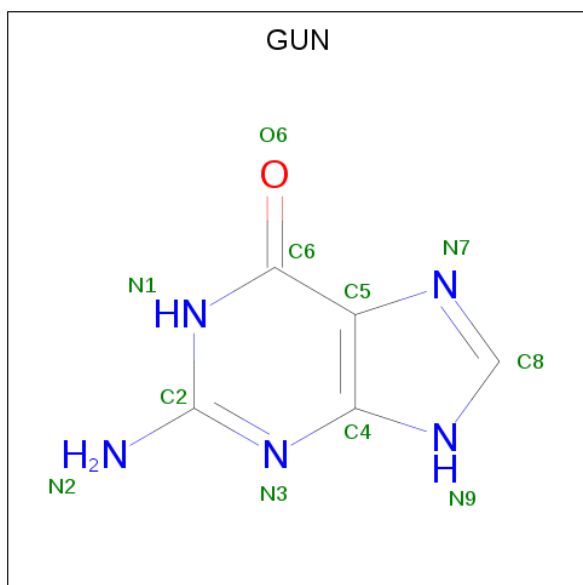
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		

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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	507	Total	O	0	0
			507	507		
69	AC	4	Total	O	0	0
			4	4		
69	AD	2	Total	O	0	0
			2	2		
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	5	Total	O	0	0
			5	5		
69	AL	7	Total	O	0	0
			7	7		
69	AM	4	Total	O	0	0
			4	4		
69	AN	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AO	1	Total 1	O 1	0	0
69	AP	1	Total 1	O 1	0	0
69	AQ	1	Total 1	O 1	0	0
69	AS	1	Total 1	O 1	0	0
69	AT	2	Total 2	O 2	0	0
69	AU	4	Total 4	O 4	0	0
69	C3	3	Total 3	O 3	0	0
69	C4	1	Total 1	O 1	0	0
69	BA	287	Total 287	O 287	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	3	Total 3	O 3	0	0
69	BN	1	Total 1	O 1	0	0
69	BO	1	Total 1	O 1	0	0
69	BP	4	Total 4	O 4	0	0
69	BR	1	Total 1	O 1	0	0
69	BT	5	Total 5	O 5	0	0
69	D1	37	Total 37	O 37	0	0
69	D2	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	D3	30	Total 30	O 30	0	0
69	D4	40	Total 40	O 40	0	0
69	D5	13	Total 13	O 13	0	0
69	D0	24	Total 24	O 24	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	11	Total 11	O 11	0	0
69	CD	4	Total 4	O 4	0	0
69	CA	696	Total 696	O 696	0	0
69	DC	100	Total 100	O 100	0	0
69	DD	97	Total 97	O 97	0	0
69	CE	5	Total 5	O 5	0	0
69	CL	1	Total 1	O 1	0	0
69	CM	3	Total 3	O 3	0	0
69	CO	1	Total 1	O 1	0	0
69	CU	2	Total 2	O 2	0	0
69	CV	1	Total 1	O 1	0	0
69	CW	1	Total 1	O 1	0	0
69	CY	1	Total 1	O 1	0	0
69	DE	54	Total 54	O 54	0	0
69	DF	13	Total 13	O 13	0	0
69	DG	9	Total 9	O 9	0	0

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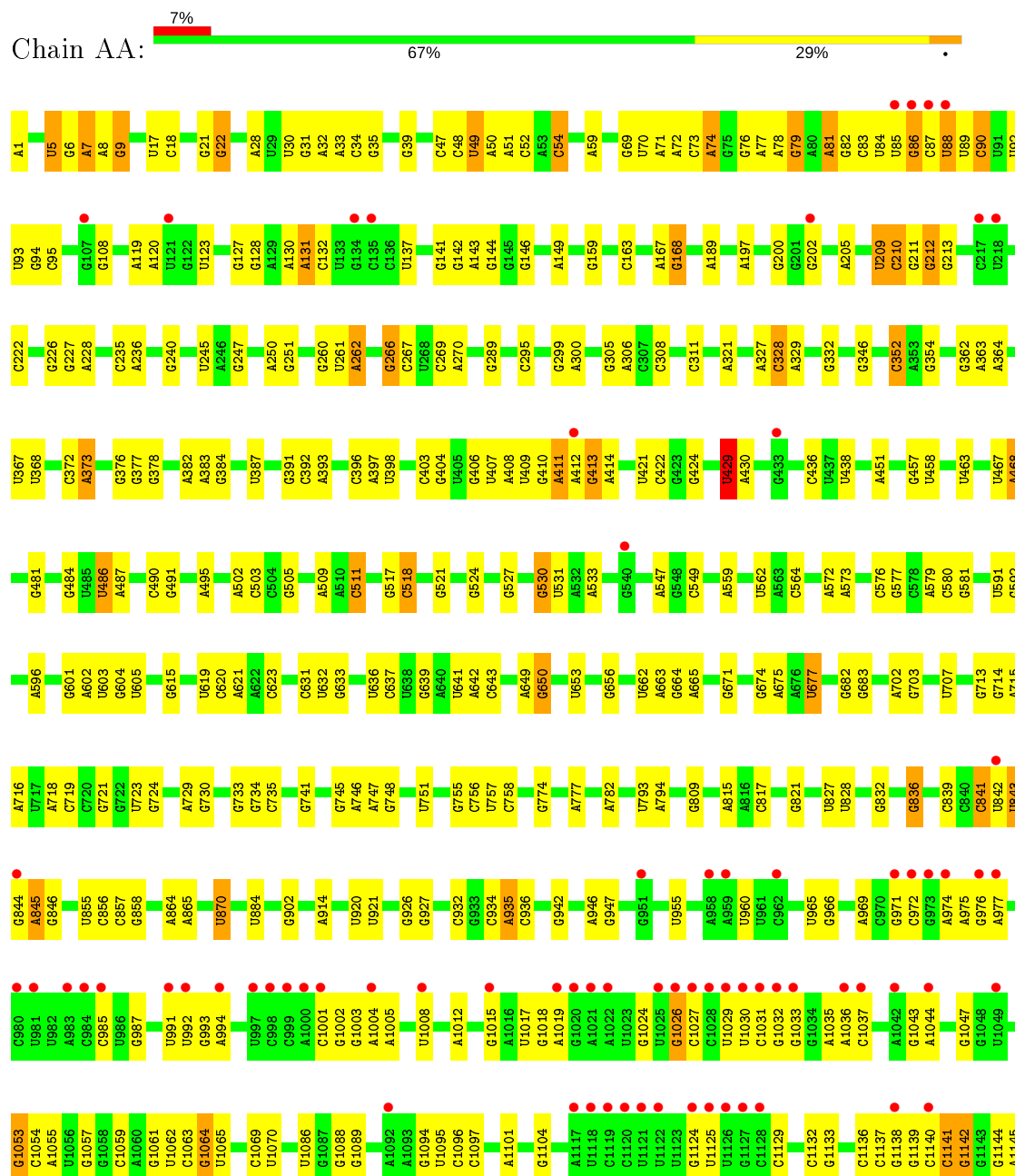
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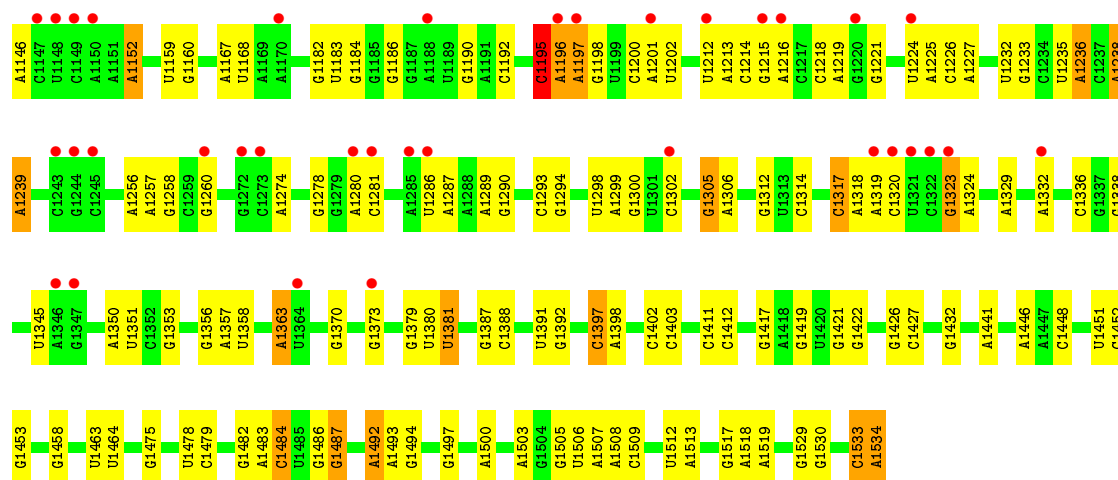
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DH	2	Total	O	0	0
			2	2		
69	DK	61	Total	O	0	0
			61	61		
69	DL	50	Total	O	0	0
			50	50		
69	DM	60	Total	O	0	0
			60	60		
69	DN	81	Total	O	0	0
			81	81		
69	DO	42	Total	O	0	0
			42	42		
69	DP	42	Total	O	0	0
			42	42		
69	DQ	32	Total	O	0	0
			32	32		
69	DR	68	Total	O	0	0
			68	68		
69	DS	52	Total	O	0	0
			52	52		
69	DT	65	Total	O	0	0
			65	65		
69	DU	24	Total	O	0	0
			24	24		
69	DV	19	Total	O	0	0
			19	19		
69	DW	33	Total	O	0	0
			33	33		
69	DX	33	Total	O	0	0
			33	33		
69	DY	11	Total	O	0	0
			11	11		
69	DZ	7	Total	O	0	0
			7	7		
69	DB	203	Total	O	0	0
			203	203		
69	DA	4824	Total	O	0	0
			4824	4824		

3 Residue-property plots [i](#)

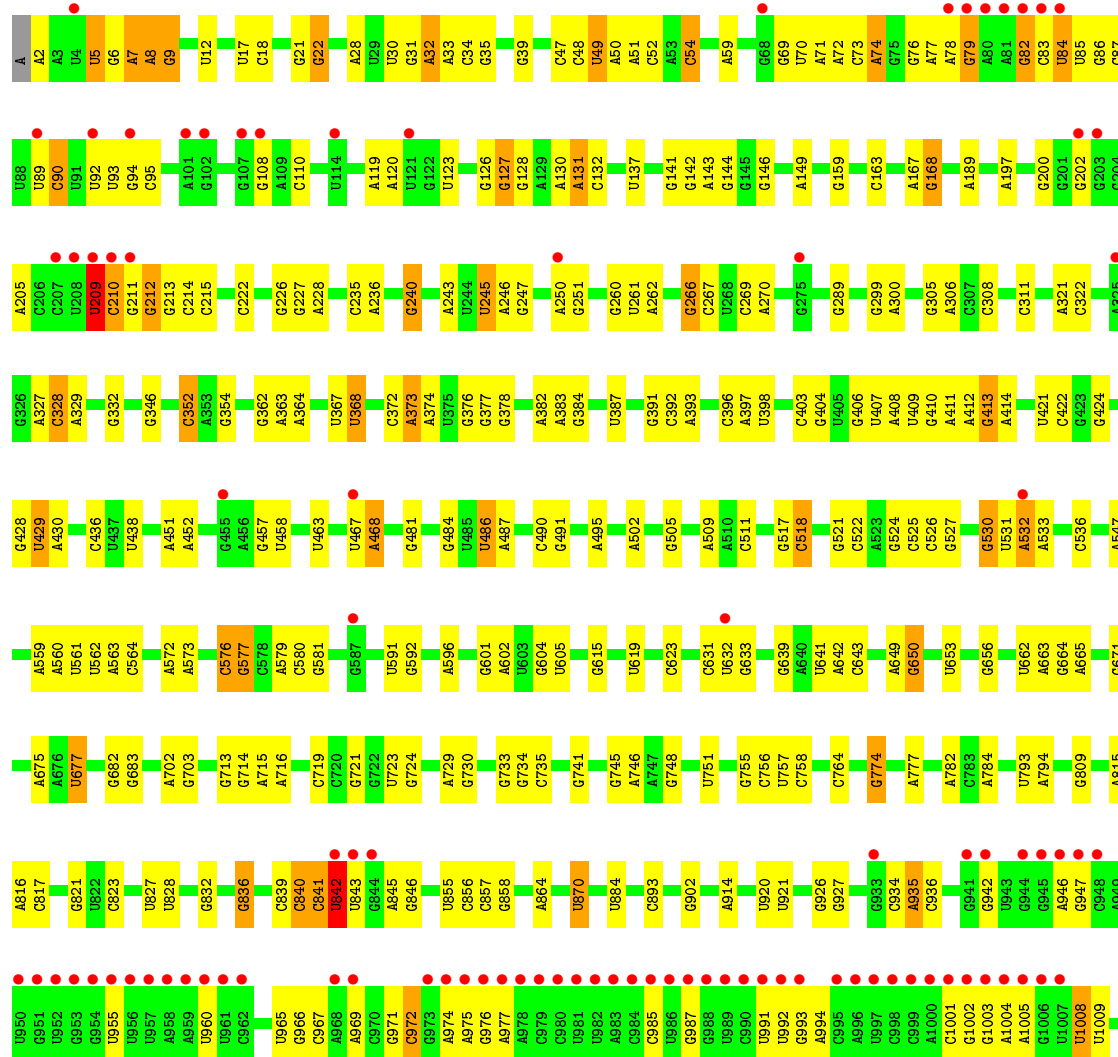
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

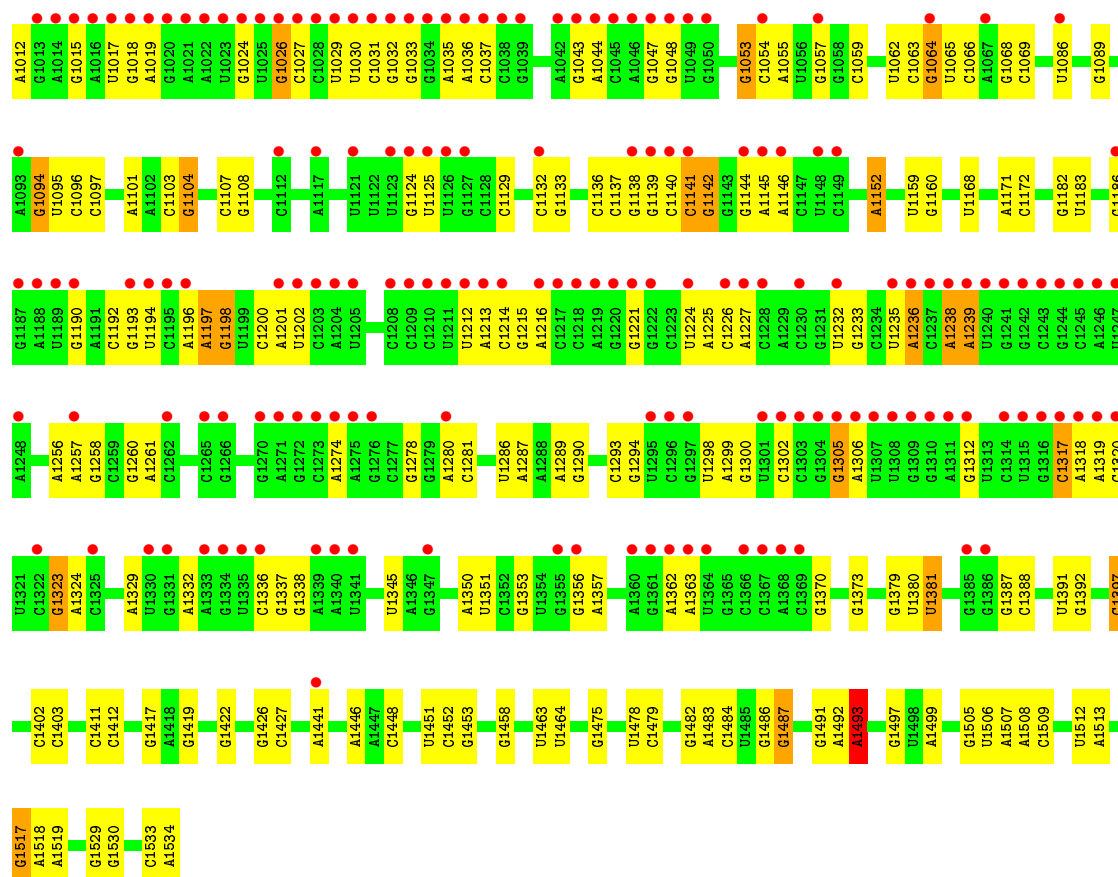
• Molecule 1: 16S rRNA



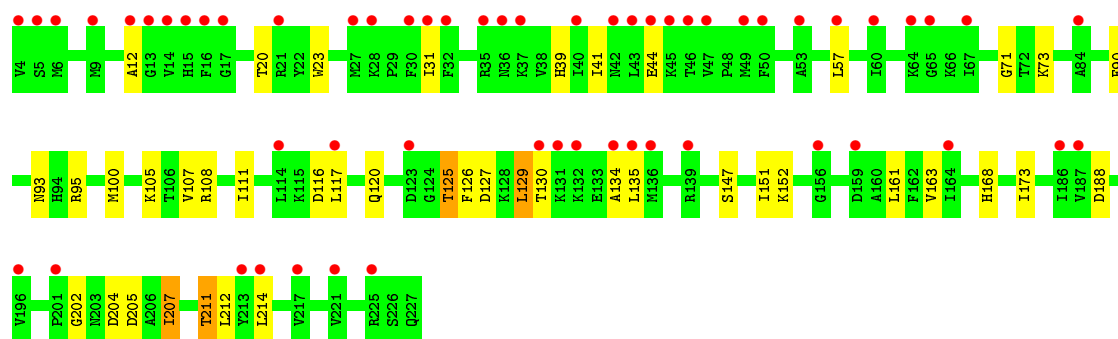
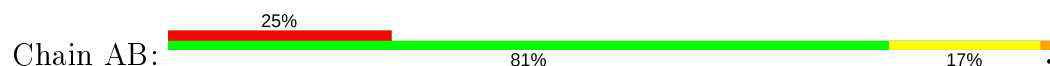


• Molecule 1: 16S rRNA

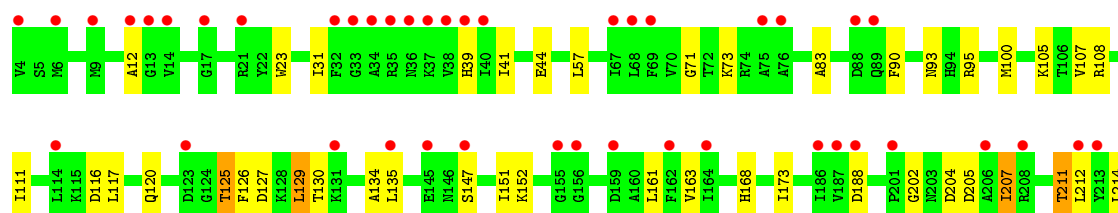
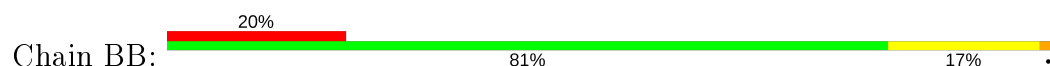




• Molecule 2: 30S ribosomal protein S2

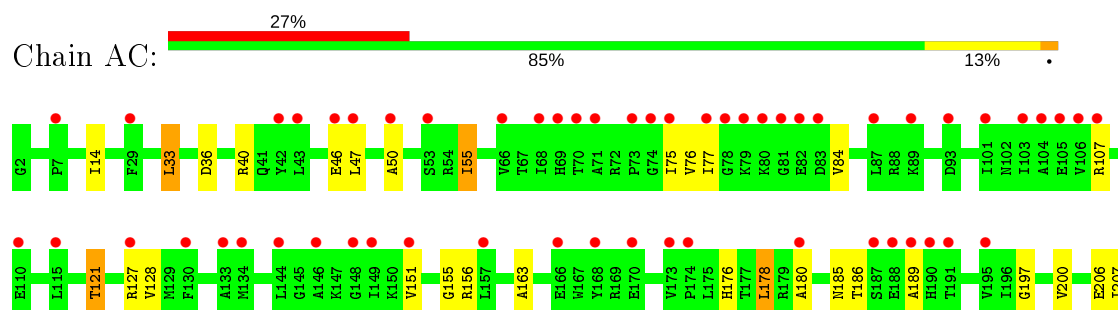


• Molecule 2: 30S ribosomal protein S2

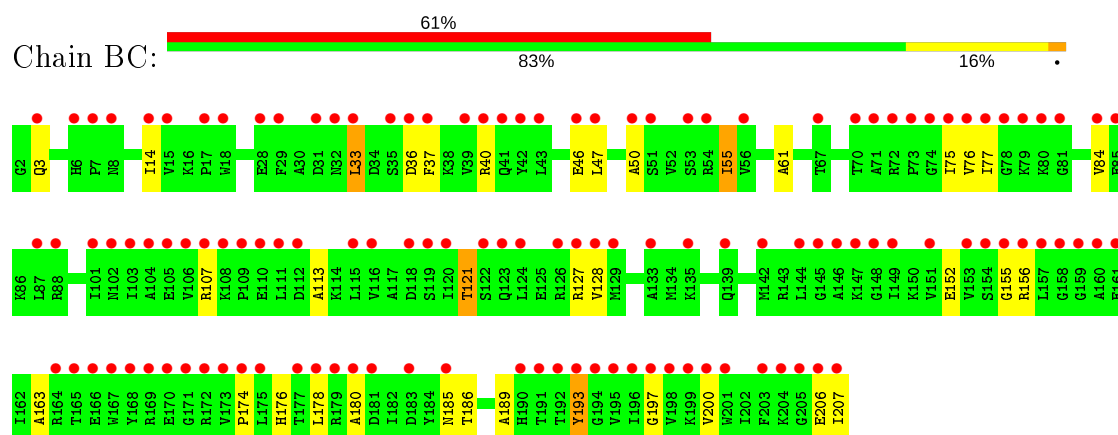




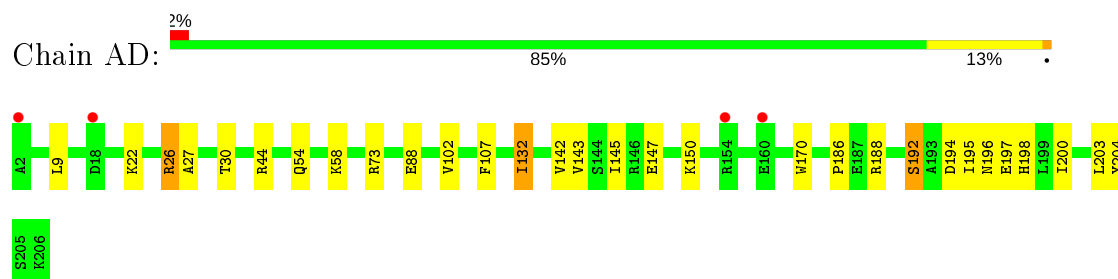
- Molecule 3: 30S ribosomal protein S3



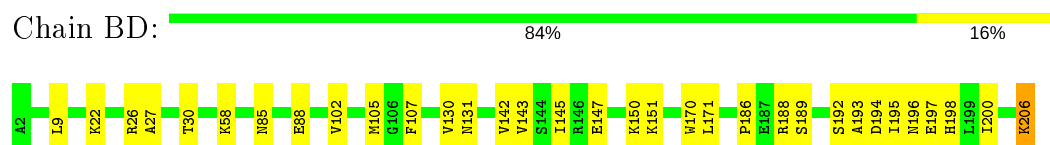
- Molecule 3: 30S ribosomal protein S3



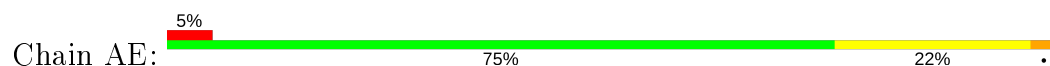
- Molecule 4: 30S ribosomal protein S4

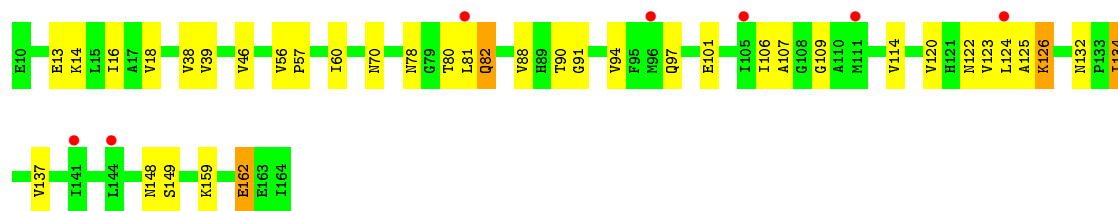


- Molecule 4: 30S ribosomal protein S4

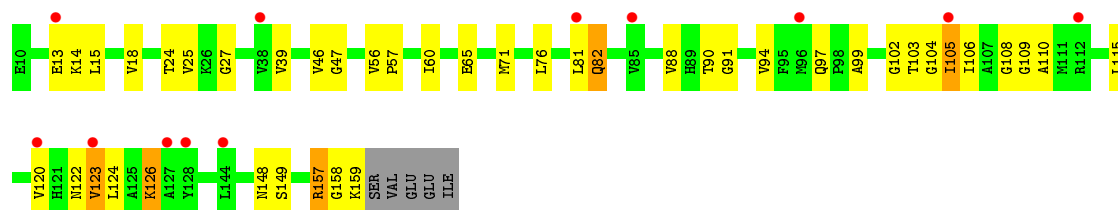


- Molecule 5: 30S ribosomal protein S5

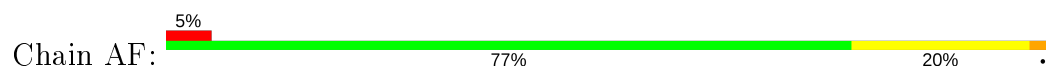




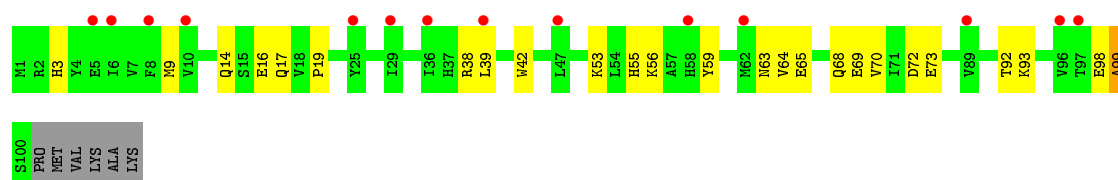
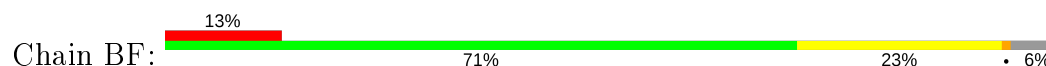
• Molecule 5: 30S ribosomal protein S5



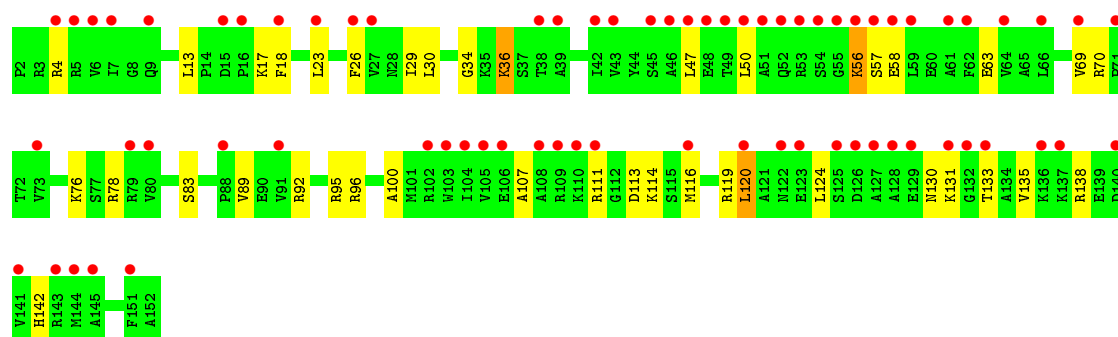
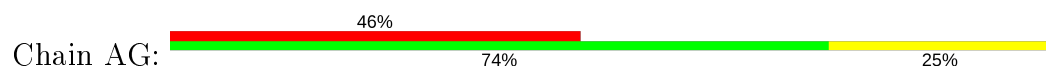
• Molecule 6: 30S ribosomal protein S6



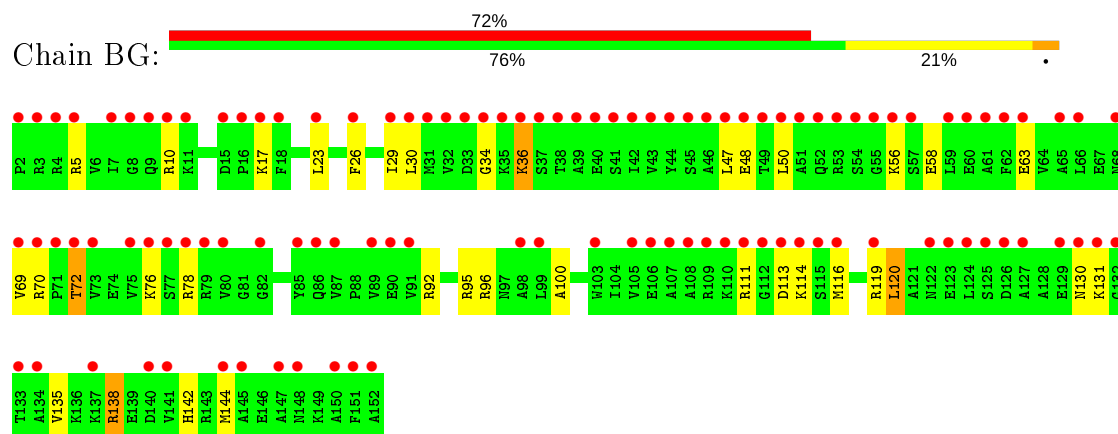
• Molecule 6: 30S ribosomal protein S6



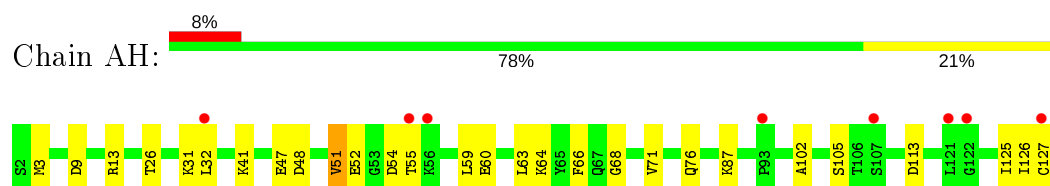
• Molecule 7: 30S ribosomal protein S7



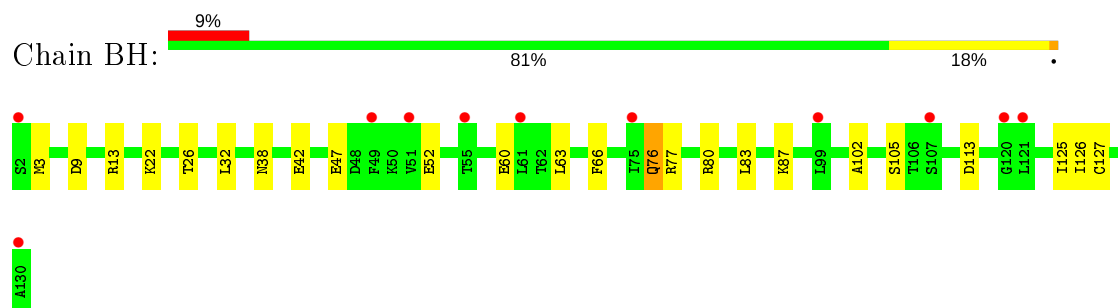
- Molecule 7: 30S ribosomal protein S7



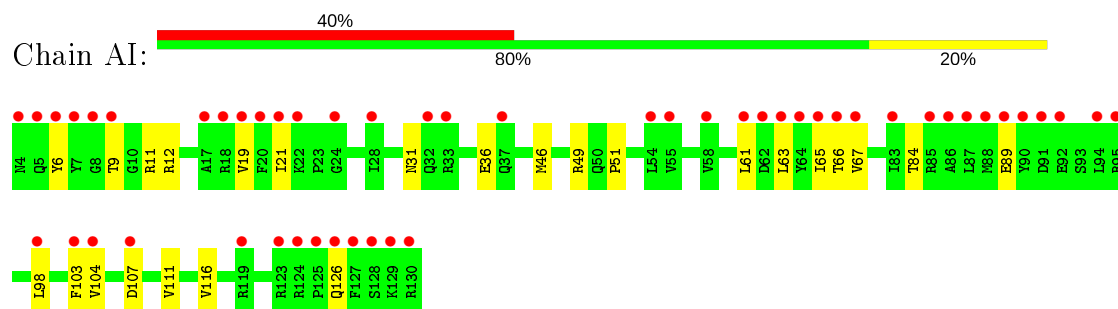
- Molecule 8: 30S ribosomal protein S8



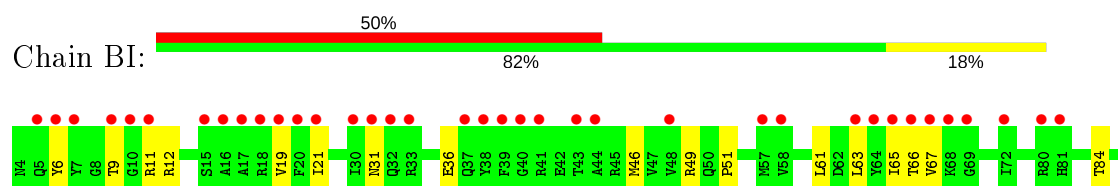
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9

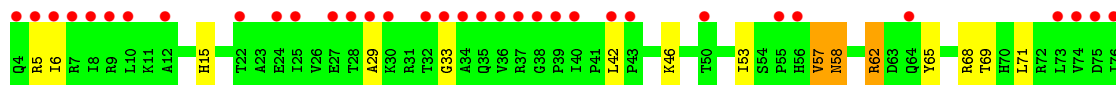
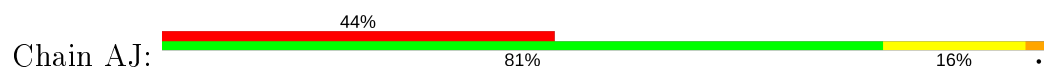


- Molecule 9: 30S ribosomal protein S9

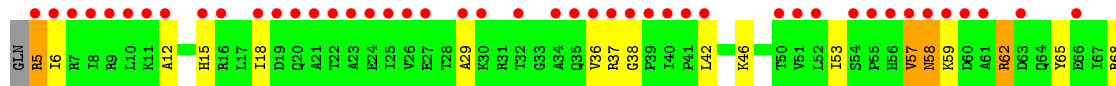
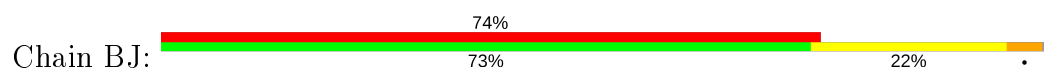




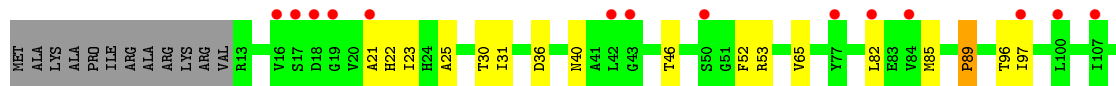
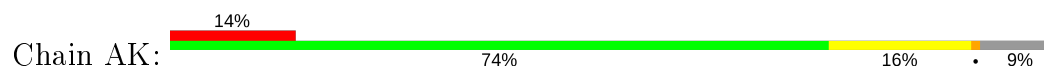
- Molecule 10: 30S ribosomal protein S10



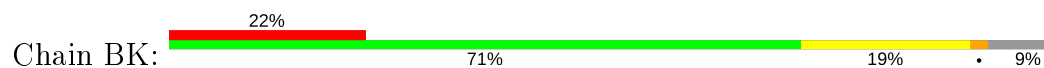
- Molecule 10: 30S ribosomal protein S10



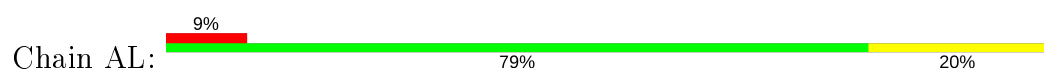
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11

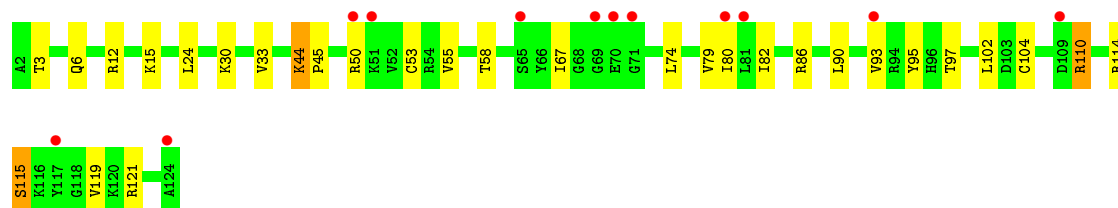
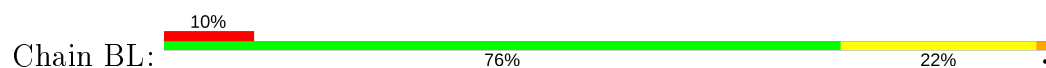


- Molecule 12: 30S ribosomal protein S12

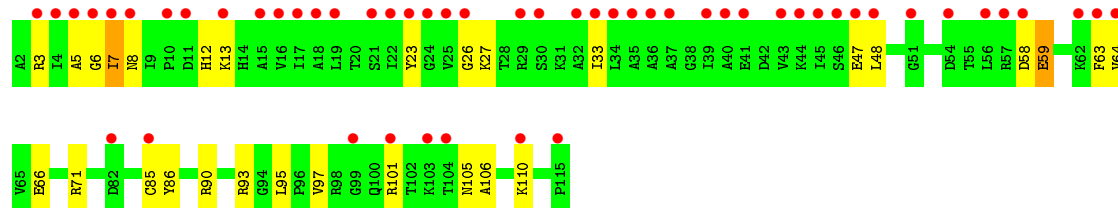
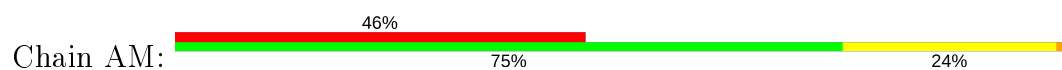




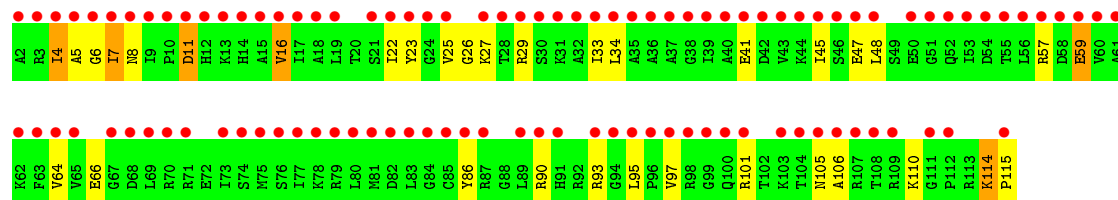
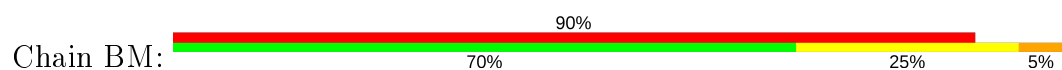
- Molecule 12: 30S ribosomal protein S12



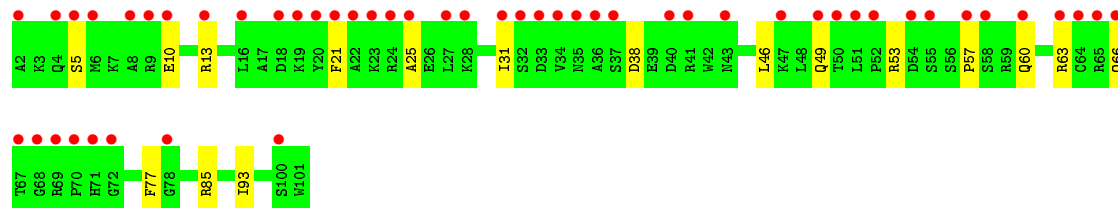
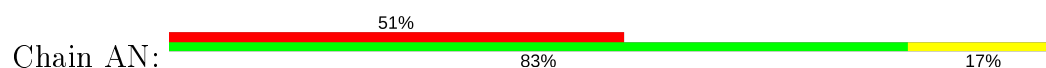
- Molecule 13: 30S ribosomal protein S13



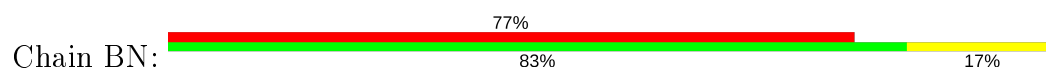
- Molecule 13: 30S ribosomal protein S13

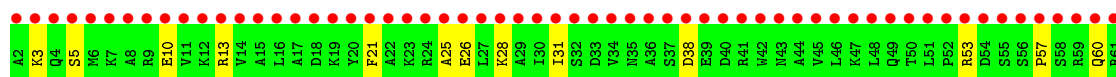


- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14

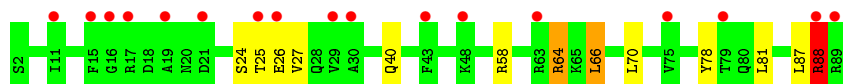
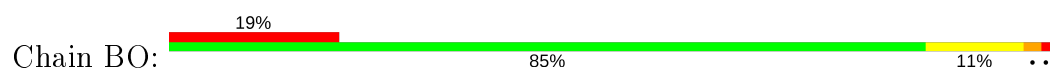




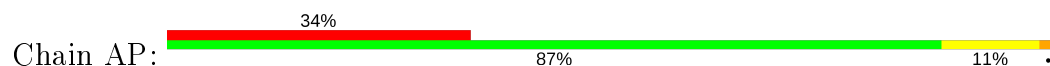
- Molecule 15: 30S ribosomal protein S15



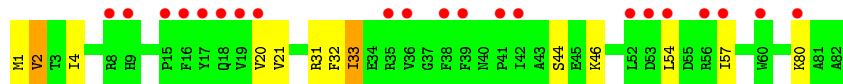
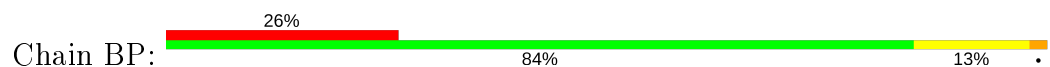
- Molecule 15: 30S ribosomal protein S15



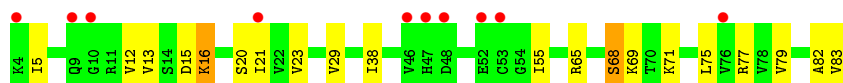
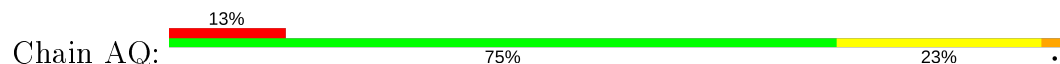
- Molecule 16: 30S ribosomal protein S16



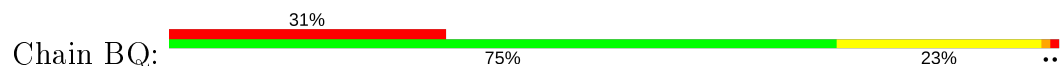
- Molecule 16: 30S ribosomal protein S16

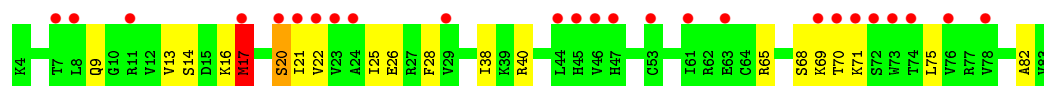


- Molecule 17: 30S ribosomal protein S17

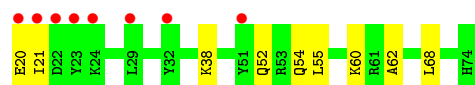
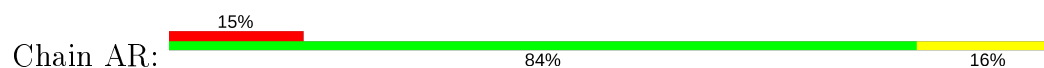


- Molecule 17: 30S ribosomal protein S17

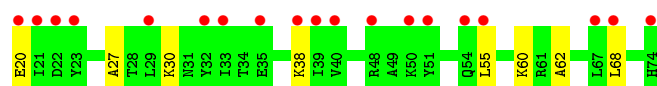
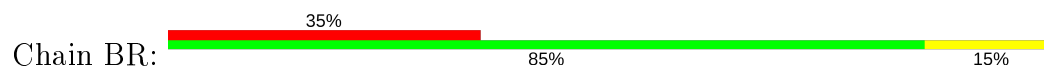




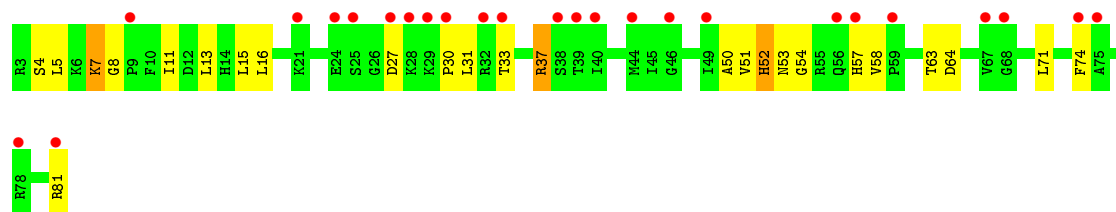
- Molecule 18: 30S ribosomal protein S18



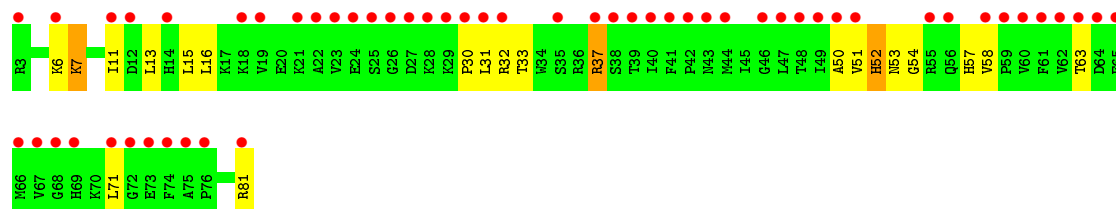
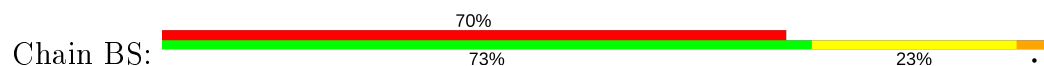
- Molecule 18: 30S ribosomal protein S18



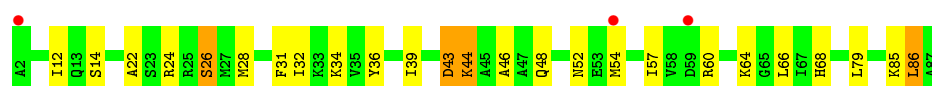
- Molecule 19: 30S ribosomal protein S19



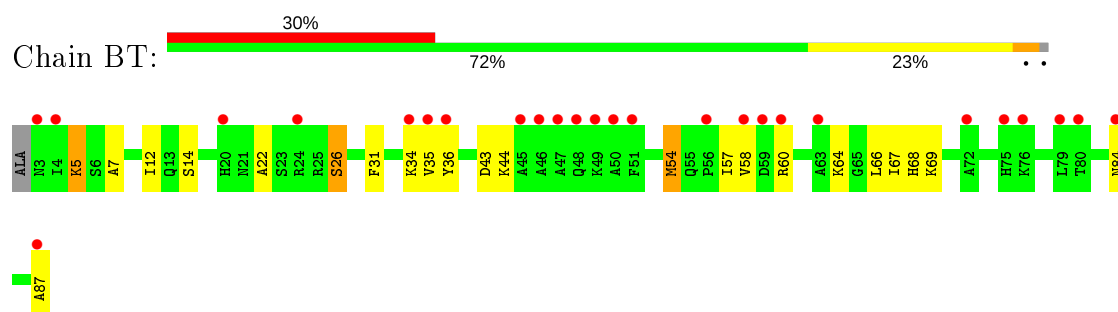
- Molecule 19: 30S ribosomal protein S19



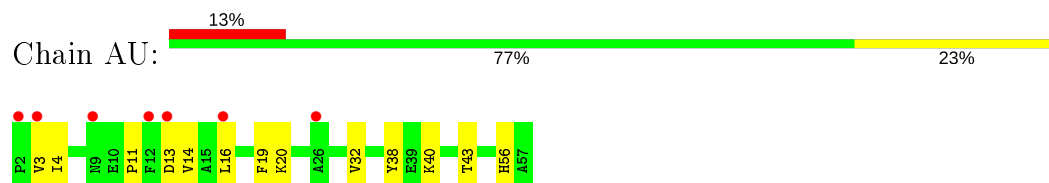
- Molecule 20: 30S ribosomal protein S20



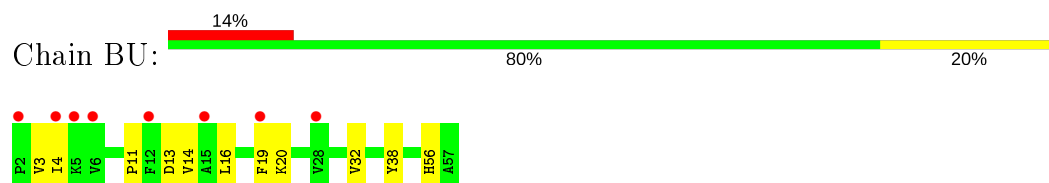
- Molecule 20: 30S ribosomal protein S20



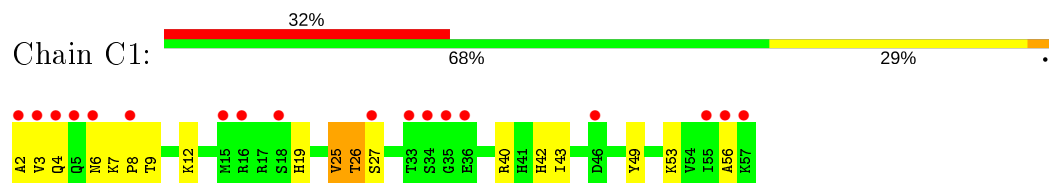
- Molecule 21: 30S ribosomal protein S21



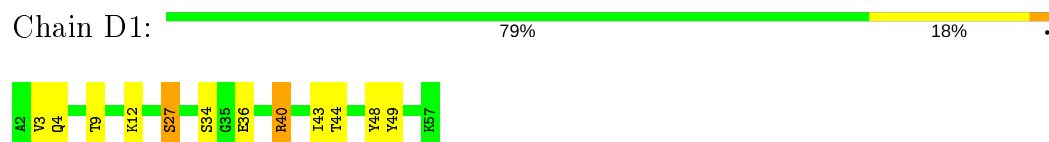
- Molecule 21: 30S ribosomal protein S21



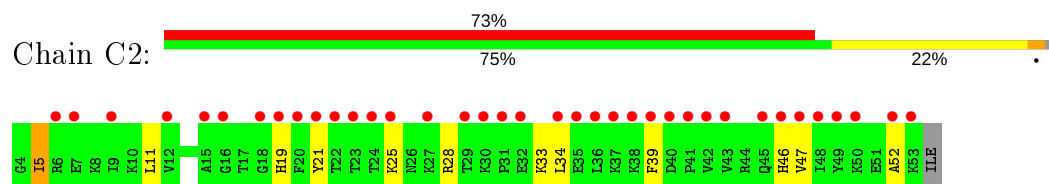
- Molecule 22: 50S ribosomal protein L32



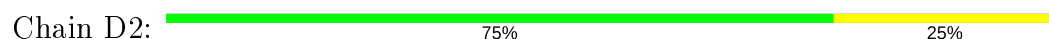
- Molecule 22: 50S ribosomal protein L32



- Molecule 23: 50S ribosomal protein L33

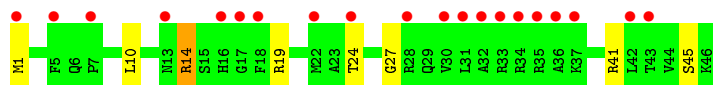
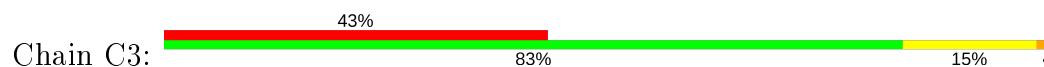


- Molecule 23: 50S ribosomal protein L33

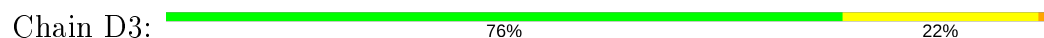




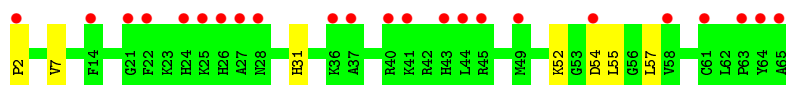
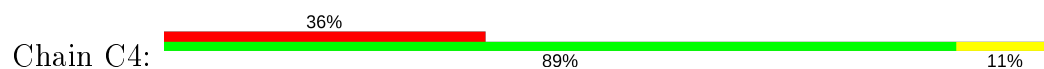
- Molecule 24: 50S ribosomal protein L34



- Molecule 24: 50S ribosomal protein L34



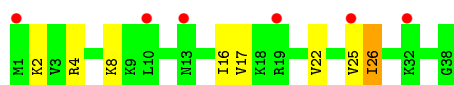
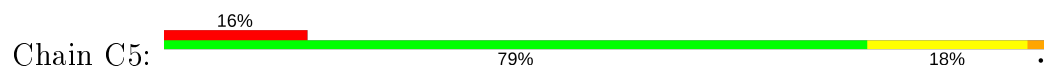
- Molecule 25: 50S ribosomal protein L35



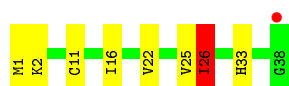
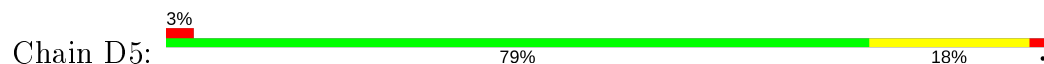
- Molecule 25: 50S ribosomal protein L35



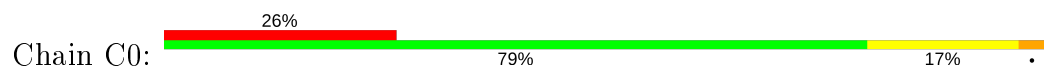
- Molecule 26: 50S ribosomal protein L36



- Molecule 26: 50S ribosomal protein L36



- Molecule 27: 50S ribosomal protein L30





- Molecule 27: 50S ribosomal protein L30

Chain D0: 74% 24%



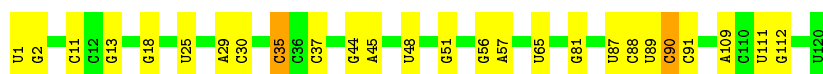
- Molecule 28: 5S rRNA

Chain CB: 6% 78% 18%



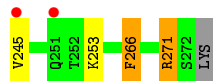
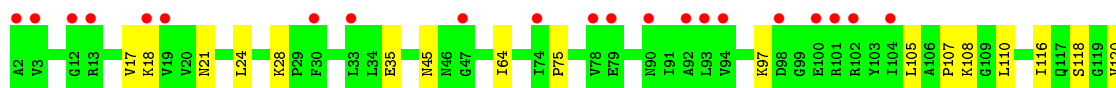
- Molecule 28: 5S rRNA

Chain DB: 78% 20%



- Molecule 29: 50S ribosomal protein L2

Chain CC: 13% 83% 15%

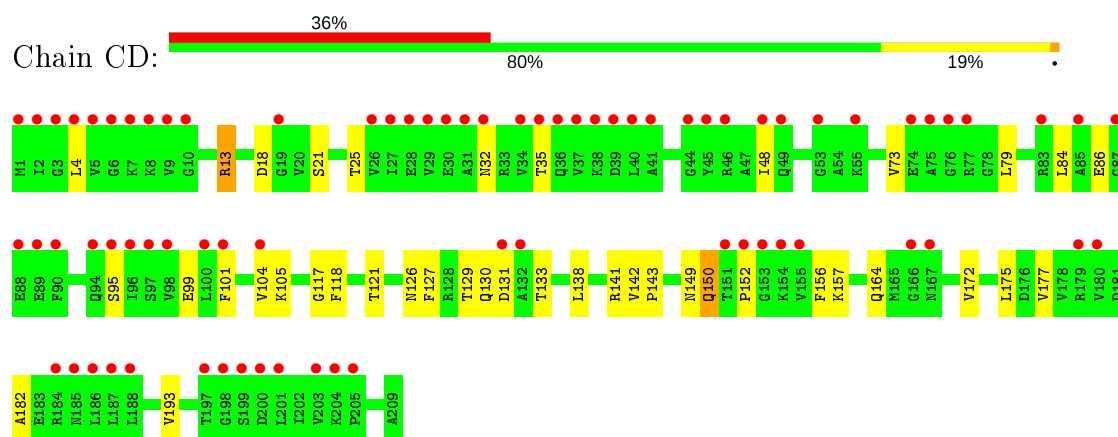


- Molecule 29: 50S ribosomal protein L2

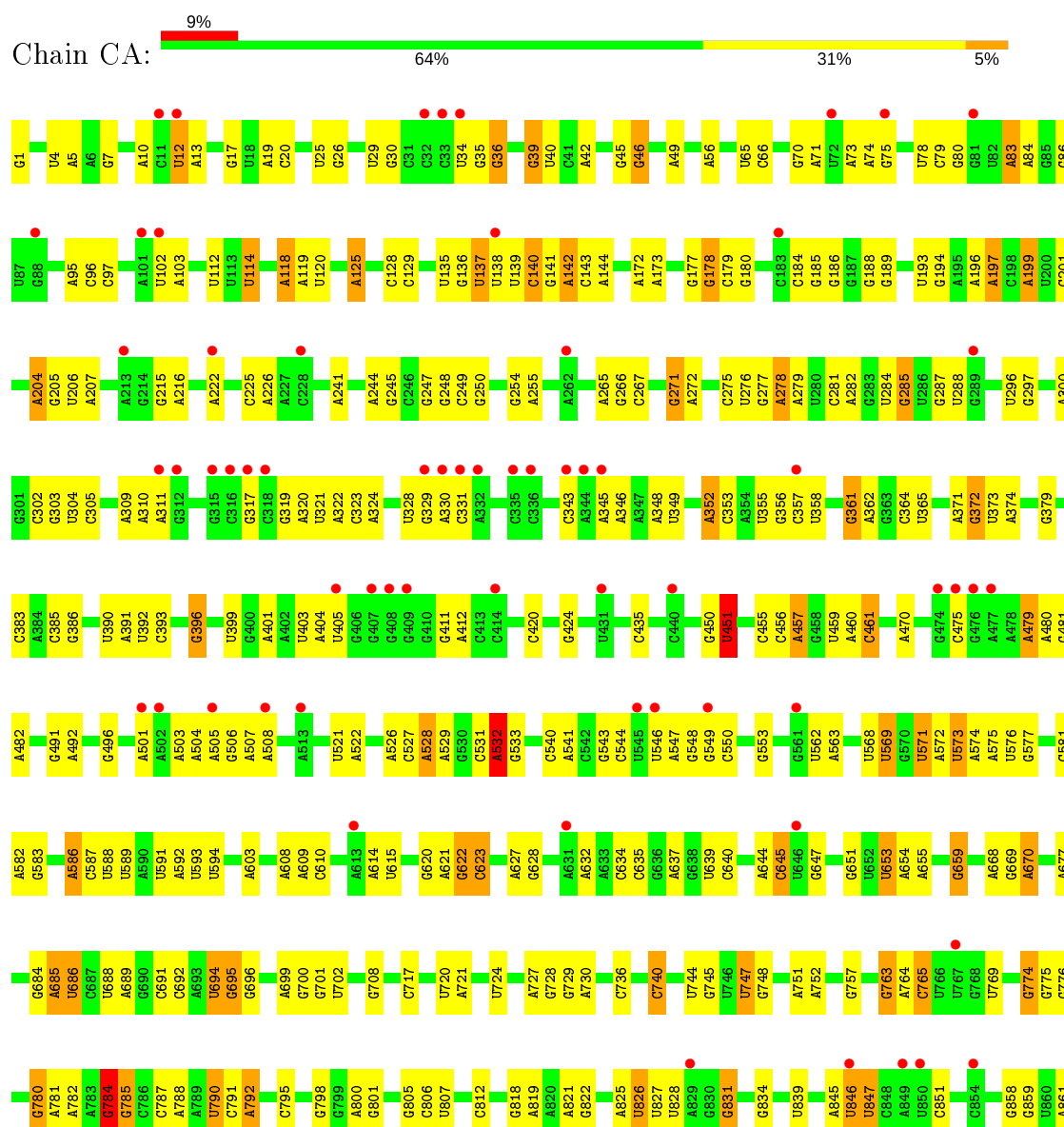
Chain DC: 82% 18%

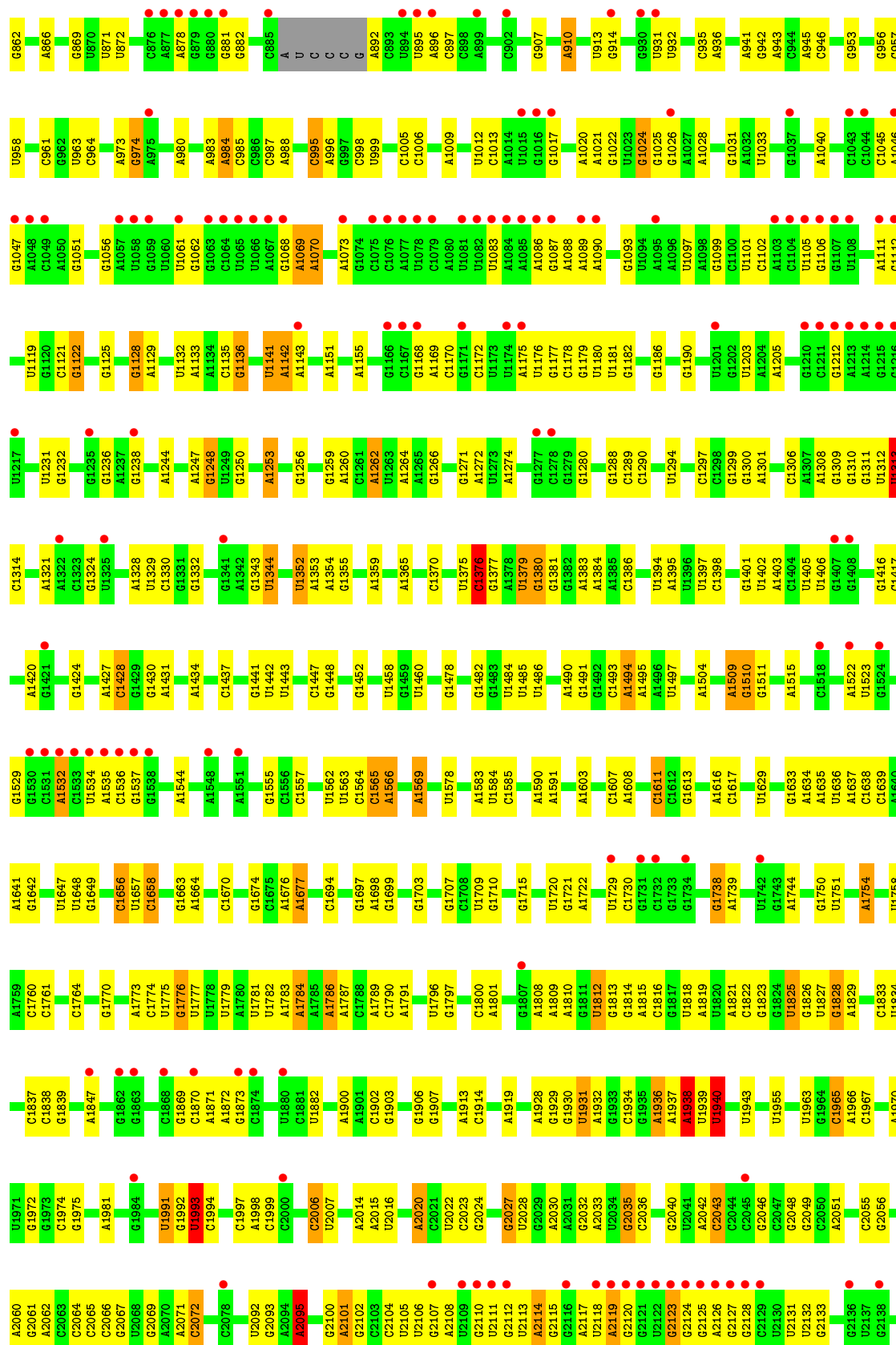


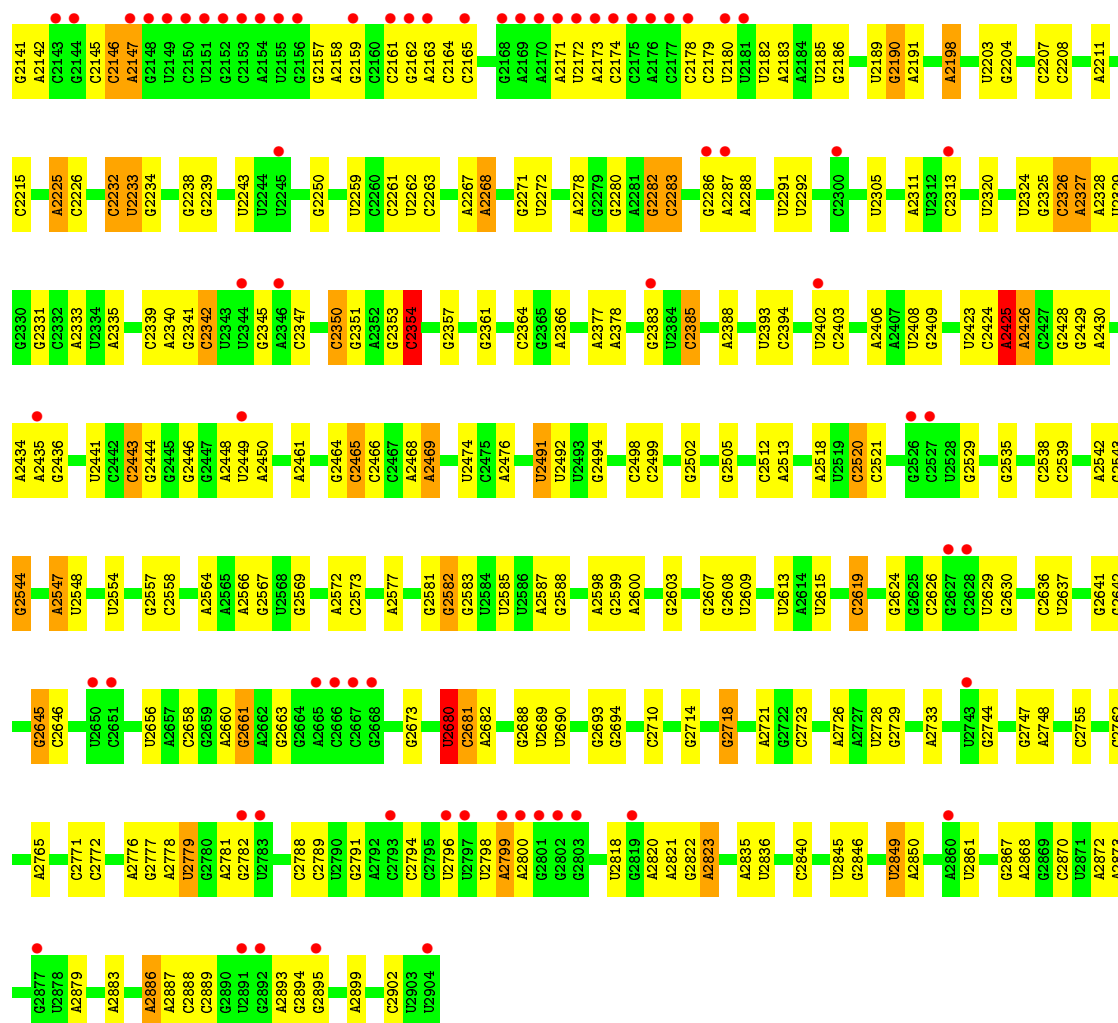
- Molecule 30: 50S ribosomal protein L3



• Molecule 31: 23S rRNA







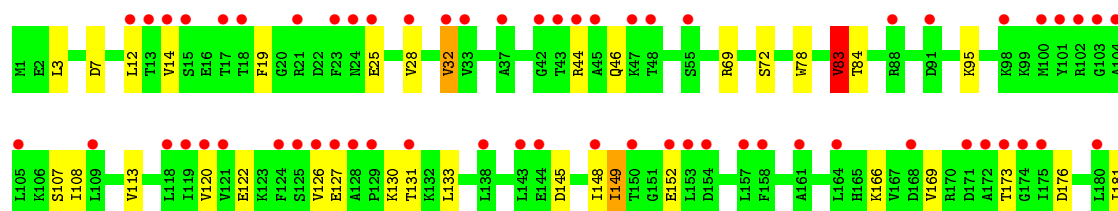
• Molecule 32: 50S ribosomal protein L3

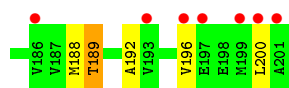
Chain DD: 79% 20% .



• Molecule 33: 50S ribosomal protein L4

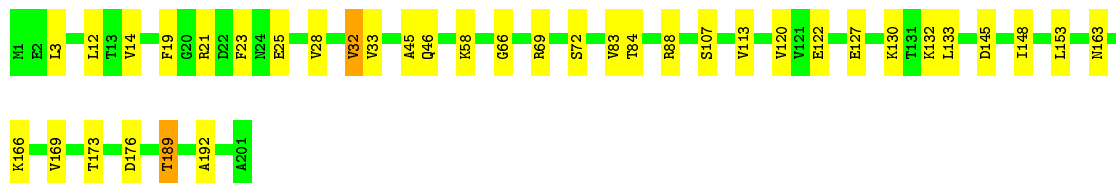
Chain CE: 34% 80% 18% .





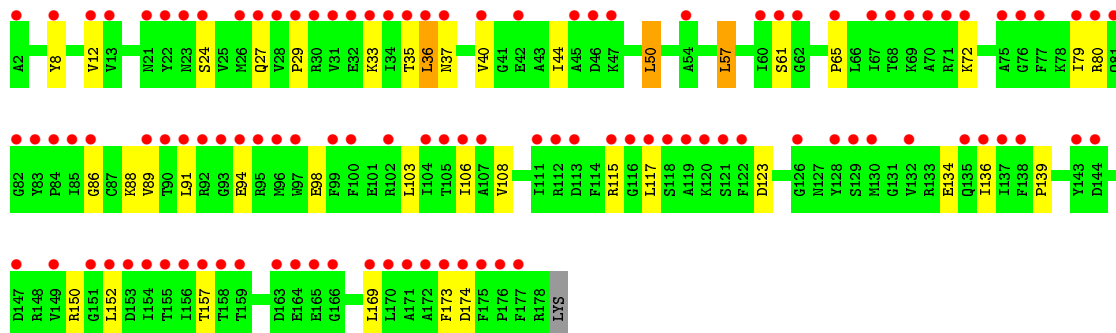
- Molecule 33: 50S ribosomal protein L4

Chain DE: 82% 17%



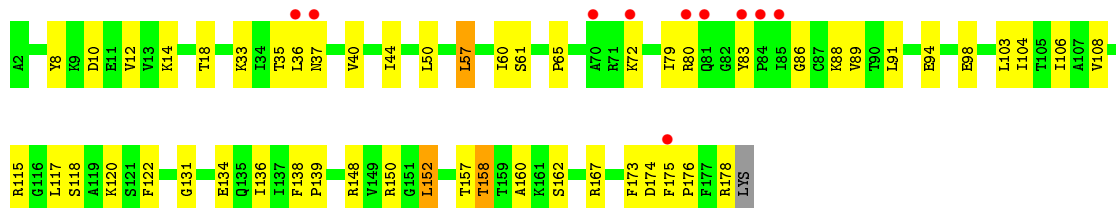
- Molecule 34: 50S ribosomal protein L5

Chain CF: 61% 78% 20%



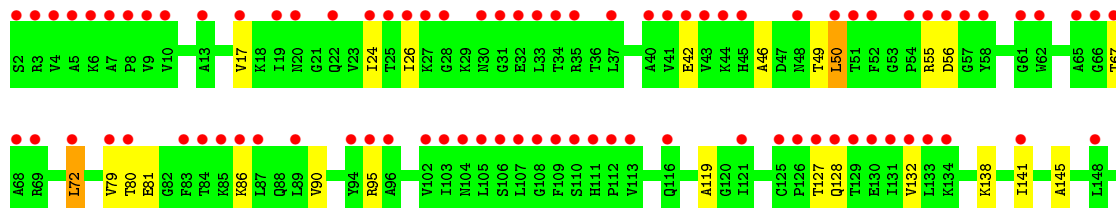
- Molecule 34: 50S ribosomal protein L5

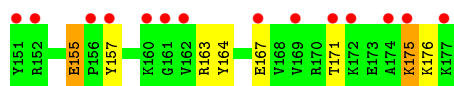
Chain DF: 6% 70% 28%



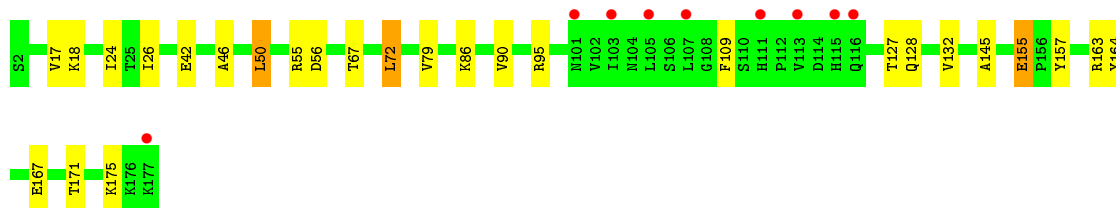
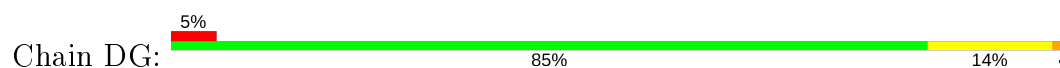
- Molecule 35: 50S ribosomal protein L6

Chain CG: 57% 82% 16%

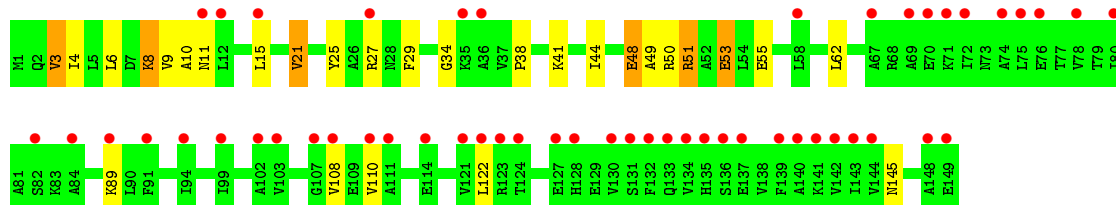
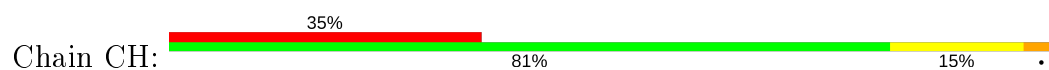




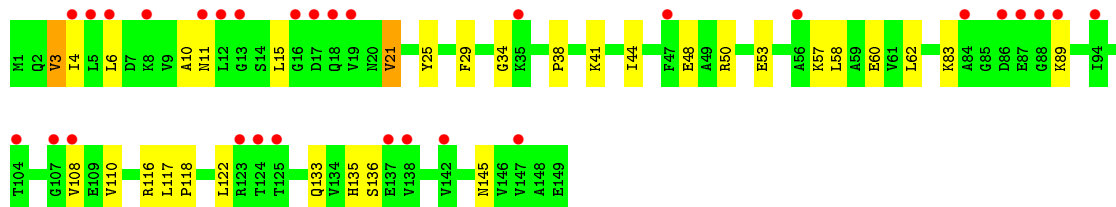
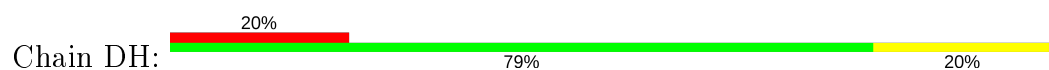
- Molecule 35: 50S ribosomal protein L6



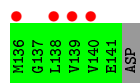
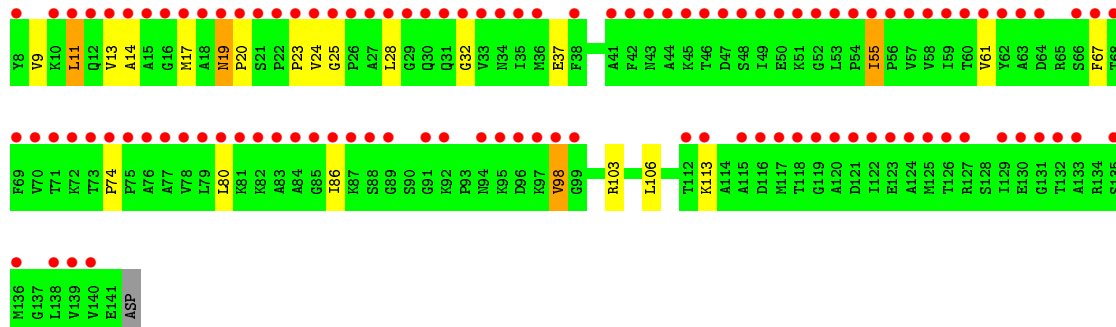
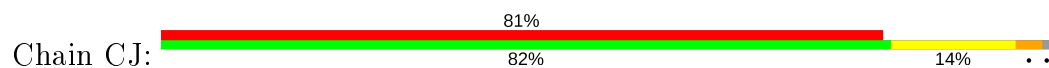
- Molecule 36: 50S ribosomal protein L9



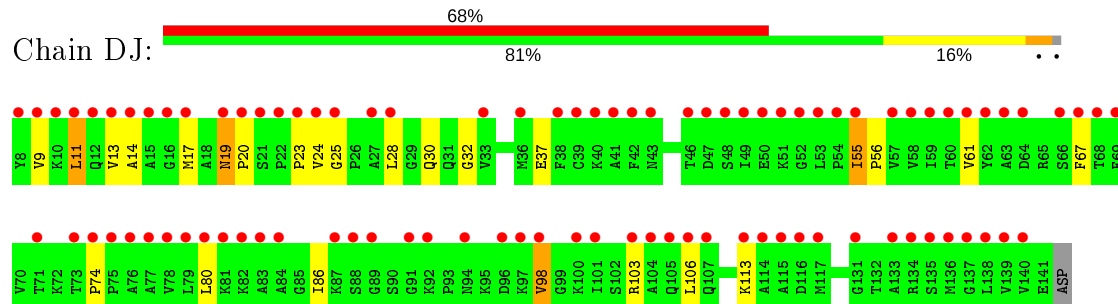
- Molecule 36: 50S ribosomal protein L9



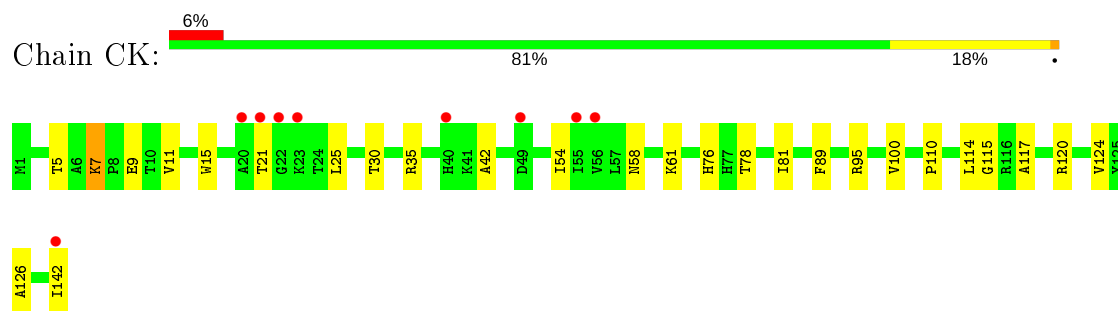
- Molecule 37: 50S ribosomal protein L11



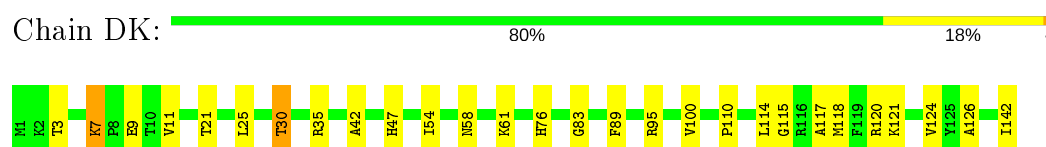
- Molecule 37: 50S ribosomal protein L11



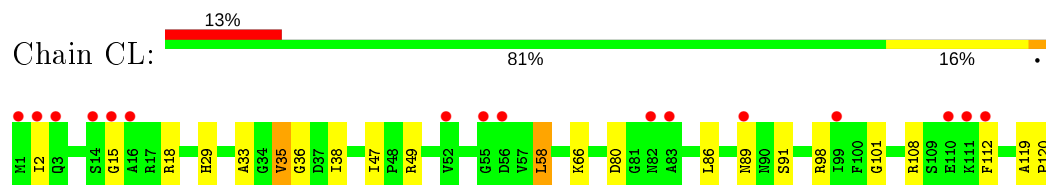
- Molecule 38: 50S ribosomal protein L13



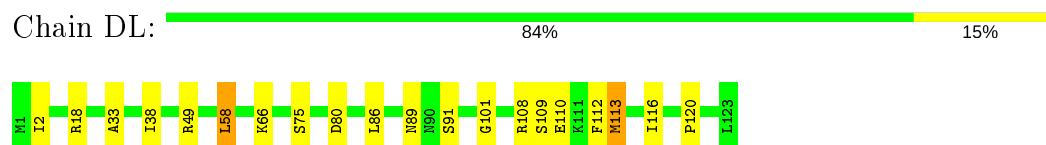
- Molecule 38: 50S ribosomal protein L13



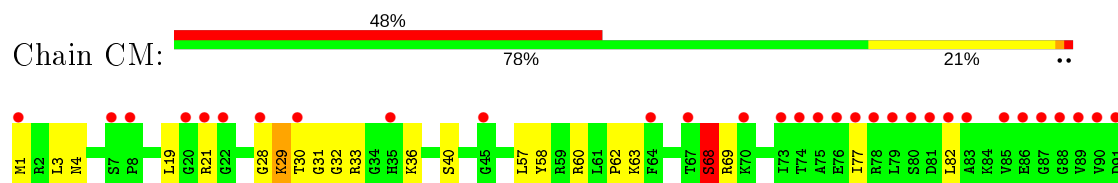
- Molecule 39: 50S ribosomal protein L14



- Molecule 39: 50S ribosomal protein L14

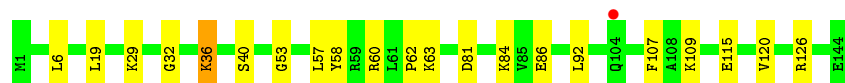
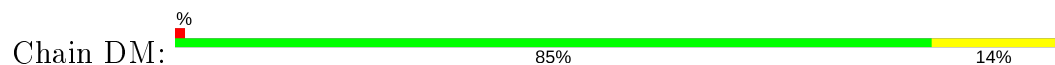


- Molecule 40: 50S ribosomal protein L15

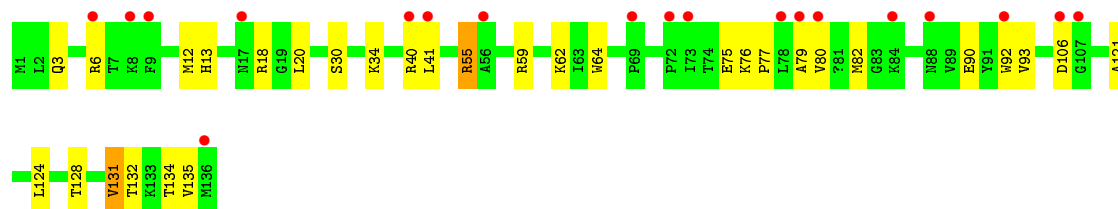
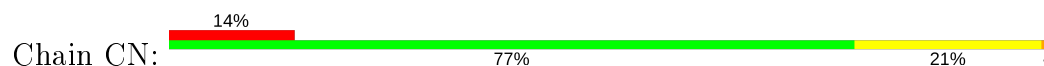




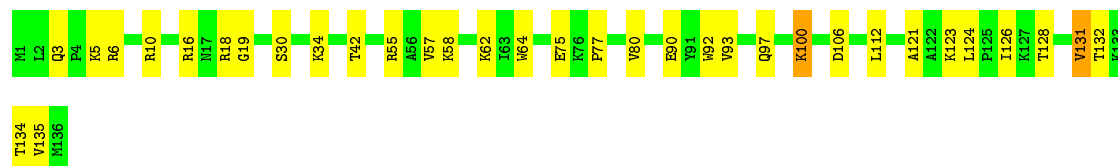
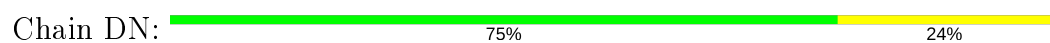
- Molecule 40: 50S ribosomal protein L15



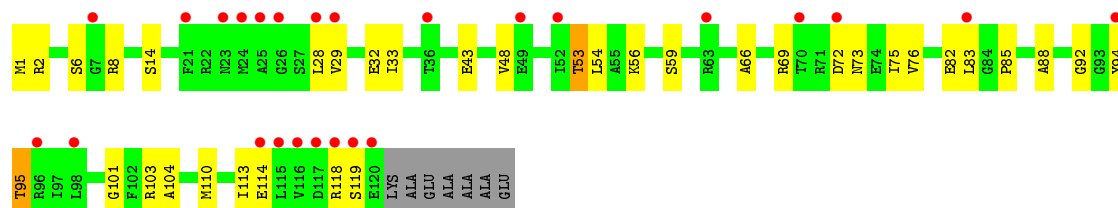
- Molecule 41: 50S ribosomal protein L16



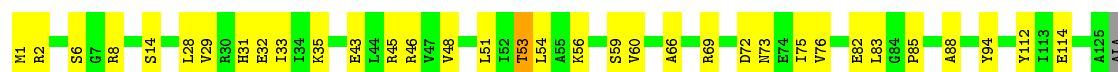
- Molecule 41: 50S ribosomal protein L16



- Molecule 42: 50S ribosomal protein L17

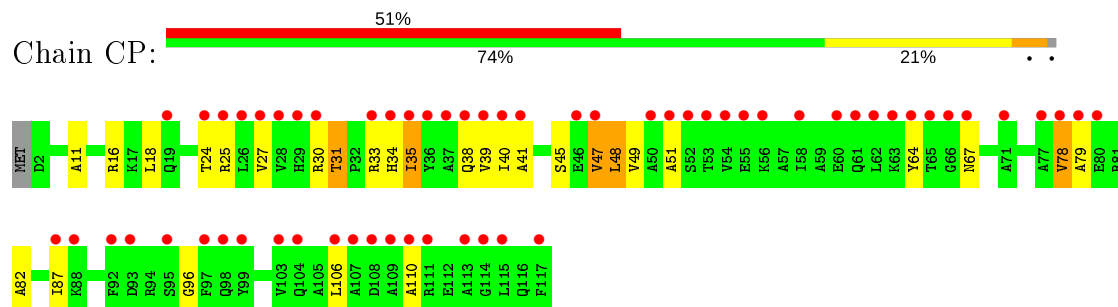


- Molecule 42: 50S ribosomal protein L17

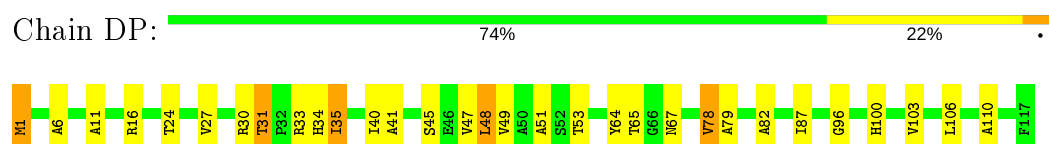


GLU

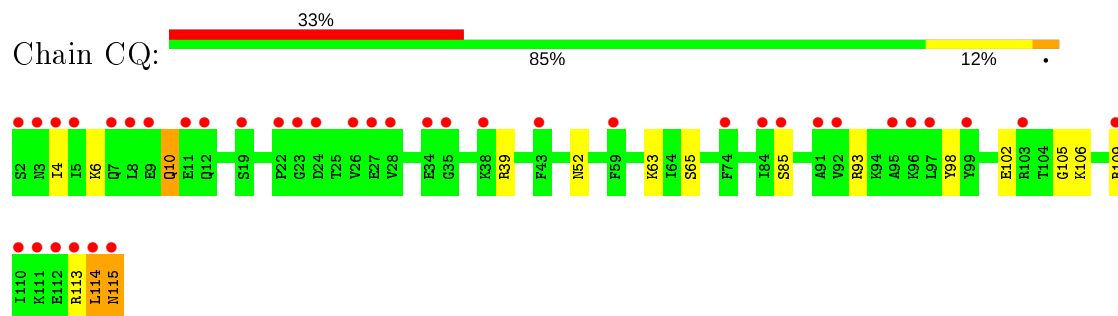
- Molecule 43: 50S ribosomal protein L18



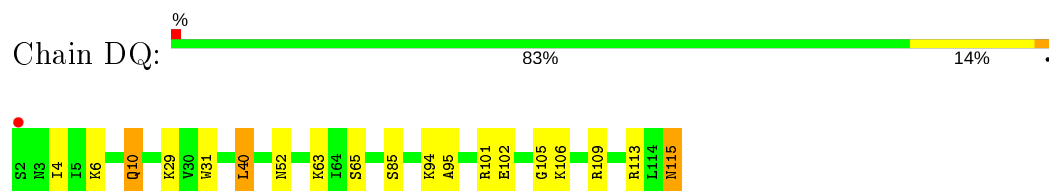
- Molecule 43: 50S ribosomal protein L18



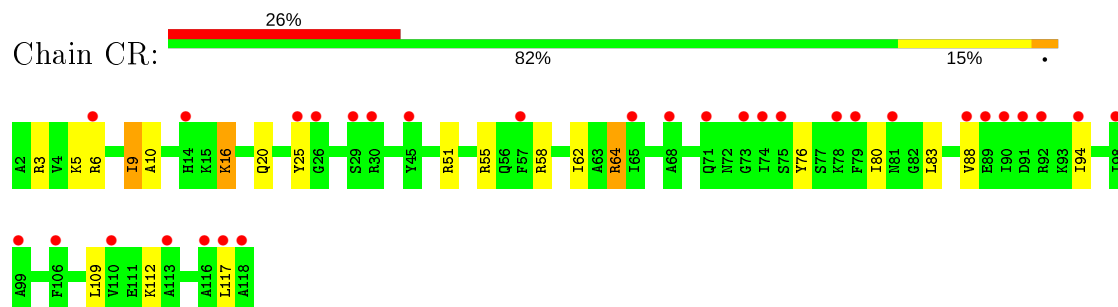
- Molecule 44: 50S ribosomal protein L19




- Molecule 44: 50S ribosomal protein L19



- Molecule 45: 50S ribosomal protein L20




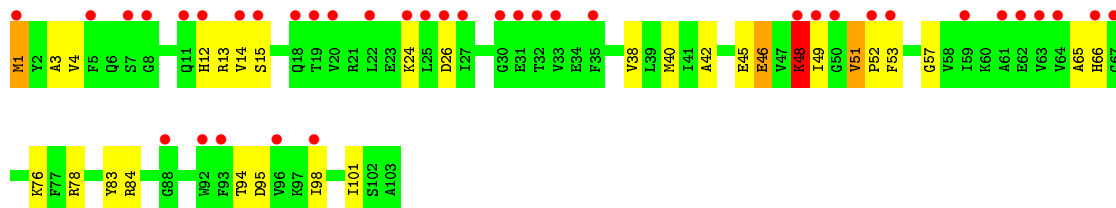
- Molecule 45: 50S ribosomal protein L20

Chain DR:  79% 19%



- Molecule 46: 50S ribosomal protein L21

Chain CS:  37% 71% 25%



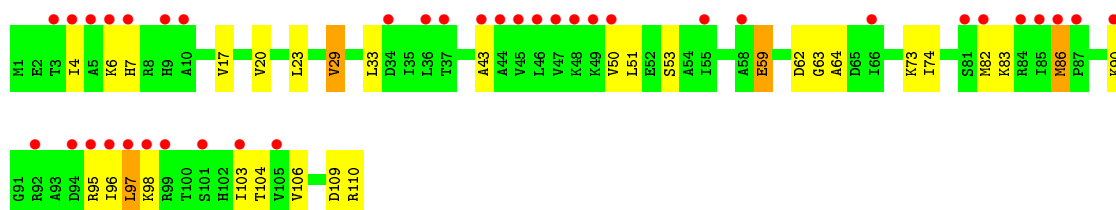
- Molecule 46: 50S ribosomal protein L21

Chain DS:  71% 26%




- Molecule 47: 50S ribosomal protein L22

Chain CT:  35% 72% 25%




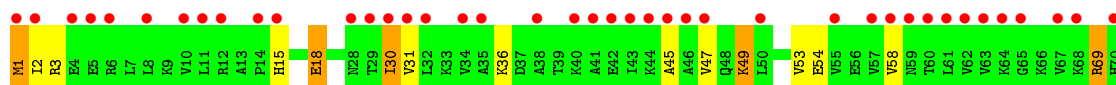
- Molecule 47: 50S ribosomal protein L22

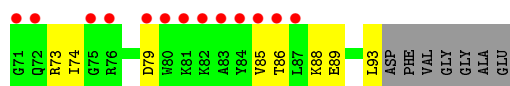
Chain DT:  78% 22%



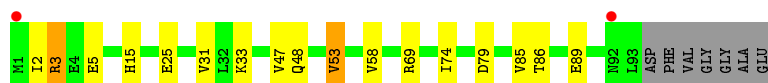
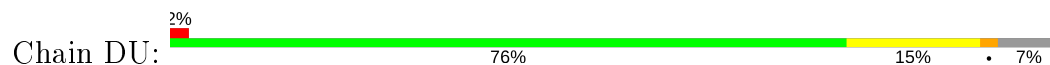
- Molecule 48: 50S ribosomal protein L23

Chain CU:  54% 70% 18% 5% 7%

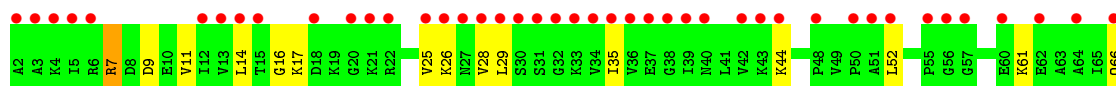
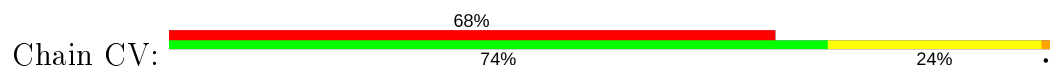




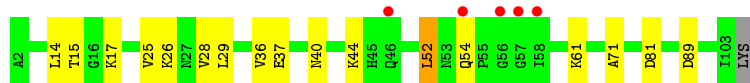
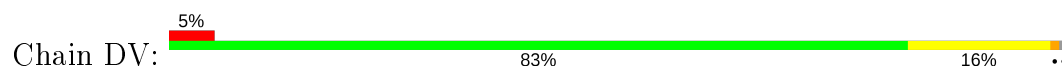
- Molecule 48: 50S ribosomal protein L23



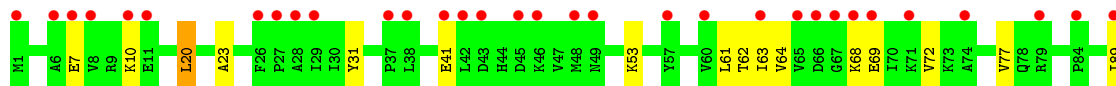
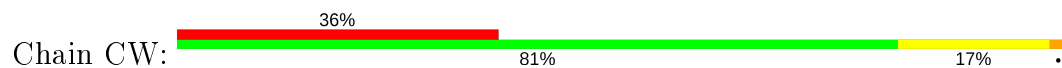
- Molecule 49: 50S ribosomal protein L24



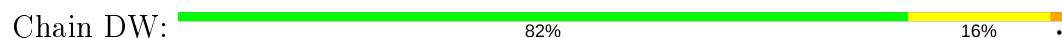
- Molecule 49: 50S ribosomal protein L24



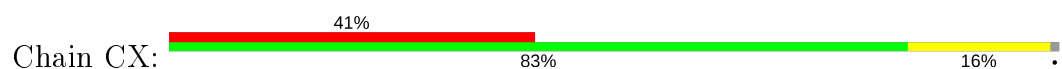
- Molecule 50: 50S ribosomal protein L25

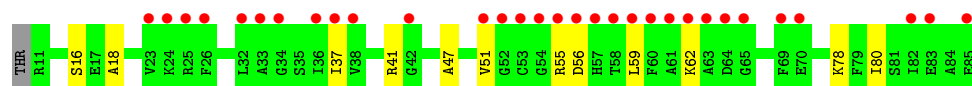


- Molecule 50: 50S ribosomal protein L25



- Molecule 51: 50S ribosomal protein L27





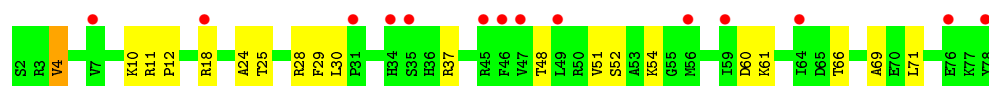
- Molecule 51: 50S ribosomal protein L27

Chain DX: 79% 20% .



- Molecule 52: 50S ribosomal protein L28

Chain CY: 18% 74% 25% .



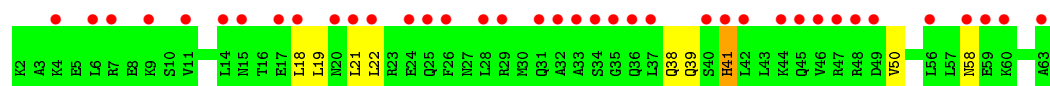
- Molecule 52: 50S ribosomal protein L28

Chain DY: % 81% 18% .



- Molecule 53: 50S ribosomal protein L29

Chain CZ: 61% 85% 13% .



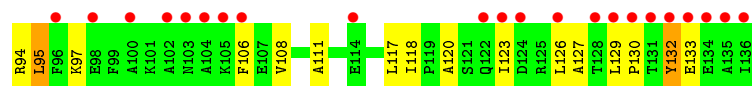
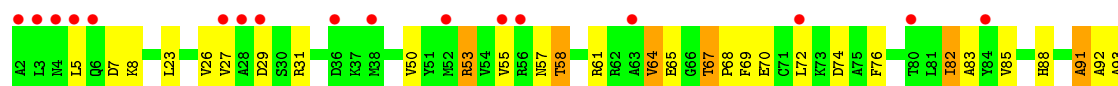
- Molecule 53: 50S ribosomal protein L29

Chain DZ: 3% 84% 13% .



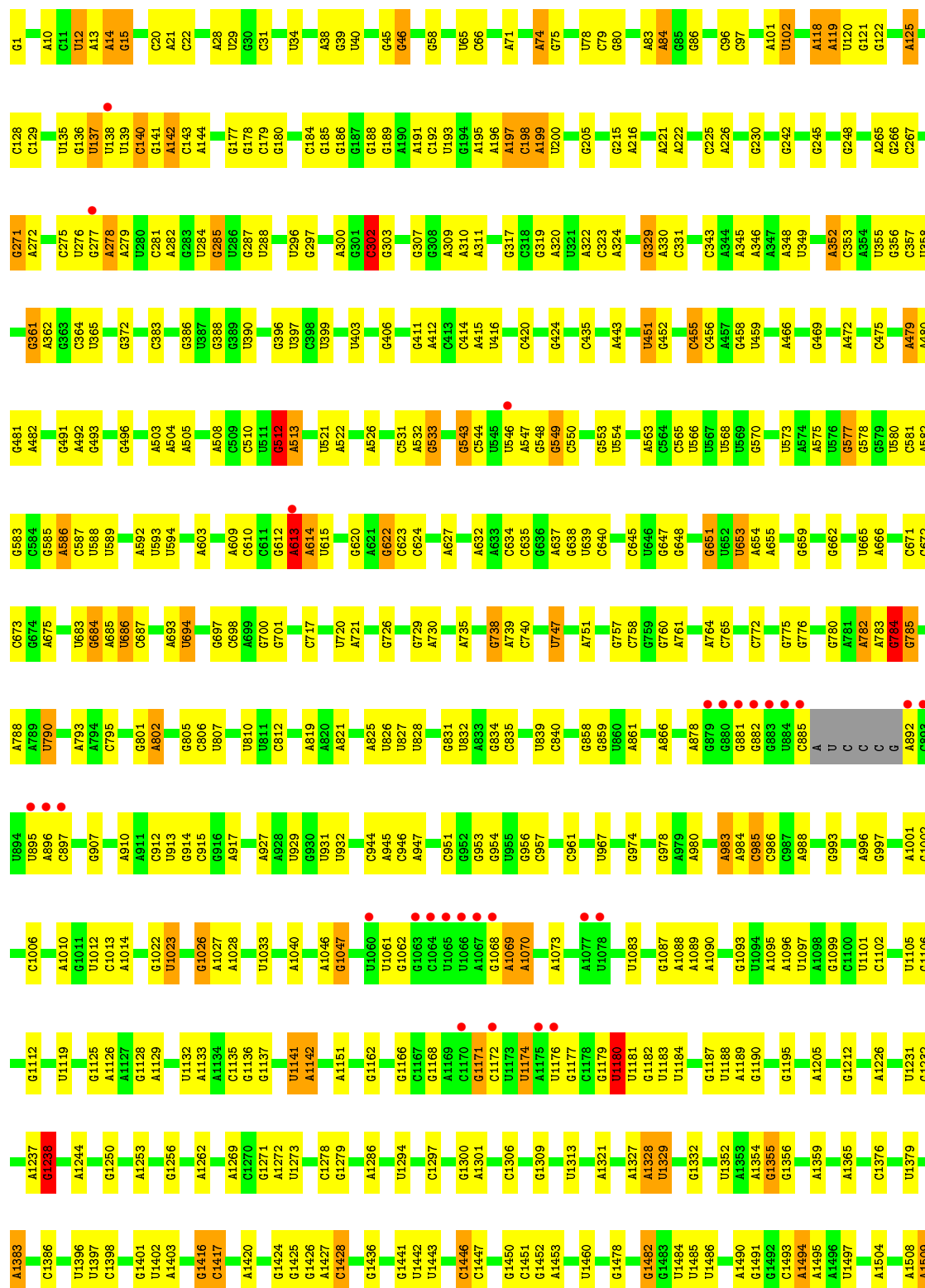
- Molecule 54: 50S ribosomal protein L10

Chain DI: 29% 66% 28% 6% .



• Molecule 55: 23S rRNA

Chain DA: 3% 67% 28% 5%



A2887	U2783	G2673	A2439	A2340	A2225	G2131	C2050	G1961	U1796	G1649	G1510
C2888	U2784	C2681	G2440	C2341	U2233	U2132	A2051	U1797	G1797	G1659	G1511
G2895	C2788	G2557	U2441	C2342	G2234	G2133	G2055	G1964	U1798	A1515	A1515
C2901	U2789	C2558	G2442	U2343	G2334	A2134	C2056	C1965	G1799	G1663	U1523
C2902	U2790	C2559	G2443	U2344	G2338	A2135	G2057	C1966	C1800	A1664	U1523
U2903	G2791	G2563	U2444	C2345	G2239	G2140	G2057	C1967	A1801	A1665	G1529
U	U2796	A2564	A2445	C2350	U2243	G2141	A2060	A1970	A1808	G1674	G1529
	U2797	A2565	A2446	C2351	G2255	A2142	G2061	U1971	A1812	A1675	A1532
	U2798	A2566	A2461	G2354	G2258	C2146	A2062	G1972	A1813	A1676	A1532
	A2799	G2567	G2464	C2357	U2259	C2147	C2063	G1973	G1813	U1534	U1534
A2800	A2706	A2572	C2465	G2357	U2260	A2147	C2064	G1974	C1816	G1682	U1535
	G2811	C2573	A2469	C2364	U2261	U2149	G2065	U1976	G1826	C1694	G1536
	G2812	A2577	G2472	C2365	U2262	C2150	G2066	G1979	G1826	G1695	G1537
A2813	C2715	G2578	U2473	A2366	A2267	U2151	G2069	U1980	A1829	A1544	A1544
A2814	G2719	C2578	U2474	A2367	A2268	G2152	G2077	A1981	G1699	C1547	C1547
C2815	U2720	G2581	U2475	A2377	A2273	C2153	A2077	C1985	C1832	U1714	U1544
	U2721	G2582	A2476	A2378	A2274	G2154	G2082	U1991	C1833	G1715	U1544
U2818	G2722	U2585	U2477	A2381	A2278	G2159	G2083	G1992	A1847	U1720	C1557
G2819	C2723	U2586	A2478	A2382	A2279	C2161	G2087	U1993	A1853	G1721	C1558
A2820	U2724	A2587	U2479	C2383	G2279	G2162	G2093	C1997	G1869	U1722	U1562
A2821	A2725	G2588	U2480	U2384	G2280	A2163	A2094	C1997	C1870	U1729	U1563
G2822	G2726	U2589	G2484	C2385	A2281	C2164	A2095	A2005	A1871	G1730	A1566
A2823	A2727	U2596	U2491	U2386	G2282	C2165	C2096	A2005	A1872	A1566	A1566
C2824	G2728	G2603	U2492	A2388	G2283	U2166	A2097	G2010	G1873	G1738	A1569
G2825	G2729	G2607	U2498	U2393	G2286	U2167	G2100	A2014	A1885	U1744	U1578
C2830	A2733	G2608	C2498	C2394	A2287	G2168	G2100	A2015	U1886	A1745	U1578
A2835	A2740	U2609	G2502	U2402	A2288	A2169	G2102	A2019	A1900	A1746	A1583
U2836	G2742	U2615	G2505	C2403	U2292	U2172	U2105	A2020	G1906	U1747	U1584
G2844	G2743	U2616	C2512	A2406	U2305	A2173	U2106	C2023	G1907	G1750	A1586
U2845	G2744	U2617	A2516	A2407	G2308	C2174	G2107	C2023	G1907	G1753	G1587
G2846	G2747	U2621	G2517	U2408	U2308	A2175	U2108	U2026	A1913	A1754	U1588
U2847	A2748	C2626	A2518	G2409	A2311	C2176	U2109	U2027	C1914	A1755	A1590
U2849	G2751	G2627	U2519	G2410	U2312	C2177	U2110	G2027	A1927	U1758	A1591
A2851	C2755	C2628	C2520	G2418	U2313	C2178	U2111	A2030	A1928	U1759	C1604
G2852	G2755	U2629	C2521	U2419	U2320	U2180	U2112	A2031	A1928	A1759	C1604
	C2762	G2630	U2522	U2420	U2321	U2181	A2114	G2032	G1929	C1764	C1607
U2861	G2763	C2636	U2523	C2421	G2325	A2182	G2115	A2033	G1930	A1608	A1608
U2866	A2764	U2637	C2524	U2422	G2326	A2183	G2116	U2034	U1931	A1773	C1612
A2868	G2765	U2638	A2423	U2423	G2327	A2184	U2117	G2035	A1932	C1774	C1612
G2869	G2766	G2643	A2424	C2424	A2328	U2185	U2118	G2036	G1935	U1775	G1613
C2870	U2768	G2644	A2425	A2425	U2329	G2186	A2119	G2037	A1938	U1778	A1614
U2871	U2769	A2660	A2426	A2426	G2330	A2198	G2120	G2038	U1939	G1622	G1622
A2872	G2770	G2661	G2427	G2427	G2331	G2204	G2121	A2042	U1940	U1781	A1641
A2873	C2771	A2662	G2428	G2428	G2332	G2204	U2122	C2043	C1941	U1782	G1642
	C2772	G2663	A2434	A2434	G2333	A2211	G2123	C2047	A1962	A1783	A1784
A2879	A2778	C2667	A2435	A2435	U2334	U2220	G2124	G2048	U1965	U1647	U1648
A2883	G2781		G2436	G2436	A2335		G2125				
U2884	G2782		G2437	G2437	A2335		G2126				
			U2438	U2438	C2339		G2128				

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.55Å 433.65Å 622.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 3.32 48.13 – 3.32	Depositor EDS
% Data completeness (in resolution range)	83.3 (48.13-3.32) 83.3 (48.13-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	40.28 (at 3.33Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, R_{free}	0.176 , 0.219 0.191 , 0.238	Depositor DCC
R_{free} test set	2784 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 128.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	295119	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, GUN, 1PE, 2MA, 2MG, ACY, PEG, 1MG, 3TD, PGE, D2T, UR3, 7MG, 4D4, 5MU, ZN, 5MC, MPD, PG4, 6MZ, TRS, OMC, MG, OMG, H2U, SPD, EDO, MEQ, OMU, PUT, 4OC, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	1.02	13/36596 (0.0%)	0.86	4/57086 (0.0%)
1	BA	1.01	12/36571 (0.0%)	0.86	3/57047 (0.0%)
2	AB	0.45	0/1784	0.65	0/2403
2	BB	0.43	0/1784	0.65	0/2403
3	AC	0.48	0/1652	0.66	0/2225
3	BC	0.48	0/1652	0.66	0/2225
4	AD	0.44	0/1665	0.69	0/2227
4	BD	0.46	0/1665	0.69	0/2227
5	AE	0.47	0/1157	0.78	0/1557
5	BE	0.45	0/1118	0.81	0/1504
6	AF	0.44	0/881	0.71	0/1189
6	BF	0.45	0/835	0.76	0/1128
7	AG	0.49	0/1196	0.65	0/1602
7	BG	0.48	0/1196	0.64	0/1602
8	AH	0.42	0/989	0.68	0/1326
8	BH	0.41	0/989	0.67	0/1326
9	AI	0.44	0/1034	0.67	0/1375
9	BI	0.45	0/1034	0.66	0/1375
10	AJ	0.46	0/806	0.67	0/1089
10	BJ	0.52	0/797	0.71	0/1077
11	AK	0.47	0/893	0.65	0/1205
11	BK	0.45	0/893	0.68	0/1205
12	AL	0.45	0/960	0.74	0/1286
12	BL	0.43	0/960	0.72	0/1286
13	AM	0.51	0/893	0.74	1/1193 (0.1%)
13	BM	0.53	0/893	0.73	0/1193
14	AN	0.48	0/817	0.65	0/1088
14	BN	0.47	0/817	0.65	0/1088
15	AO	0.47	0/722	0.65	0/964
15	BO	0.43	0/722	0.64	0/964
16	AP	0.48	0/659	0.73	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BP	0.47	0/659	0.75	0/884
17	AQ	0.47	0/658	0.73	0/881
17	BQ	0.47	0/658	0.75	0/881
18	AR	0.50	0/463	0.70	0/621
18	BR	0.49	0/463	0.69	0/621
19	AS	0.51	0/653	0.63	0/877
19	BS	0.51	0/653	0.64	0/877
20	AT	0.47	0/676	0.68	0/895
20	BT	0.50	0/671	0.70	0/888
21	AU	0.42	0/472	0.62	0/627
21	BU	0.40	0/472	0.63	0/627
22	C1	0.49	0/450	0.69	0/599
22	D1	0.61	0/450	0.75	0/599
23	C2	0.46	0/416	0.73	0/554
23	D2	0.49	0/421	0.70	0/561
24	C3	0.44	0/380	0.71	0/498
24	D3	0.54	0/380	0.74	0/498
25	C4	0.44	0/513	0.64	0/676
25	D4	0.52	0/513	0.68	0/676
26	C5	0.44	0/303	0.74	0/397
26	D5	0.60	1/303 (0.3%)	0.75	0/397
27	C0	0.53	0/453	0.75	0/605
27	D0	0.61	0/467	0.79	0/623
28	CB	1.01	1/2828 (0.0%)	0.90	1/4410 (0.0%)
28	DB	1.10	3/2872 (0.1%)	0.91	0/4478
29	CC	0.45	0/2121	0.74	0/2852
29	DC	0.49	0/2121	0.75	0/2852
30	CD	0.44	0/1586	0.68	0/2134
31	CA	1.05	65/69165 (0.1%)	0.88	16/107896 (0.0%)
32	DD	0.53	0/1576	0.70	0/2119
33	CE	0.43	0/1571	0.72	0/2113
33	DE	0.48	0/1571	0.72	0/2113
34	CF	0.43	0/1434	0.69	0/1926
34	DF	0.47	0/1434	0.73	0/1926
35	CG	0.41	0/1343	0.68	1/1816 (0.1%)
35	DG	0.45	0/1343	0.67	0/1816
36	CH	0.46	0/1121	0.72	1/1515 (0.1%)
36	DH	0.47	0/1121	0.70	0/1515
37	CJ	0.54	0/993	0.68	0/1341
37	DJ	0.54	0/993	0.68	0/1341
38	CK	0.43	0/1152	0.71	0/1551
38	DK	0.58	0/1152	0.75	0/1551
39	CL	0.47	0/947	0.75	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DL	0.53	0/955	0.77	0/1279
40	CM	0.45	0/1062	0.73	1/1413 (0.1%)
40	DM	0.51	0/1062	0.71	0/1413
41	CN	0.45	0/1081	0.72	0/1443
41	DN	0.55	0/1092	0.78	0/1457
42	CO	0.45	0/973	0.72	0/1301
42	DO	0.59	0/1006	0.78	0/1345
43	CP	0.44	0/902	0.70	0/1209
43	DP	0.51	0/910	0.70	0/1219
44	CQ	0.42	0/929	0.75	0/1242
44	DQ	0.50	0/929	0.74	0/1242
45	CR	0.47	0/960	0.70	0/1278
45	DR	0.61	0/960	0.75	0/1278
46	CS	0.45	0/829	0.77	0/1107
46	DS	0.59	0/829	0.82	0/1107
47	CT	0.42	0/864	0.78	0/1156
47	DT	0.57	0/864	0.80	0/1156
48	CU	0.46	0/744	0.72	0/994
48	DU	0.52	0/744	0.72	0/994
49	CV	0.47	0/787	0.79	0/1051
49	DV	0.49	0/787	0.82	0/1051
50	CW	0.42	0/766	0.69	0/1025
50	DW	0.52	0/766	0.71	0/1025
51	CX	0.39	0/576	0.66	0/762
51	DX	0.51	0/598	0.69	0/790
52	CY	0.40	0/635	0.70	0/848
52	DY	0.46	0/635	0.72	0/848
53	CZ	0.44	0/502	0.69	0/667
53	DZ	0.50	0/502	0.69	0/667
54	DI	0.52	0/1037	0.78	1/1402 (0.1%)
55	DA	1.19	83/69364 (0.1%)	0.93	24/108207 (0.0%)
All	All	0.95	178/309271 (0.1%)	0.85	53/462220 (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
10	BJ	0	1
28	DB	0	1
31	CA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	DA	0	26
All	All	0	29

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-10.08	1.26	1.42
31	CA	2225	A	C3'-O3'	9.82	1.55	1.42
31	CA	1936	A	N9-C4	-9.23	1.32	1.37
55	DA	2097	A	O5'-C5'	-8.54	1.29	1.42
55	DA	2585	U	C1'-N1	8.38	1.61	1.48
1	BA	5	U	C1'-N1	7.67	1.60	1.48
55	DA	12	U	C1'-N1	7.64	1.60	1.48
31	CA	769	U	C1'-N1	7.56	1.60	1.48
31	CA	2232	C	C1'-N1	7.42	1.59	1.48
55	DA	673	C	C3'-O3'	-7.20	1.32	1.42
55	DA	790	U	C1'-N1	7.15	1.59	1.48
55	DA	2585	U	C3'-O3'	7.08	1.52	1.42
55	DA	2068	U	C3'-O3'	-7.06	1.32	1.42
1	AA	632	U	C1'-N1	6.96	1.59	1.48
55	DA	2426	A	C3'-O3'	6.89	1.51	1.42
31	CA	1657	U	C1'-N1	6.82	1.58	1.48
1	AA	1195	C	C1'-N1	6.80	1.58	1.48
55	DA	2127	G	C3'-O3'	6.79	1.51	1.42
31	CA	1825	U	C1'-N1	6.69	1.58	1.48
31	CA	1313	U	C1'-N1	6.65	1.58	1.48
31	CA	995	C	O5'-C5'	-6.62	1.32	1.42
31	CA	12	U	C1'-N1	6.57	1.58	1.48
31	CA	1938	A	N9-C4	6.54	1.41	1.37
31	CA	2465	C	C1'-N1	6.54	1.58	1.48
31	CA	790	U	C1'-N1	6.54	1.58	1.48
31	CA	2215	C	C1'-N1	6.52	1.58	1.48
31	CA	1940	U	C3'-O3'	6.50	1.51	1.42
1	BA	1397	C	N1-C2	6.45	1.46	1.40
55	DA	784	G	C3'-O3'	6.42	1.51	1.42
1	BA	632	U	C1'-N1	6.37	1.58	1.48
1	AA	5	U	C1'-N1	6.33	1.58	1.48
31	CA	2425	A	C3'-O3'	6.33	1.51	1.42
55	DA	1126	A	N9-C4	6.32	1.41	1.37
55	DA	1188	U	C2-N3	-6.30	1.33	1.37
31	CA	1670	C	C3'-O3'	6.19	1.50	1.42
55	DA	2402	U	N1-C2	6.19	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	2585	U	N1-C2	6.18	1.44	1.38
1	AA	1397	C	N1-C6	6.15	1.40	1.37
31	CA	461	C	C1'-N1	6.15	1.57	1.48
55	DA	2031	A	N7-C5	-6.09	1.35	1.39
31	CA	1777	U	C1'-N1	6.08	1.57	1.48
31	CA	2263	C	C1'-N1	6.06	1.57	1.48
55	DA	793	A	N7-C5	-6.04	1.35	1.39
55	DA	1547	C	C1'-N1	6.02	1.57	1.48
55	DA	2729	G	C3'-O3'	-6.02	1.33	1.42
55	DA	1778	U	C4'-C3'	-6.01	1.46	1.53
31	CA	532	A	C3'-O3'	6.01	1.50	1.42
31	CA	1993	U	C1'-N1	6.01	1.57	1.48
1	BA	764	C	C1'-N1	5.99	1.57	1.48
31	CA	271	G	C3'-O3'	5.99	1.50	1.42
31	CA	1376	C	C1'-N1	5.94	1.57	1.48
55	DA	2502	G	O5'-C5'	-5.94	1.33	1.42
55	DA	662	G	N7-C5	-5.93	1.35	1.39
31	CA	2354	C	C1'-N1	5.91	1.57	1.48
31	CA	1584	U	C1'-N1	5.91	1.57	1.48
55	DA	12	U	P-O5'	5.89	1.65	1.59
31	CA	2443	C	C1'-N1	5.88	1.57	1.48
55	DA	1534	U	C1'-N1	5.88	1.57	1.48
55	DA	140	C	C1'-N1	5.87	1.57	1.48
31	CA	2779	U	C1'-N1	5.85	1.57	1.48
55	DA	954	G	C5-C6	5.79	1.48	1.42
55	DA	1785	A	N7-C5	-5.79	1.35	1.39
55	DA	526	A	N3-C4	5.76	1.38	1.34
55	DA	416	U	C1'-N1	5.75	1.57	1.48
31	CA	2006	C	C1'-N1	5.74	1.57	1.48
1	BA	1008	U	O5'-C5'	-5.71	1.33	1.42
1	AA	1059	C	C1'-N1	5.70	1.57	1.48
31	CA	653	U	C1'-N1	5.70	1.57	1.48
55	DA	2268	A	N7-C5	-5.68	1.35	1.39
31	CA	784	G	C3'-O3'	5.68	1.50	1.42
55	DA	102	U	N1-C2	5.67	1.43	1.38
31	CA	2680	U	C3'-O3'	5.67	1.50	1.42
31	CA	20	C	C1'-N1	5.63	1.57	1.48
1	BA	842	U	C3'-O3'	5.63	1.50	1.42
1	AA	295	C	C1'-N1	5.62	1.57	1.48
55	DA	585	G	C2-N3	5.60	1.37	1.32
31	CA	1633	G	C3'-O3'	5.59	1.50	1.42
31	CA	1656	C	C1'-N1	5.57	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	2586	U	C1'-N1	5.57	1.57	1.48
55	DA	653	U	C1'-N1	5.56	1.57	1.48
55	DA	1383	A	N7-C5	-5.56	1.35	1.39
55	DA	2781	A	N7-C5	-5.56	1.35	1.39
28	DB	35	C	N1-C6	5.55	1.40	1.37
31	CA	691	C	C1'-N1	5.55	1.57	1.48
31	CA	2233	U	C1'-N1	5.55	1.57	1.48
31	CA	1352	U	C1'-N1	5.54	1.57	1.48
55	DA	978	G	C6-N1	5.51	1.43	1.39
1	AA	932	C	C1'-N1	5.51	1.57	1.48
31	CA	1314	C	C1'-N1	5.50	1.57	1.48
55	DA	1664	A	N7-C5	-5.50	1.35	1.39
55	DA	2220	U	C1'-N1	5.50	1.56	1.48
31	CA	1774	C	C1'-N1	5.49	1.56	1.48
55	DA	790	U	P-O5'	5.49	1.65	1.59
55	DA	2239	G	C3'-O3'	-5.48	1.34	1.42
1	AA	137	U	C1'-N1	5.47	1.56	1.48
1	BA	209	U	C1'-N1	5.47	1.56	1.48
55	DA	2055	C	C3'-O3'	-5.47	1.34	1.42
28	DB	11	C	C1'-N1	5.47	1.56	1.48
55	DA	1584	U	C1'-N1	5.45	1.56	1.48
55	DA	2077	A	N7-C5	-5.45	1.35	1.39
1	BA	1059	C	C1'-N1	5.44	1.56	1.48
31	CA	2104	C	C1'-N1	5.44	1.56	1.48
55	DA	2850	A	N7-C5	-5.42	1.35	1.39
1	BA	137	U	C1'-N1	5.42	1.56	1.48
55	DA	2542	A	C6-N6	-5.40	1.29	1.33
1	BA	222	C	C1'-N1	5.40	1.56	1.48
1	AA	603	U	C1'-N1	5.40	1.56	1.48
55	DA	2354	C	O5'-C5'	-5.39	1.34	1.42
55	DA	2005	A	C6-N1	5.38	1.39	1.35
31	CA	1253	A	P-O5'	5.37	1.65	1.59
55	DA	1446	C	C1'-N1	5.37	1.56	1.48
55	DA	2158	A	C3'-O3'	5.36	1.49	1.42
31	CA	1557	C	C1'-N1	5.36	1.56	1.48
31	CA	2320	U	C1'-N1	5.36	1.56	1.48
55	DA	967	U	C1'-N1	5.36	1.56	1.48
55	DA	2425	A	C3'-O3'	5.35	1.49	1.42
55	DA	2506	U	C1'-N1	5.35	1.56	1.48
55	DA	2342	C	C1'-N1	5.35	1.56	1.48
55	DA	1659	G	C3'-O3'	-5.34	1.34	1.42
31	CA	140	C	C1'-N1	5.32	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	692	C	C1'-N1	5.31	1.56	1.48
1	AA	222	C	C1'-N1	5.28	1.56	1.48
55	DA	549	G	C3'-O3'	5.27	1.49	1.42
31	CA	826	U	C1'-N1	5.26	1.56	1.48
55	DA	2901	C	C1'-N1	5.26	1.56	1.48
55	DA	275	C	C1'-N1	5.25	1.56	1.48
28	DB	91	C	C1'-N1	5.24	1.56	1.48
31	CA	623	C	C1'-N1	5.23	1.56	1.48
55	DA	2472	G	N7-C5	-5.23	1.36	1.39
31	CA	1981	A	C3'-O3'	5.21	1.49	1.42
55	DA	443	A	N7-C5	-5.21	1.36	1.39
55	DA	613	A	N9-C4	5.21	1.41	1.37
1	AA	549	C	C1'-N1	5.20	1.56	1.48
55	DA	2578	G	C5-C4	-5.19	1.34	1.38
55	DA	2402	U	C1'-N1	5.19	1.56	1.48
31	CA	1658	C	C1'-N1	5.18	1.56	1.48
31	CA	2619	C	C1'-N1	5.18	1.56	1.48
31	CA	562	U	C1'-N1	5.17	1.56	1.48
55	DA	735	A	N3-C4	5.17	1.38	1.34
55	DA	694	U	C1'-N1	5.16	1.56	1.48
55	DA	1180	U	C1'-N1	5.15	1.56	1.48
1	AA	503	C	C1'-N1	5.15	1.56	1.48
31	CA	1375	U	C1'-N1	5.14	1.56	1.48
31	CA	635	C	C1'-N1	5.13	1.56	1.48
55	DA	2406	A	P-O5'	5.12	1.64	1.59
31	CA	114	U	C1'-N1	5.12	1.56	1.48
1	BA	1493	A	C3'-O3'	5.11	1.49	1.42
31	CA	801	G	C3'-O3'	5.10	1.49	1.42
55	DA	810	U	N1-C2	5.10	1.43	1.38
55	DA	1913	A	C3'-O3'	5.10	1.49	1.42
55	DA	2491	U	C1'-N1	5.10	1.56	1.48
31	CA	275	C	C1'-N1	5.10	1.56	1.48
31	CA	2385	C	C1'-N1	5.09	1.56	1.48
55	DA	951	C	N1-C6	5.09	1.40	1.37
31	CA	2823	A	C3'-O3'	5.09	1.49	1.42
31	CA	2656	U	C1'-N1	5.08	1.56	1.48
55	DA	533	G	N7-C5	-5.08	1.36	1.39
55	DA	635	C	C1'-N1	5.08	1.56	1.48
1	BA	823	C	C1'-N1	5.08	1.56	1.48
28	CB	11	C	C1'-N1	5.08	1.56	1.48
31	CA	1994	C	C1'-N1	5.08	1.56	1.48
55	DA	1174	U	C1'-N1	5.08	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	29	U	C1'-N1	5.08	1.56	1.48
55	DA	578	G	N7-C5	-5.07	1.36	1.39
55	DA	469	G	C3'-O3'	-5.06	1.35	1.42
31	CA	2581	G	N3-C4	5.06	1.39	1.35
55	DA	1714	U	C1'-N1	5.05	1.56	1.48
55	DA	701	G	N3-C4	5.05	1.39	1.35
55	DA	1665	A	N7-C5	-5.04	1.36	1.39
31	CA	1629	U	C1'-N1	5.04	1.56	1.48
31	CA	2658	C	C1'-N1	5.04	1.56	1.48
55	DA	458	G	N3-C4	5.03	1.39	1.35
55	DA	2442	C	C3'-O3'	-5.03	1.35	1.42
1	AA	1196	A	N9-C4	5.02	1.40	1.37
55	DA	2769	U	C3'-O3'	-5.02	1.35	1.42
26	D5	26	ILE	CG1-CD1	5.01	1.85	1.50
55	DA	632	A	N7-C5	-5.01	1.36	1.39
31	CA	2342	C	C1'-N1	5.00	1.56	1.48

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CB	15	A	O4'-C1'-N9	9.57	115.86	108.20
31	CA	2425	A	P-O3'-C3'	8.79	130.24	119.70
31	CA	271	G	P-O3'-C3'	7.72	128.96	119.70
1	BA	2	A	OP1-P-OP2	-7.50	108.34	119.60
1	AA	1	A	OP1-P-OP2	-7.15	108.88	119.60
55	DA	892	A	OP1-P-OP2	-7.06	109.01	119.60
54	DI	132	TYR	C-N-CA	7.02	139.24	121.70
55	DA	2585	U	P-O3'-C3'	6.93	128.01	119.70
55	DA	1	G	OP1-P-OP2	-6.92	109.23	119.60
31	CA	892	A	OP1-P-OP2	-6.85	109.32	119.60
31	CA	1786	A	C1'-O4'-C4'	-6.60	104.62	109.90
55	DA	512	G	O4'-C1'-N9	6.55	113.44	108.20
55	DA	2825	G	O4'-C1'-N9	6.38	113.31	108.20
55	DA	199	A	C1'-O4'-C4'	-6.29	104.87	109.90
1	BA	7	A	C1'-O4'-C4'	-6.22	104.93	109.90
1	BA	893	C	C3'-C2'-C1'	-6.15	96.58	101.50
55	DA	479	A	C3'-C2'-C1'	-6.12	96.60	101.50
55	DA	613	A	O4'-C1'-N9	6.05	113.04	108.20
55	DA	1023	U	C4'-C3'-C2'	-6.03	96.58	102.60
55	DA	2848	G	O4'-C1'-N9	5.97	112.98	108.20
55	DA	271	G	P-O3'-C3'	5.84	126.71	119.70
31	CA	974	G	N9-C1'-C2'	5.79	121.52	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2225	A	P-O3'-C3'	5.78	126.63	119.70
31	CA	199	A	C1'-O4'-C4'	-5.76	105.29	109.90
31	CA	784	G	P-O3'-C3'	5.75	126.61	119.70
31	CA	479	A	C3'-C2'-C1'	-5.73	96.92	101.50
1	AA	7	A	C1'-O4'-C4'	-5.68	105.35	109.90
55	DA	1648	U	O4'-C1'-N1	5.58	112.66	108.20
40	CM	68	SER	C-N-CA	5.57	135.63	121.70
55	DA	2825	G	C4'-C3'-C2'	-5.49	97.11	102.60
55	DA	242	G	C3'-C2'-C1'	-5.47	97.12	101.50
31	CA	2680	U	P-O3'-C3'	5.47	126.27	119.70
13	AM	12	HIS	C-N-CA	5.47	135.37	121.70
31	CA	1128	G	C1'-O4'-C4'	-5.46	105.53	109.90
1	AA	841	C	P-O3'-C3'	5.43	126.21	119.70
31	CA	2095	A	C5'-C4'-C3'	-5.39	107.37	116.00
55	DA	242	G	C1'-O4'-C4'	-5.37	105.60	109.90
55	DA	2436	G	C4'-C3'-C2'	-5.34	97.26	102.60
55	DA	451	U	C1'-O4'-C4'	-5.33	105.64	109.90
36	CH	8	LYS	C-N-CA	5.31	134.98	121.70
55	DA	458	G	C3'-C2'-C1'	-5.31	97.25	101.50
31	CA	2035	G	C1'-O4'-C4'	-5.28	105.67	109.90
55	DA	302	C	C5'-C4'-O4'	5.21	115.35	109.10
55	DA	2238	G	C1'-O4'-C4'	-5.18	105.76	109.90
35	CG	175	LYS	C-N-CA	5.17	134.62	121.70
31	CA	1379	U	P-O3'-C3'	5.14	125.87	119.70
55	DA	2447	G	C3'-C2'-C1'	-5.14	97.39	101.50
31	CA	451	U	C1'-O4'-C4'	-5.12	105.80	109.90
55	DA	2127	G	P-O3'-C3'	5.12	125.84	119.70
55	DA	1800	C	C1'-O4'-C4'	-5.11	105.81	109.90
1	AA	429	U	C1'-O4'-C4'	-5.10	105.82	109.90
31	CA	204	A	C3'-C2'-C1'	-5.03	97.47	101.50
55	DA	479	A	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	BJ	37	ARG	Mainchain
31	CA	780	G	Sidechain
55	DA	1047	G	Sidechain
55	DA	1162	G	Sidechain
55	DA	1238	G	Sidechain
55	DA	1682	G	Sidechain

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Mol	Chain	Res	Type	Group
55	DA	1773	A	Sidechain
55	DA	1985	C	Sidechain
55	DA	2010	G	Sidechain
55	DA	2286	G	Sidechain
55	DA	2351	G	Sidechain
55	DA	2512	C	Sidechain
55	DA	2516	A	Sidechain
55	DA	2518	A	Sidechain
55	DA	2582	G	Sidechain
55	DA	2588	G	Sidechain
55	DA	2728	U	Sidechain
55	DA	2825	G	Sidechain
55	DA	329	G	Sidechain
55	DA	452	G	Sidechain
55	DA	512	G	Sidechain
55	DA	577	G	Sidechain
55	DA	700	G	Sidechain
55	DA	726	G	Sidechain
55	DA	953	G	Sidechain
55	DA	956	G	Sidechain
55	DA	980	A	Sidechain
55	DA	983	A	Sidechain
28	DB	13	G	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	32932	0	16593	164	0
1	BA	32910	0	16582	182	0
2	AB	1753	0	1780	14	0
2	BB	1753	0	1780	15	0
3	AC	1625	0	1696	13	0
3	BC	1625	0	1696	17	0
4	AD	1643	0	1707	18	0
4	BD	1643	0	1707	19	0
5	AE	1144	0	1185	17	0
5	BE	1105	0	1148	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AF	862	0	864	12	0
6	BF	817	0	808	9	0
7	AG	1182	0	1238	17	0
7	BG	1182	0	1238	16	0
8	AH	979	0	1031	9	0
8	BH	979	0	1031	7	0
9	AI	1022	0	1070	11	0
9	BI	1022	0	1070	10	0
10	AJ	796	0	836	8	0
10	BJ	787	0	828	11	0
11	AK	877	0	887	11	0
11	BK	877	0	887	13	0
12	AL	957	0	1017	14	0
12	BL	957	0	1017	16	0
13	AM	884	0	941	11	0
13	BM	884	0	941	14	0
14	AN	805	0	844	10	0
14	BN	805	0	844	10	0
15	AO	714	0	734	3	0
15	BO	714	0	734	7	0
16	AP	649	0	666	5	0
16	BP	649	0	666	8	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	5	0
18	AR	456	0	478	5	0
18	BR	456	0	478	5	0
19	AS	638	0	665	13	0
19	BS	638	0	665	11	0
20	AT	670	0	719	11	0
20	BT	665	0	714	8	0
21	AU	465	0	491	6	0
21	BU	465	0	491	5	0
22	C1	444	0	458	17	0
22	D1	444	0	458	10	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	7	0
25	C4	504	0	572	3	0
25	D4	504	0	572	7	0
26	C5	302	0	340	5	0
26	D5	302	0	340	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	C0	449	0	488	4	0
27	D0	463	0	504	7	0
28	CB	2529	0	1281	7	0
28	DB	2569	0	1301	10	0
29	CC	2082	0	2154	24	0
29	DC	2082	0	2154	22	0
30	CD	1565	0	1616	22	0
31	CA	62229	0	31319	399	0
32	DD	1576	0	1627	29	0
33	CE	1552	0	1619	20	0
33	DE	1552	0	1619	20	0
34	CF	1410	0	1444	18	0
34	DF	1410	0	1444	26	0
35	CG	1323	0	1371	16	0
35	DG	1323	0	1371	14	0
36	CH	1110	0	1148	9	0
36	DH	1110	0	1148	10	0
37	CJ	979	0	1028	7	0
37	DJ	979	0	1028	10	0
38	CK	1129	0	1162	13	0
38	DK	1129	0	1162	14	0
39	CL	938	0	1012	9	0
39	DL	946	0	1023	7	0
40	CM	1053	0	1129	21	0
40	DM	1053	0	1129	16	0
41	CN	1075	0	1154	15	0
41	DN	1092	0	1177	17	0
42	CO	960	0	1000	16	0
42	DO	993	0	1034	16	0
43	CP	892	0	923	14	0
43	DP	900	0	935	17	0
44	CQ	917	0	962	8	0
44	DQ	917	0	962	14	0
45	CR	947	0	1019	13	0
45	DR	947	0	1019	20	0
46	CS	816	0	839	16	0
46	DS	816	0	839	20	0
47	CT	857	0	922	16	0
47	DT	857	0	922	14	0
48	CU	738	0	807	9	0
48	DU	738	0	807	6	0
49	CV	779	0	831	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	DV	779	0	831	8	0
50	CW	753	0	780	6	0
50	DW	753	0	780	7	0
51	CX	569	0	581	8	0
51	DX	591	0	606	14	0
52	CY	625	0	652	11	0
52	DY	625	0	652	8	0
53	CZ	501	0	531	5	0
53	DZ	501	0	531	6	0
54	DI	1023	0	1052	26	0
55	DA	62423	0	31411	382	0
56	AA	70	0	0	0	0
56	BA	41	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	184	0	0	0	0
56	DB	9	0	0	0	0
56	DD	1	0	0	0	0
56	DM	1	0	0	0	0
56	DR	1	0	0	0	0
57	AA	13	0	18	0	0
57	BA	13	0	18	1	0
57	DA	26	0	36	0	0
57	DQ	13	0	18	0	0
57	DR	13	0	18	1	0
57	DS	13	0	18	0	0
58	AA	16	0	28	0	0
58	DA	40	0	70	2	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	4	0
58	DT	16	0	28	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
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D3	7	0	10	1	0
61	DA	42	0	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DL	7	0	10	0	0
61	DP	7	0	10	0	0
61	DQ	7	0	10	1	0
62	D0	4	0	6	0	0
62	D1	4	0	6	0	0
62	DA	32	0	48	4	0
62	DB	8	0	12	0	0
63	D1	10	0	14	0	0
63	D3	10	0	14	0	0
63	DA	40	0	56	5	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	0	0
65	DA	32	0	44	1	0
66	DA	12	0	9	2	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	507	0	0	3	0
69	AC	4	0	0	0	0
69	AD	2	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	5	0	0	0	0
69	AL	7	0	0	0	0
69	AM	4	0	0	0	0
69	AN	6	0	0	1	0
69	AO	1	0	0	0	0
69	AP	1	0	0	0	0
69	AQ	1	0	0	0	0
69	AS	1	0	0	0	0
69	AT	2	0	0	0	0
69	AU	4	0	0	0	0
69	BA	287	0	0	2	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
69	BL	3	0	0	0	0
69	BN	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	BO	1	0	0	0	0
69	BP	4	0	0	0	0
69	BR	1	0	0	0	0
69	BT	5	0	0	0	0
69	C3	3	0	0	0	0
69	C4	1	0	0	0	0
69	CA	696	0	0	3	0
69	CB	13	0	0	0	0
69	CC	11	0	0	0	0
69	CD	4	0	0	0	0
69	CE	5	0	0	0	0
69	CL	1	0	0	0	0
69	CM	3	0	0	0	0
69	CO	1	0	0	0	0
69	CU	2	0	0	0	0
69	CV	1	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	24	0	0	2	0
69	D1	37	0	0	0	0
69	D2	5	0	0	0	0
69	D3	30	0	0	0	0
69	D4	40	0	0	1	0
69	D5	13	0	0	1	0
69	DA	4824	0	0	39	0
69	DB	203	0	0	3	0
69	DC	100	0	0	1	0
69	DD	97	0	0	5	0
69	DE	54	0	0	2	0
69	DF	13	0	0	1	0
69	DG	9	0	0	0	0
69	DH	2	0	0	0	0
69	DK	61	0	0	0	0
69	DL	50	0	0	0	0
69	DM	60	0	0	0	0
69	DN	81	0	0	1	0
69	DO	42	0	0	1	0
69	DP	42	0	0	2	0
69	DQ	32	0	0	1	0
69	DR	68	0	0	3	0
69	DS	52	0	0	5	0
69	DT	65	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	DU	24	0	0	0	0
69	DV	19	0	0	1	0
69	DW	33	0	0	1	0
69	DX	33	0	0	2	0
69	DY	11	0	0	1	0
69	DZ	7	0	0	0	0
All	All	295119	0	194415	2066	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 4.

All (2066) 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	1.85	1.50
46:CS:14:VAL:HG21	46:CS:98:ILE:HG13	1.26	1.16
31:CA:1005:C:O2'	38:CK:30:THR:HG21	1.62	0.99
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.44	0.95
31:CA:1311:G:H21	31:CA:1603:A:H62	1.16	0.94
54:DI:67:THR:HG22	54:DI:68:PRO:HA	1.52	0.91
31:CA:1936:A:H2	31:CA:1943:U:H3	1.15	0.91
51:DX:41[A]:ARG:HH12	55:DA:2262:U:H5''	1.39	0.88
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.56	0.87
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.56	0.87
55:DA:1975:G:H21	63:DA:3225:PGE:H22	1.39	0.86
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.57	0.86
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.57	0.86
40:DM:60:ARG:HH21	55:DA:2428:G:N2	1.72	0.86
2:AB:31:ILE:HG21	2:AB:39:HIS:HD2	1.42	0.85
46:CS:14:VAL:HG21	46:CS:98:ILE:CG1	2.07	0.84
1:AA:1492:A:H5''	12:AL:44:LYS:HG2	1.60	0.84
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.60	0.83
32:DD:140:HIS:HB3	69:DD:485:HOH:O	1.76	0.83
49:DV:52:LEU:HB3	49:DV:54:GLN:HB2	1.59	0.83
2:BB:31:ILE:HG21	2:BB:39:HIS:HD2	1.43	0.82
33:DE:33:VAL:HG22	58:DA:3192:MPD:H12	1.62	0.82
31:CA:2796:U:H3	31:CA:2799:A:H61	1.23	0.82
55:DA:1927:A:H2'	55:DA:1928:A:C8	2.15	0.82
1:AA:1063:C:H2'	1:AA:1064:G:C8	2.15	0.82
55:DA:2796:U:H3	55:DA:2799:A:H61	1.24	0.82
29:CC:17:VAL:HB	29:CC:204:VAL:CG1	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:CM:77:ILE:HD11	40:CM:108:ALA:HB1	1.62	0.80
31:CA:694:U:OP1	31:CA:1569:A:H1'	1.83	0.79
31:CA:206:U:H2'	31:CA:207:A:H8	1.46	0.79
47:DT:90:LYS:HA	55:DA:751:A:H5'	1.62	0.79
46:CS:14:VAL:CG2	46:CS:98:ILE:HG13	2.09	0.78
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.63	0.78
31:CA:2428:G:N2	40:CM:60:ARG:HH21	1.79	0.78
1:AA:81:A:H61	1:AA:86:G:H1	1.29	0.78
11:BK:24:HIS:HB3	11:BK:31:ILE:HG23	1.66	0.78
31:CA:751:A:H5'	47:CT:90:LYS:HA	1.66	0.78
1:BA:841:C:H3'	1:BA:842:U:H5''	1.66	0.78
31:CA:193:U:H2'	31:CA:194:G:H8	1.49	0.77
31:CA:450:G:H2'	31:CA:451:U:H5''	1.65	0.76
34:DF:158:THR:HG23	34:DF:160:ALA:H	1.50	0.76
47:DT:73:LYS:HB2	47:DT:106:VAL:HB	1.67	0.76
33:DE:21:ARG:HD2	69:DE:432:HOH:O	1.85	0.76
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	1.68	0.76
55:DA:758:C:O2	55:DA:1981:A:H2	1.69	0.75
29:DC:41:GLY:O	29:DC:43:ARG:HD2	1.87	0.75
40:DM:60:ARG:HH21	55:DA:2428:G:H21	1.33	0.75
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.69	0.75
36:CH:27:ARG:HH11	52:CY:60:ASP:HA	1.52	0.75
47:CT:73:LYS:HB2	47:CT:106:VAL:HB	1.68	0.74
33:DE:130:LYS:HB2	33:DE:133:LEU:HD12	1.69	0.74
43:DP:103:VAL:HG23	69:DP:313:HOH:O	1.87	0.74
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.68	0.74
49:DV:37:GLU:HB3	69:DV:206:HOH:O	1.88	0.74
31:CA:2641:G:H5''	38:CK:78:THR:HB	1.69	0.73
5:AE:106:ILE:HD11	5:AE:124:LEU:HD23	1.69	0.73
29:CC:266:PHE:CD1	29:CC:266:PHE:N	2.57	0.73
31:CA:1203:U:H5'	40:CM:3:LEU:HD12	1.70	0.73
29:CC:266:PHE:H	29:CC:266:PHE:HD1	1.33	0.73
42:DO:33:ILE:HD12	42:DO:114:GLU:HB3	1.70	0.72
1:BA:82:G:H1	1:BA:84:U:H5	1.37	0.72
1:BA:1107:C:OP1	3:BC:174:PRO:HB3	1.90	0.71
55:DA:568:U:H1'	55:DA:2030:6MZ:H9C1	1.71	0.71
1:BA:518:C:H2'	1:BA:530:G:C8	2.25	0.71
45:DR:20:GLN:HG2	57:DR:201:PG4:H42	1.73	0.71
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.72	0.71
39:CL:38:ILE:HD11	39:CL:112:PHE:HZ	1.54	0.71
1:BA:664:G:H22	1:BA:741:G:H1	1.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.72	0.71
31:CA:118:A:N3	31:CA:178:G:H1'	2.06	0.71
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.57	0.70
31:CA:1936:A:N6	31:CA:1963:U:H3	1.90	0.70
1:AA:518:C:H2'	1:AA:530:G:C8	2.27	0.70
29:DC:258:ARG:HD2	55:DA:1799:G:OP1	1.92	0.70
55:DA:671:C:O2'	55:DA:672:C:H5'	1.92	0.70
29:CC:107:PRO:HD2	29:CC:110:LEU:HD22	1.74	0.70
55:DA:1137:G:H5''	59:DA:3213:PUT:H12	1.73	0.69
1:AA:202:G:HO2'	1:AA:468:A:H8	1.40	0.69
42:CO:33:ILE:HD12	42:CO:114:GLU:HB3	1.73	0.69
1:BA:967:5MC:HM53	1:BA:1197:A:N6	2.07	0.69
1:AA:403:C:H5'	4:AD:132:ILE:HG23	1.74	0.69
35:DG:95:ARG:HG2	35:DG:128:GLN:HB3	1.75	0.69
34:DF:80:ARG:HB3	34:DF:83:TYR:CZ	2.28	0.69
33:CE:130:LYS:HB2	33:CE:133:LEU:HD12	1.73	0.69
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	1.75	0.68
1:AA:664:G:H22	1:AA:741:G:H1	1.39	0.68
31:CA:784:G:H5'	31:CA:785:G:OP1	1.93	0.68
35:CG:95:ARG:HG2	35:CG:128:GLN:HB3	1.76	0.68
31:CA:532:A:N1	31:CA:2020:A:H1'	2.08	0.68
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.76	0.68
31:CA:1936:A:H2	31:CA:1943:U:N3	1.90	0.68
31:CA:2428:G:H21	40:CM:60:ARG:HH21	1.40	0.68
45:DR:28:ARG:HD3	69:DR:310:HOH:O	1.94	0.68
12:AL:114:ARG:HB3	12:AL:119:VAL:HB	1.76	0.68
29:CC:17:VAL:HB	29:CC:204:VAL:HG13	1.75	0.68
55:DA:414:C:H2'	55:DA:415:A:C8	2.29	0.68
39:DL:38:ILE:HD11	39:DL:112:PHE:HZ	1.58	0.68
39:DL:2:ILE:HB	39:DL:33:ALA:HB3	1.76	0.67
1:BA:841:C:H3'	1:BA:842:U:C5'	2.24	0.67
33:CE:126:VAL:CG2	33:CE:133:LEU:HB3	2.24	0.67
29:DC:107:PRO:HD2	29:DC:110:LEU:HD22	1.76	0.67
54:DI:85:VAL:HG11	54:DI:91:ALA:HB3	1.75	0.67
6:AF:16:GLU:HG2	4:BD:193:ALA:HB2	1.77	0.67
41:DN:19:GLY:HA2	69:DB:338:HOH:O	1.92	0.67
35:CG:80:THR:HG23	35:CG:81:GLU:H	1.58	0.67
42:DO:53:THR:HA	42:DO:56:LYS:HD2	1.77	0.67
1:BA:715:A:H2'	1:BA:716:A:C8	2.30	0.67
55:DA:1028:A:N6	55:DA:1125:G:H2'	2.09	0.67
1:AA:715:A:H2'	1:AA:716:A:C8	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:774:G:H21	57:BA:1642:PG4:H62	1.60	0.67
31:CA:910:A:H62	41:CN:12:MET:HA	1.57	0.67
49:CV:7:ARG:O	49:CV:25:VAL:HB	1.94	0.67
1:BA:1305:G:H21	1:BA:1332:A:H2	1.44	0.66
43:CP:18:LEU:HD23	43:CP:25:ARG:HD3	1.76	0.66
31:CA:2189:U:H2'	31:CA:2190:G:H8	1.60	0.66
31:CA:2394:C:H5''	40:CM:63:LYS:HE2	1.76	0.66
31:CA:1779:U:H5	31:CA:1784:A:N7	1.93	0.66
55:DA:1026:G:H2'	55:DA:1027:A:C8	2.31	0.66
39:CL:2:ILE:HB	39:CL:33:ALA:HB3	1.76	0.66
55:DA:2751:G:H2'	69:DA:4887:HOH:O	1.94	0.66
4:BD:85:ASN:HA	5:BE:102:GLY:CA	2.26	0.66
49:CV:82:ARG:HB2	49:CV:97:LYS:HG3	1.78	0.66
54:DI:132:TYR:H	54:DI:133:GLU:HB2	1.60	0.66
1:AA:1197:A:H3'	1:AA:1197:A:OP2	1.96	0.66
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.78	0.66
55:DA:74:A:N3	55:DA:74:A:H5''	2.11	0.66
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.77	0.66
43:DP:64:TYR:HB3	43:DP:67:ASN:HD22	1.61	0.65
43:CP:64:TYR:HB3	43:CP:67:ASN:HD22	1.62	0.65
55:DA:1002:G:H5'	61:DA:3201:PEG:H32	1.78	0.65
40:DM:63:LYS:HE2	55:DA:2394:C:H5''	1.78	0.65
43:DP:51:ALA:HB3	43:DP:78:VAL:HG13	1.77	0.65
45:DR:94:ILE:HG21	46:DS:4:VAL:HG11	1.79	0.65
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.77	0.65
31:CA:2326:C:O2'	31:CA:2327:A:H8	1.80	0.65
55:DA:1026:G:H2'	55:DA:1027:A:H8	1.62	0.65
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.79	0.65
31:CA:2366:A:H4'	51:CX:62:LYS:HE3	1.79	0.65
9:BI:116:VAL:HG21	10:BJ:62:ARG:HB2	1.77	0.65
55:DA:2255:G:H21	68:DA:3220:TRS:H12	1.62	0.65
47:CT:29:VAL:HG22	47:CT:51:LEU:HD11	1.79	0.64
2:AB:31:ILE:HG21	2:AB:39:HIS:CD2	2.30	0.64
42:CO:53:THR:HA	42:CO:56:LYS:HD2	1.78	0.64
32:DD:122:VAL:HG23	69:DD:411:HOH:O	1.97	0.64
46:DS:73:LYS:HZ2	58:DS:203:MPD:H53	1.60	0.64
43:CP:51:ALA:HB3	43:CP:78:VAL:HG13	1.80	0.64
55:DA:2127:G:H4'	55:DA:2128:G:OP1	1.96	0.64
12:BL:114:ARG:HB3	12:BL:119:VAL:HB	1.78	0.64
55:DA:2052:A:H3'	69:DA:3584:HOH:O	1.96	0.64
45:CR:94:ILE:HG21	46:CS:4:VAL:HG11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DI:64:VAL:HG22	54:DI:69:PHE:HB2	1.79	0.64
1:AA:1144:G:H21	1:AA:1146:A:H62	1.46	0.64
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.80	0.64
33:DE:3:LEU:HD12	33:DE:14:VAL:HG11	1.80	0.63
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.79	0.63
32:DD:186:LEU:HD21	44:DQ:4:ILE:HG21	1.81	0.63
55:DA:1778:U:H2'	55:DA:1784:A:N6	2.13	0.63
44:DQ:31:TRP:CE2	44:DQ:40:LEU:HD21	2.34	0.63
1:AA:1305:G:H21	1:AA:1332:A:H2	1.44	0.63
38:CK:117:ALA:HA	38:CK:120:ARG:HD2	1.81	0.63
36:CH:4:ILE:HD11	36:CH:44:ILE:HG22	1.80	0.63
1:AA:677:U:H3	1:AA:713:G:H22	1.45	0.63
31:CA:1709:U:H2'	31:CA:1710:G:C8	2.34	0.63
40:DM:36:LYS:HE2	55:DA:807:U:OP1	1.98	0.63
1:BA:1063:C:H42	1:BA:1193:G:H1	1.47	0.63
1:BA:202:G:HO2'	1:BA:468:A:H8	1.45	0.63
1:BA:677:U:H3	1:BA:713:G:H22	1.43	0.63
34:CF:36:LEU:HD21	34:CF:91:LEU:HD11	1.80	0.63
55:DA:1975:G:H21	63:DA:3225:PGE:C2	2.07	0.63
29:DC:38:SER:HA	69:DA:5917:HOH:O	1.98	0.63
3:BC:77:ILE:HA	3:BC:84:VAL:HG23	1.81	0.62
43:CP:31:THR:HG22	43:CP:34:HIS:H	1.62	0.62
43:DP:31:THR:HG22	43:DP:34:HIS:H	1.64	0.62
27:D0:39:GLU:HB2	27:D0:41:THR:HG23	1.80	0.62
55:DA:1965:C:OP1	55:DA:1966:A:H2'	1.99	0.62
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.34	0.62
27:C0:39:GLU:HB2	27:C0:41:THR:HG23	1.81	0.62
24:C3:19:ARG:HD3	31:CA:125:A:OP2	1.99	0.62
29:CC:17:VAL:HB	29:CC:204:VAL:HG12	1.78	0.62
29:CC:45:ASN:ND2	31:CA:1812:U:H1'	2.14	0.62
53:DZ:2:LYS:HB3	53:DZ:6:LEU:HD12	1.80	0.62
1:BA:1144:G:H21	1:BA:1146:A:H62	1.47	0.62
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.34	0.62
31:CA:1827:U:H2'	31:CA:1828:G:O4'	2.00	0.62
18:AR:62:ALA:HB3	18:AR:68:LEU:HD12	1.82	0.62
31:CA:528:A:H3'	31:CA:528:A:C8	2.35	0.62
33:CE:3:LEU:HD12	33:CE:14:VAL:HG11	1.82	0.62
55:DA:588:U:H2'	55:DA:589:U:C6	2.34	0.62
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.82	0.62
22:D1:34:SER:OG	22:D1:36:GLU:HB2	2.00	0.62
54:DI:50:VAL:HG11	54:DI:92:ALA:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:197:A:H2	31:CA:2434:A:H62	1.48	0.62
31:CA:571:U:H4'	31:CA:573:U:H5	1.64	0.62
1:BA:663:A:H5'	1:BA:836:G:OP1	1.98	0.62
55:DA:2162:G:H5''	55:DA:2171:A:H2'	1.82	0.62
1:AA:663:A:H5'	1:AA:836:G:OP1	1.99	0.61
31:CA:1707:G:H1	31:CA:1751:U:H3	1.47	0.61
31:CA:1931:U:H2'	31:CA:1932:A:H8	1.64	0.61
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.35	0.61
1:BA:209:U:H4'	1:BA:210:C:OP2	2.00	0.61
11:BK:88:GLY:N	11:BK:114:THR:HG22	2.15	0.61
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.81	0.61
18:BR:62:ALA:HB3	18:BR:68:LEU:HD12	1.82	0.61
31:CA:320:A:H4'	31:CA:322:A:N7	2.15	0.61
38:DK:117:ALA:HA	38:DK:120:ARG:HD2	1.81	0.61
41:DN:62:LYS:HD3	41:DN:64:TRP:CZ2	2.36	0.61
31:CA:1760:C:H2'	31:CA:1761:C:O4'	2.00	0.61
1:BA:1063:C:N4	1:BA:1193:G:H1	1.97	0.61
45:DR:78:LYS:HA	69:DA:6376:HOH:O	2.01	0.61
1:AA:209:U:H4'	1:AA:210:C:OP2	1.99	0.61
31:CA:806:C:H2'	31:CA:807:U:C6	2.36	0.61
14:AN:66:GLN:HB2	69:AN:202:HOH:O	2.01	0.61
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.83	0.61
38:CK:110:PRO:O	38:CK:115:GLY:HA3	2.01	0.61
55:DA:1141:U:H4'	55:DA:1142:A:O4'	2.01	0.61
1:AA:1314:C:H41	19:AS:4:SER:HA	1.66	0.60
31:CA:1155:A:H5''	45:CR:55:ARG:HD3	1.81	0.60
42:DO:60:VAL:HB	69:DO:217:HOH:O	2.00	0.60
31:CA:588:U:H2'	31:CA:589:U:C6	2.36	0.60
54:DI:5:LEU:HA	54:DI:8:LYS:HB2	1.83	0.60
50:DW:63:ILE:HD12	50:DW:72:VAL:HG21	1.83	0.60
1:BA:562:U:H1'	12:BL:12:ARG:HD2	1.84	0.60
1:AA:707:U:H5''	11:AK:22:HIS:CD2	2.37	0.60
55:DA:1913:A:H4'	55:DA:1913:A:OP1	2.01	0.60
1:AA:1421:G:H3'	69:AA:1814:HOH:O	2.02	0.60
2:BB:163:VAL:HG11	2:BB:173:ILE:HD11	1.82	0.60
31:CA:1006:C:O4'	38:CK:30:THR:HG23	2.01	0.60
31:CA:2443:C:H2'	31:CA:2444:G:O4'	2.01	0.60
37:CJ:19:ASN:H	37:CJ:20:PRO:HD2	1.67	0.60
48:CU:18:GLU:H	48:CU:18:GLU:CD	2.03	0.60
29:DC:45:ASN:ND2	55:DA:1812:U:H1'	2.15	0.60
1:BA:1289:A:H3'	1:BA:1290:G:H8	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:58:LYS:HA	4:BD:200:ILE:HG12	1.84	0.60
31:CA:1709:U:H2'	31:CA:1710:G:H8	1.66	0.60
31:CA:2326:C:O2'	31:CA:2327:A:C8	2.55	0.60
55:DA:2402:U:O2	55:DA:2402:U:H2'	2.01	0.60
54:DI:94:ARG:HG2	54:DI:127:ALA:HA	1.83	0.60
26:D5:1:MET:HG2	69:D5:202:HOH:O	2.01	0.60
42:CO:73:ASN:HA	42:CO:76:VAL:HG22	1.84	0.60
22:D1:9:THR:CG2	55:DA:2020:A:H5'	2.32	0.60
41:DN:18[B]:ARG:HG3	28:DB:90:C:H5'	1.83	0.60
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	1.84	0.59
48:CU:69:ARG:HB2	48:CU:74:ILE:HG22	1.84	0.59
33:DE:189:THR:HG22	33:DE:192:ALA:H	1.66	0.59
43:CP:49:VAL:HG21	43:CP:82:ALA:HA	1.84	0.59
51:DX:56:ASP:OD1	55:DA:2364:C:H4'	2.02	0.59
32:DD:150[B]:MEQ:HG3	55:DA:2032:G:N3	2.17	0.59
31:CA:1974:C:H3'	69:CA:3320:HOH:O	2.03	0.59
45:DR:50:ARG:O	45:DR:54:LYS:HD2	2.02	0.59
2:AB:163:VAL:HG11	2:AB:173:ILE:HD11	1.84	0.59
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.83	0.59
4:AD:58:LYS:HA	4:AD:200:ILE:HG12	1.84	0.59
1:BA:33:A:H2'	1:BA:34:C:C6	2.37	0.59
45:CR:58:ARG:NH1	45:CR:62:ILE:HD11	2.17	0.59
1:AA:1289:A:H3'	1:AA:1290:G:H8	1.67	0.59
55:DA:1424:G:H21	63:DA:3214:PGE:H32	1.67	0.59
32:DD:30:GLU:HB3	69:DD:457:HOH:O	2.03	0.59
1:BA:967:5MC:HN42	1:BA:1197:A:H61	1.48	0.59
55:DA:2783:U:H2'	55:DA:2784:U:H6	1.67	0.59
2:BB:31:ILE:HG21	2:BB:39:HIS:CD2	2.31	0.59
31:CA:135:U:H3	31:CA:144:A:H61	1.51	0.59
29:CC:160:THR:HG22	29:CC:177:ARG:HG2	1.84	0.59
37:DJ:19:ASN:H	37:DJ:20:PRO:HD2	1.67	0.59
1:AA:562:U:H1'	12:AL:12:ARG:HD2	1.83	0.59
50:CW:63:ILE:HD12	50:CW:72:VAL:HG21	1.85	0.59
3:BC:113:ALA:O	3:BC:200:VAL:HG11	2.03	0.59
54:DI:67:THR:CG2	54:DI:68:PRO:HA	2.29	0.59
6:AF:92:THR:HG22	6:AF:93:LYS:HE2	1.85	0.58
31:CA:320:A:H2'	33:CE:131:THR:HG21	1.83	0.58
33:CE:189:THR:HG22	33:CE:192:ALA:H	1.67	0.58
55:DA:1105:U:H2'	55:DA:1106:G:H8	1.68	0.58
55:DA:45:G:H5''	55:DA:46:G:H5'	1.85	0.58
14:AN:10:GLU:HG3	14:AN:63:ARG:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1770:G:H4'	31:CA:1938:A:OP1	2.03	0.58
55:DA:2771:C:H2'	55:DA:2772:C:H6	1.68	0.58
36:DH:4:ILE:HD11	36:DH:44:ILE:HG22	1.84	0.58
31:CA:729:G:H2'	31:CA:1775:U:H1'	1.85	0.58
31:CA:29:U:H2'	31:CA:30:G:C8	2.37	0.58
55:DA:1853:A:N1	55:DA:2087:G:H1'	2.19	0.58
31:CA:2728:U:HO2'	31:CA:2729:G:H8	1.49	0.58
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	1.85	0.58
51:DX:21:LEU:HD11	51:DX:41[A]:ARG:HE	1.68	0.58
31:CA:142:A:H1'	48:CU:1:MET:HB3	1.85	0.58
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.85	0.58
33:CE:28:VAL:O	33:CE:32:VAL:HG23	2.04	0.58
41:CN:62:LYS:HD3	41:CN:64:TRP:CZ2	2.37	0.58
53:DZ:41:HIS:CD2	55:DA:96:C:H4'	2.38	0.58
1:AA:54:C:H2'	1:AA:352:C:H41	1.69	0.58
1:AA:73:C:HO2'	1:AA:74:A:H8	1.51	0.58
3:AC:40:ARG:HG2	3:AC:55:ILE:HG21	1.85	0.58
1:BA:54:C:H2'	1:BA:352:C:H41	1.69	0.58
31:CA:45:G:H5''	31:CA:46:G:H5'	1.85	0.58
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	1.85	0.58
31:CA:2469:A:H4'	41:CN:55:ARG:HD3	1.86	0.58
24:D3:29:GLN:HG2	61:D3:102:PEG:H21	1.86	0.58
40:DM:32:GLY:HA2	55:DA:1190:G:H5''	1.84	0.58
55:DA:2557:G:H2'	55:DA:2558:C:C6	2.39	0.58
32:DD:152:PRO:HG3	32:DD:156:PHE:CZ	2.39	0.58
42:DO:73:ASN:HA	42:DO:76:VAL:HG22	1.85	0.58
12:BL:80:ILE:HD12	12:BL:97:THR:HG22	1.86	0.58
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.68	0.58
31:CA:1796:U:H2'	31:CA:1797:G:C8	2.39	0.58
31:CA:1812:U:H2'	31:CA:1813:G:C8	2.38	0.58
31:CA:1936:A:H61	31:CA:1963:U:H3	1.50	0.58
31:CA:586:A:H5'	33:CE:84:THR:HG21	1.84	0.58
31:CA:846:U:H1'	31:CA:847:U:H5	1.68	0.58
33:CE:108:ILE:HG22	40:CM:1:MET:SD	2.43	0.57
31:CA:2106:U:H2'	31:CA:2107:G:H8	1.70	0.57
41:CN:30:SER:H	41:CN:106:ASP:HB3	1.68	0.57
55:DA:1417:C:H5'	55:DA:1588:G:H1'	1.86	0.57
47:DT:75:PHE:CZ	65:DA:3185:1PE:H142	2.39	0.57
17:BQ:68:SER:OG	17:BQ:71:LYS:HB3	2.03	0.57
1:BA:73:C:HO2'	1:BA:74:A:H8	1.50	0.57
31:CA:1311:G:H21	31:CA:1603:A:N6	1.95	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:582:A:H2'	31:CA:583:G:C8	2.39	0.57
55:DA:944:C:H2'	69:DA:6066:HOH:O	2.04	0.57
41:DN:30:SER:H	41:DN:106:ASP:HB3	1.69	0.57
43:DP:49:VAL:HG21	43:DP:82:ALA:HA	1.86	0.57
1:AA:79:G:H22	1:AA:90:C:H42	1.52	0.57
37:CJ:14:ALA:HB3	37:CJ:17:MET:HB2	1.87	0.57
55:DA:2063:C:O2	55:DA:2450:A:N1	2.37	0.57
51:DX:40:GLN:HG3	51:DX:42:GLY:O	2.05	0.57
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.85	0.57
22:C1:7:LYS:HD2	31:CA:1262:A:C2	2.39	0.57
50:CW:20:LEU:HD21	50:CW:41:GLU:HB2	1.85	0.57
37:DJ:14:ALA:HB3	37:DJ:17:MET:HB2	1.86	0.57
1:AA:1063:C:H2'	1:AA:1064:G:H8	1.64	0.57
14:AN:21:PHE:HA	14:AN:25:ALA:HB3	1.86	0.57
22:C1:9:THR:CG2	31:CA:2020:A:H5'	2.34	0.57
50:DW:20:LEU:HD21	50:DW:41:GLU:HB2	1.85	0.57
5:BE:104:GLY:HA3	5:BE:122:ASN:HA	1.86	0.57
31:CA:35:G:H2'	31:CA:36:G:O4'	2.04	0.57
34:CF:36:LEU:HD21	34:CF:91:LEU:CD1	2.35	0.57
31:CA:96:C:H4'	53:CZ:41:HIS:CD2	2.40	0.57
55:DA:2728:U:HO2'	55:DA:2729:G:H8	1.51	0.57
55:DA:2783:U:H2'	55:DA:2784:U:C6	2.39	0.57
38:DK:110:PRO:O	38:DK:115:GLY:HA3	2.04	0.57
43:DP:48:LEU:HD12	43:DP:87:ILE:HD11	1.87	0.57
14:BN:10:GLU:HG3	14:BN:63:ARG:HD2	1.87	0.57
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.86	0.57
31:CA:528:A:C2	31:CA:2043:C:H4'	2.40	0.57
30:CD:152:PRO:HG3	30:CD:156:PHE:CZ	2.39	0.57
31:CA:1203:U:H1'	40:CM:4:ASN:HB3	1.87	0.57
55:DA:1885:A:H2'	55:DA:1886:U:O4'	2.04	0.57
10:BJ:42:LEU:HB2	10:BJ:71:LEU:HB3	1.86	0.56
45:DR:31:VAL:HG13	55:DA:580:U:O3'	2.05	0.56
1:AA:33:A:H2'	1:AA:34:C:C6	2.39	0.56
22:D1:4:GLN:HA	55:DA:2615:U:C2	2.41	0.56
31:CA:2491:U:HO2'	31:CA:2492:U:H5	1.54	0.56
34:CF:24:SER:H	34:CF:27:GLN:NE2	2.03	0.56
29:DC:158:ALA:HB1	29:DC:197:ASN:O	2.04	0.56
45:DR:16:LYS:O	45:DR:20:GLN:HG3	2.05	0.56
14:AN:13:ARG:HB3	14:AN:60:GLN:HG2	1.87	0.56
45:DR:22:LYS:HE3	55:DA:20:C:OP1	2.06	0.56
47:DT:17:VAL:HG11	47:DT:103:ILE:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:1327:A:H2'	55:DA:1328:A:O4'	2.06	0.56
55:DA:135:U:H3	55:DA:144:A:H61	1.51	0.56
54:DI:69:PHE:HB3	54:DI:72:LEU:HD12	1.86	0.56
39:CL:38:ILE:HD11	39:CL:112:PHE:CZ	2.38	0.56
28:CB:114:C:H1'	43:CP:47:VAL:HG11	1.86	0.56
47:CT:17:VAL:HG11	47:CT:103:ILE:HG12	1.86	0.56
3:BC:40:ARG:HG2	3:BC:55:ILE:HG21	1.87	0.56
31:CA:677:A:O2'	31:CA:2071:A:H5'	2.05	0.56
29:CC:105:LEU:H	29:CC:105:LEU:HD12	1.70	0.56
55:DA:320:A:H4'	55:DA:322:A:N7	2.20	0.56
1:BA:576:C:H3'	1:BA:577:G:H5''	1.86	0.56
1:BA:840:C:H2'	1:BA:841:C:O4'	2.06	0.56
35:DG:86:LYS:HG2	35:DG:132:VAL:HG22	1.87	0.56
43:DP:16:ARG:HD3	69:DP:310:HOH:O	2.06	0.56
5:AE:97:GLN:HE21	5:AE:124:LEU:HD13	1.71	0.56
31:CA:2636:C:H2'	31:CA:2637:U:C6	2.41	0.56
33:CE:46:GLN:HB3	33:CE:83:VAL:HG21	1.87	0.56
35:CG:90:VAL:HG21	35:CG:163:ARG:HE	1.71	0.56
32:DD:48:ILE:HG23	32:DD:84:LEU:HD11	1.88	0.56
35:DG:90:VAL:HG21	35:DG:163:ARG:HE	1.70	0.56
1:BA:79:G:H22	1:BA:90:C:H42	1.54	0.56
14:BN:13:ARG:HB3	14:BN:60:GLN:HG2	1.88	0.56
31:CA:2114:A:N6	31:CA:2119:A:H62	2.03	0.56
31:CA:2728:U:O2'	31:CA:2729:G:H5''	2.05	0.56
31:CA:459:U:H2'	31:CA:460:A:H8	1.69	0.56
34:DF:138:PHE:HE2	34:DF:152:LEU:HD21	1.71	0.56
35:DG:26:ILE:HG22	35:DG:79:VAL:HG21	1.88	0.56
16:BP:20:VAL:CG1	16:BP:32:PHE:HB2	2.36	0.56
52:CY:37:ARG:HG2	52:CY:48:THR:HG22	1.87	0.56
24:D3:7:PRO:HG2	55:DA:1309:G:H4'	1.87	0.56
1:AA:1350:A:H2	7:AG:34:GLY:HA3	1.70	0.55
2:AB:188:ASP:HB2	2:AB:204:ASP:OD2	2.06	0.55
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.87	0.55
55:DA:683:U:H2'	55:DA:684:G:H5''	1.88	0.55
55:DA:760:G:H2'	55:DA:761:A:O4'	2.06	0.55
32:DD:121:THR:HB	32:DD:127:PHE:CD2	2.42	0.55
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.87	0.55
2:BB:188:ASP:HB2	2:BB:204:ASP:OD2	2.07	0.55
31:CA:744:U:H4'	31:CA:1658:C:H4'	1.88	0.55
31:CA:822:G:O6	31:CA:943:A:H2	1.89	0.55
31:CA:659:G:H4'	33:CE:95:LYS:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:CH:27:ARG:HH12	36:CH:38:PRO:HG3	1.71	0.55
55:DA:2636:C:H2'	55:DA:2637:U:C6	2.41	0.55
1:AA:674:G:H3'	69:AA:1714:HOH:O	2.05	0.55
31:CA:540:C:H2'	31:CA:541:A:C8	2.41	0.55
39:DL:113:MET:CE	39:DL:116:ILE:HD11	2.37	0.55
35:DG:67:THR:HG23	55:DA:2747:G:O2'	2.06	0.55
1:AA:1012:A:H61	1:AA:1017:U:H3	1.55	0.55
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	1.88	0.55
11:BK:25:ALA:HA	11:BK:30:THR:HG22	1.89	0.55
31:CA:528:A:H3'	31:CA:528:A:H8	1.71	0.55
55:DA:912:C:O2'	55:DA:913:U:H5'	2.07	0.55
29:DC:17:VAL:HB	29:DC:204:VAL:HB	1.88	0.55
50:DW:39:ALA:HB3	69:DW:105:HOH:O	2.06	0.55
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.86	0.55
4:BD:197:GLU:HA	4:BD:200:ILE:HD12	1.89	0.55
31:CA:792:A:H1'	31:CA:2072:C:O2'	2.06	0.55
55:DA:2771:C:H2'	55:DA:2772:C:C6	2.41	0.55
12:AL:3:THR:HB	12:AL:6:GLN:HB2	1.86	0.55
1:BA:1350:A:H2	7:BG:34:GLY:HA3	1.70	0.55
55:DA:1952:A:H4'	69:DA:5281:HOH:O	2.07	0.55
40:DM:60:ARG:NH2	55:DA:2428:G:N2	2.51	0.55
34:DF:60:ILE:HG12	34:DF:138:PHE:CD2	2.42	0.55
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.72	0.55
16:BP:2:VAL:CG2	16:BP:33:ILE:HD11	2.36	0.55
31:CA:321:U:H5''	33:CE:131:THR:HG23	1.89	0.55
31:CA:373:U:H2'	31:CA:374:A:H8	1.71	0.55
55:DA:1532:A:H5''	55:DA:1532:A:H8	1.72	0.55
37:DJ:30:GLN:HE22	55:DA:1095:A:H61	1.54	0.55
39:DL:38:ILE:HD11	39:DL:112:PHE:CZ	2.42	0.55
4:BD:27:ALA:HB3	4:BD:30:THR:HG23	1.88	0.55
41:DN:75:GLU:HB2	41:DN:90:GLU:HG3	1.89	0.55
49:DV:52:LEU:HD13	49:DV:54:GLN:HE21	1.72	0.55
5:AE:57:PRO:O	5:AE:60:ILE:HG13	2.07	0.54
31:CA:1509:A:O2'	31:CA:1510:G:H8	1.90	0.54
31:CA:2557:G:H2'	31:CA:2558:C:C6	2.42	0.54
31:CA:373:U:H2'	31:CA:374:A:C8	2.41	0.54
1:AA:269:C:H2'	1:AA:270:A:C8	2.42	0.54
1:AA:76:G:H1	1:AA:93:U:H3	1.55	0.54
31:CA:2064:C:H2'	31:CA:2065:C:C6	2.43	0.54
33:CE:149:ILE:HG23	33:CE:188:MET:HG2	1.90	0.54
34:CF:24:SER:H	34:CF:27:GLN:HE21	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:CM:77:ILE:CD1	40:CM:108:ALA:HB1	2.36	0.54
55:DA:20:C:H2'	55:DA:21:A:H8	1.72	0.54
55:DA:784:G:H5'	55:DA:785:G:OP1	2.08	0.54
1:BA:751:U:H4'	15:BO:24:SER:HA	1.89	0.54
14:BN:21:PHE:HA	14:BN:25:ALA:HB3	1.87	0.54
31:CA:2425:A:H4'	31:CA:2426:A:O5'	2.07	0.54
55:DA:1509:A:O2'	55:DA:1510:G:H8	1.89	0.54
35:DG:24:ILE:HG21	35:DG:72:LEU:HD21	1.88	0.54
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.73	0.54
2:AB:111:ILE:HD12	2:AB:152:LYS:HA	1.89	0.54
12:BL:79:VAL:HG12	12:BL:102:LEU:HD23	1.90	0.54
31:CA:2105:U:H2'	31:CA:2106:U:C6	2.42	0.54
31:CA:2267:A:H5''	31:CA:2268:A:H5'	1.90	0.54
52:CY:4:VAL:HG13	52:CY:11:ARG:HG3	1.89	0.54
55:DA:414:C:H2'	55:DA:415:A:H8	1.73	0.54
32:DD:99:GLU:HG2	32:DD:182:ALA:HB2	1.87	0.54
3:AC:121:THR:HA	3:AC:189:ALA:HB2	1.88	0.54
45:CR:16:LYS:O	45:CR:20:GLN:HG3	2.08	0.54
34:DF:65:PRO:HA	34:DF:89:VAL:HG23	1.89	0.54
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.89	0.54
55:DA:2887[B]:A:N3	55:DA:2887[B]:A:H2'	2.22	0.54
1:BA:1012:A:H61	1:BA:1017:U:H3	1.54	0.54
1:BA:209:U:O2	1:BA:209:U:H2'	2.08	0.54
1:BA:76:G:H1	1:BA:93:U:H3	1.54	0.54
42:CO:28:LEU:HD23	42:CO:48:VAL:HG11	1.90	0.54
34:DF:8:TYR:HB2	34:DF:173:PHE:HZ	1.73	0.54
42:DO:28:LEU:HD23	42:DO:48:VAL:HG11	1.88	0.54
1:BA:591:U:H2'	1:BA:592:G:C8	2.42	0.54
3:BC:121:THR:HA	3:BC:189:ALA:HB2	1.89	0.54
31:CA:1936:A:N6	31:CA:1963:U:N3	2.54	0.54
35:CG:86:LYS:HG2	35:CG:132:VAL:HG22	1.89	0.54
46:CS:49:ILE:HD12	46:CS:52:PRO:HA	1.90	0.54
6:AF:42:TRP:HB2	6:AF:59:TYR:HB2	1.90	0.54
11:AK:25:ALA:HA	11:AK:30:THR:HG22	1.89	0.54
31:CA:1738:G:HO2'	31:CA:1739:A:H8	1.55	0.54
31:CA:1796:U:H2'	31:CA:1797:G:H8	1.73	0.54
39:CL:58:LEU:HD11	39:CL:86:LEU:HD13	1.89	0.54
55:DA:2767:C:H2'	55:DA:2768:U:H6	1.73	0.54
46:DS:20:VAL:HG22	69:DS:339:HOH:O	2.07	0.54
4:AD:197:GLU:HA	4:AD:200:ILE:HD12	1.89	0.53
13:BM:33:ILE:HG23	13:BM:59:GLU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:241:A:N1	31:CA:255:A:H5''	2.23	0.53
27:D0:3[B]:LYS:O	27:D0:40:ASP:HB2	2.08	0.53
44:DQ:94:LYS:CE	55:DA:1754:A:C8	2.92	0.53
53:DZ:39:GLN:HB3	53:DZ:41:HIS:CE1	2.44	0.53
1:AA:1411:C:H2'	1:AA:1412:C:C6	2.44	0.53
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.08	0.53
31:CA:685:A:H5''	31:CA:774:G:O6	2.08	0.53
31:CA:699:A:H2'	31:CA:700:G:O4'	2.09	0.53
33:DE:84:THR:HG21	55:DA:586:A:H5'	1.90	0.53
13:AM:90:ARG:HD3	13:AM:97:VAL:HA	1.91	0.53
1:BA:1411:C:H2'	1:BA:1412:C:C6	2.43	0.53
23:D2:9:ILE:HD13	23:D2:51:GLU:HG3	1.88	0.53
55:DA:1812:U:H2'	55:DA:1813:G:C8	2.44	0.53
30:CD:121:THR:HB	30:CD:127:PHE:CD2	2.43	0.53
34:CF:8:TYR:HB2	34:CF:173:PHE:HZ	1.73	0.53
44:CQ:4:ILE:H	44:CQ:4:ILE:HD12	1.73	0.53
55:DA:985:C:H2'	55:DA:986:C:H6	1.73	0.53
1:AA:260:G:H2'	1:AA:261:U:C6	2.44	0.53
1:AA:591:U:H2'	1:AA:592:G:C8	2.43	0.53
1:BA:490:C:H2'	1:BA:491:G:H8	1.74	0.53
31:CA:2598:A:H2'	31:CA:2599:G:O4'	2.09	0.53
33:CE:149:ILE:HG12	33:CE:188:MET:HG2	1.91	0.53
55:DA:2233:U:H2'	55:DA:2234:G:C8	2.44	0.53
31:CA:1532:A:H8	31:CA:1532:A:H5''	1.73	0.53
47:CT:4:ILE:HG12	47:CT:106:VAL:HG22	1.91	0.53
47:DT:93:ALA:HB2	55:DA:1614:A:C2	2.44	0.53
1:AA:1373:G:H5'	7:AG:36:LYS:HB2	1.91	0.53
31:CA:1564:C:H2'	31:CA:1565:C:C6	2.44	0.53
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.91	0.53
55:DA:693:A:H2'	55:DA:694:U:O4'	2.08	0.53
43:DP:79:ALA:HB2	43:DP:110:ALA:HA	1.91	0.53
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.73	0.53
1:BA:269:C:H2'	1:BA:270:A:C8	2.43	0.53
31:CA:1308:A:H2'	31:CA:1309:G:O4'	2.09	0.53
31:CA:2106:U:H2'	31:CA:2107:G:C8	2.44	0.53
55:DA:2105:U:O4	55:DA:2184:A:H2	1.92	0.53
1:BA:260:G:H2'	1:BA:261:U:C6	2.44	0.53
31:CA:2747:G:O2'	35:CG:67:THR:HG23	2.09	0.53
22:D1:44:THR:HG23	22:D1:48:TYR:O	2.09	0.53
55:DA:2128:G:H1	55:DA:2160:C:H42	1.57	0.53
22:D1:40:ARG:NH2	55:DA:2884[B]:U:H2'	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2800:A:C2	55:DA:2895:G:H1'	2.43	0.53
55:DA:623:C:H2'	55:DA:624:C:C6	2.44	0.53
39:DL:58:LEU:HD11	39:DL:86:LEU:HD13	1.91	0.53
43:DP:27:VAL:HG21	43:DP:40:ILE:HD12	1.91	0.53
1:AA:751:U:H4'	15:AO:24:SER:HA	1.90	0.53
12:AL:79:VAL:HG12	12:AL:102:LEU:HD23	1.90	0.53
31:CA:2189:U:H2'	31:CA:2190:G:C8	2.43	0.53
31:CA:2261:C:C2	31:CA:2280:G:N2	2.77	0.53
31:CA:457:A:N1	31:CA:470:A:H5''	2.24	0.53
31:CA:780:G:H8	31:CA:780:G:O5'	1.90	0.53
55:DA:1166:G:N2	55:DA:1184:U:H1'	2.24	0.53
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.74	0.52
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	1.92	0.52
55:DA:1722:A:N6	55:DA:1738:G:H1'	2.24	0.52
55:DA:1753:G:N2	55:DA:1755:A:H3'	2.25	0.52
26:C5:4:ARG:HB2	31:CA:2466:C:OP1	2.09	0.52
35:CG:24:ILE:HG21	35:CG:72:LEU:HD21	1.90	0.52
52:CY:10:LYS:HE3	52:CY:54:LYS:HG2	1.90	0.52
55:DA:795:C:H1'	69:DA:4280:HOH:O	2.08	0.52
29:DC:43:ARG:HG3	29:DC:49:ILE:HA	1.91	0.52
40:DM:60:ARG:HD3	55:DA:2428:G:H21	1.74	0.52
50:DW:72:VAL:HG12	50:DW:93:ARG:HA	1.91	0.52
31:CA:2064:C:H1'	31:CA:2450:A:C6	2.45	0.52
41:CN:75:GLU:HB2	41:CN:90:GLU:HG3	1.91	0.52
55:DA:14:A:H5''	55:DA:15:G:OP2	2.09	0.52
55:DA:612:G:H4'	55:DA:613:A:C2	2.43	0.52
32:DD:134:HIS:HE1	69:DA:5373:HOH:O	1.92	0.52
44:DQ:4:ILE:H	44:DQ:4:ILE:HD12	1.74	0.52
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.44	0.52
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.45	0.52
4:AD:27:ALA:HB3	4:AD:30:THR:HG23	1.90	0.52
1:AA:1381:U:H1'	7:AG:78:ARG:HE	1.75	0.52
6:BF:42:TRP:HB2	6:BF:59:TYR:HB2	1.92	0.52
31:CA:581:C:H2'	31:CA:582:A:C8	2.44	0.52
30:CD:129:THR:HG22	30:CD:141:ARG:HA	1.91	0.52
53:CZ:39:GLN:HB3	53:CZ:41:HIS:CE1	2.44	0.52
55:DA:2183:A:H2'	55:DA:2184:A:C8	2.44	0.52
55:DA:2408:U:H2'	55:DA:2409:G:C8	2.45	0.52
1:BA:1001:C:H2'	1:BA:1002:G:C8	2.45	0.52
19:BS:52:HIS:HD2	19:BS:54:GLY:H	1.58	0.52
31:CA:861:A:H2'	31:CA:862:G:O4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:587:C:O2'	40:CM:19:LEU:HD13	2.09	0.52
43:CP:79:ALA:HB2	43:CP:110:ALA:HA	1.90	0.52
55:DA:2037:A:H2'	55:DA:2038:G:C8	2.44	0.52
55:DA:2703:C:H2'	55:DA:2704:C:H6	1.74	0.52
13:BM:90:ARG:HD3	13:BM:97:VAL:HA	1.91	0.52
31:CA:568:U:C1'	31:CA:2030:6MZ:H9C1	2.31	0.52
37:CJ:11:LEU:HD22	37:CJ:24:VAL:HG23	1.92	0.52
44:DQ:101:ARG:HD2	69:DQ:322:HOH:O	2.10	0.52
44:DQ:106:LYS:HA	44:DQ:109:ARG:HD3	1.92	0.52
1:BA:1373:G:H5'	7:BG:36:LYS:HB2	1.92	0.52
31:CA:2888:C:H2'	31:CA:2889:C:C6	2.45	0.52
40:DM:57:LEU:HA	40:DM:60:ARG:HE	1.75	0.52
1:AA:718:A:C8	11:AK:118:HIS:HB3	2.45	0.52
16:AP:2:VAL:CG2	16:AP:33:ILE:HD11	2.40	0.52
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	1.90	0.52
31:CA:1248:G:O2'	45:CR:3:ARG:HA	2.10	0.52
31:CA:568:U:H1'	31:CA:2030:6MZ:C9	2.29	0.52
30:CD:121:THR:HG21	30:CD:143:PRO:HB3	1.92	0.52
55:DA:1105:U:H2'	55:DA:1106:G:C8	2.45	0.52
43:DP:11:ALA:HB2	43:DP:96:GLY:N	2.25	0.52
13:AM:33:ILE:HG23	13:AM:59:GLU:HB3	1.91	0.52
55:DA:2097:A:H8	55:DA:2097:A:H5''	1.76	0.52
55:DA:2402:U:H2'	55:DA:2403:C:H5'	1.91	0.52
33:DE:46:GLN:HB3	33:DE:83:VAL:HG21	1.92	0.52
38:DK:21:THR:HG23	38:DK:61:LYS:HB3	1.92	0.52
1:BA:403:C:H2'	1:BA:404:G:O4'	2.10	0.51
27:C0:9:GLN:HB3	27:C0:32:ILE:HA	1.91	0.51
31:CA:1722:A:N6	31:CA:1738:G:H1'	2.24	0.51
31:CA:2262:U:OP2	51:CX:16:SER:HB2	2.10	0.51
35:DG:175:LYS:HG3	55:DA:2529:G:H4'	1.92	0.51
47:DT:4:ILE:HG12	47:DT:106:VAL:HG22	1.92	0.51
1:BA:967:5MC:N4	1:BA:1197:A:H61	2.08	0.51
1:BA:212:G:H2'	1:BA:213:G:C8	2.44	0.51
40:CM:19:LEU:HD23	40:CM:31:GLY:O	2.11	0.51
40:CM:57:LEU:HA	40:CM:60:ARG:HE	1.75	0.51
42:CO:103:ARG:HD3	42:CO:110:MET:SD	2.50	0.51
55:DA:20:C:H2'	55:DA:21:A:C8	2.44	0.51
1:AA:412:A:H3'	1:AA:413:G:H5'	1.92	0.51
6:AF:70:VAL:HA	6:AF:73:GLU:HG2	1.92	0.51
1:BA:1458:G:H5''	20:BT:26:SER:HB3	1.93	0.51
55:DA:2563:U:H1'	55:DA:2566:A:N6	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:582:A:H2'	55:DA:583:G:C8	2.46	0.51
37:DJ:11:LEU:HD22	37:DJ:24:VAL:HG23	1.92	0.51
42:DO:82:GLU:O	42:DO:85:PRO:HD2	2.10	0.51
1:AA:1001:C:H2'	1:AA:1002:G:C8	2.45	0.51
1:BA:12:U:H4'	1:BA:526:C:H4'	1.93	0.51
35:CG:26:ILE:HG22	35:CG:79:VAL:HG21	1.91	0.51
38:CK:21:THR:HG23	38:CK:61:LYS:HB3	1.93	0.51
55:DA:1416:G:HO2'	55:DA:1417:C:H6	1.59	0.51
32:DD:150[A]:MEQ:HE3	55:DA:2032:G:C8	2.45	0.51
42:CO:82:GLU:O	42:CO:85:PRO:HD2	2.10	0.51
25:D4:57:LEU:HD11	55:DA:834:G:H5'	1.93	0.51
39:DL:101:GLY:O	39:DL:120:PRO:HD2	2.11	0.51
1:AA:619:U:C2	4:AD:132:ILE:HD11	2.46	0.51
6:AF:17:GLN:HG3	4:BD:189:SER:HB2	1.92	0.51
4:BD:170:TRP:CD2	4:BD:186:PRO:HB3	2.45	0.51
1:BA:429:U:H5''	4:BD:9:LEU:HD12	1.92	0.51
46:DS:65:ALA:HB3	46:DS:95:ASP:HB2	1.92	0.51
52:DY:10:LYS:HE3	52:DY:54:LYS:HG2	1.92	0.51
8:AH:51:VAL:HG13	8:AH:59:LEU:HD12	1.93	0.51
46:CS:65:ALA:HB3	46:CS:95:ASP:HB2	1.93	0.51
23:D2:11:LEU:HD21	23:D2:34:LEU:HD23	1.92	0.51
40:DM:57:LEU:HB2	40:DM:60:ARG:HH11	1.75	0.51
38:DK:42:ALA:O	45:DR:64:ARG:HD3	2.10	0.51
1:AA:1317:C:OP1	14:AN:57:PRO:HD2	2.11	0.51
1:AA:77:A:H2'	1:AA:78:A:C8	2.46	0.51
5:AE:82:GLN:HG2	5:AE:149:SER:HA	1.93	0.51
16:BP:2:VAL:HG21	16:BP:33:ILE:HD11	1.93	0.51
45:CR:9:ILE:HG13	45:CR:10:ALA:N	2.26	0.51
35:DG:42:GLU:HA	35:DG:55:ARG:HH21	1.75	0.51
33:DE:32:VAL:HG21	40:DM:6:LEU:HD13	1.93	0.51
45:DR:64:ARG:HD2	69:DR:323:HOH:O	2.09	0.51
46:DS:24:LYS:HE3	69:DS:312:HOH:O	2.10	0.51
10:AJ:53:ILE:HG13	14:AN:85:ARG:HD2	1.92	0.51
31:CA:1353:A:H2'	31:CA:1354:A:C8	2.46	0.51
31:CA:1380:G:H2'	31:CA:1381:G:H8	1.75	0.51
31:CA:2408:U:H2'	31:CA:2409:G:C8	2.46	0.51
35:CG:42:GLU:HA	35:CG:55:ARG:HH21	1.75	0.51
55:DA:1720:U:H2'	55:DA:1721:G:O4'	2.11	0.51
55:DA:296:U:H2'	55:DA:297:G:C8	2.46	0.51
36:DH:3:VAL:HG12	36:DH:38:PRO:HA	1.93	0.51
54:DI:132:TYR:N	54:DI:133:GLU:HB2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DI:27:VAL:HG22	54:DI:82:ILE:HG22	1.93	0.51
11:AK:23:ILE:HG21	11:AK:96:THR:HG21	1.93	0.51
1:BA:579:A:H2'	1:BA:580:C:C6	2.46	0.51
1:BA:643:C:H5'	8:BH:32:LEU:HD13	1.93	0.51
31:CA:1991:U:H6	31:CA:1991:U:H5''	1.76	0.51
30:CD:48:ILE:HG23	30:CD:84:LEU:HD11	1.91	0.51
33:CE:148:ILE:HB	33:CE:169:VAL:HG22	1.93	0.51
44:CQ:106:LYS:HA	44:CQ:109:ARG:HD3	1.93	0.51
23:D2:19:HIS:HE1	23:D2:21:TYR:CE1	2.29	0.51
55:DA:2788:C:H2'	55:DA:2789:C:C6	2.46	0.51
32:DD:35:THR:HG22	32:DD:73:VAL:HG21	1.93	0.51
54:DI:26:VAL:HB	54:DI:83:ALA:HB3	1.93	0.51
4:AD:192:SER:HB3	4:AD:195:ILE:HD12	1.93	0.50
5:AE:107:ALA:CB	5:AE:125:ALA:HB3	2.40	0.50
8:AH:102:ALA:HB3	8:AH:113:ASP:HB3	1.93	0.50
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.76	0.50
22:C1:7:LYS:HD2	31:CA:1262:A:H2	1.76	0.50
22:C1:3:VAL:HG21	31:CA:2016:U:H1'	1.93	0.50
34:CF:65:PRO:HA	34:CF:89:VAL:HG23	1.91	0.50
41:DN:3:GLN:HG3	41:DN:92:TRP:CD1	2.46	0.50
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.93	0.50
1:BA:1197:A:H3'	1:BA:1198:G:C5'	2.42	0.50
1:BA:17:U:H2'	1:BA:18:C:C6	2.47	0.50
9:BI:84:THR:HG21	9:BI:103:PHE:HB2	1.93	0.50
22:C1:25:VAL:HG13	22:C1:26:THR:H	1.76	0.50
23:C2:11:LEU:HD21	23:C2:34:LEU:HD23	1.92	0.50
31:CA:1170:C:H42	31:CA:1178:C:H41	1.58	0.50
35:CG:90:VAL:HG21	35:CG:163:ARG:NE	2.27	0.50
36:CH:3:VAL:HG12	36:CH:38:PRO:HA	1.91	0.50
55:DA:118:A:N3	55:DA:178:G:H1'	2.25	0.50
55:DA:2126:A:H61	55:DA:2163:A:H5'	1.75	0.50
32:DD:121:THR:HG21	32:DD:143:PRO:HB3	1.92	0.50
35:DG:90:VAL:HG21	35:DG:163:ARG:NE	2.26	0.50
4:AD:170:TRP:CD2	4:AD:186:PRO:HB3	2.47	0.50
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.77	0.50
10:BJ:53:ILE:HG13	14:BN:85:ARG:HD2	1.93	0.50
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.47	0.50
22:C1:19:HIS:HE1	31:CA:2624:G:H1'	1.75	0.50
31:CA:296:U:H2'	31:CA:297:G:C8	2.46	0.50
31:CA:526:A:N6	31:CA:2626:C:H4'	2.26	0.50
35:CG:80:THR:HG23	35:CG:81:GLU:N	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2339:C:H2'	55:DA:2340:A:C8	2.46	0.50
55:DA:284:U:H2'	55:DA:285:G:H8	1.75	0.50
19:AS:52:HIS:HD2	19:AS:54:GLY:H	1.59	0.50
11:BK:23:ILE:HG21	11:BK:96:THR:HG21	1.94	0.50
14:BN:53:ARG:HH21	19:BS:37:ARG:HH22	1.60	0.50
31:CA:806:C:H2'	31:CA:807:U:H6	1.76	0.50
50:CW:64:VAL:HG22	50:CW:69:GLU:HG2	1.94	0.50
55:DA:2133:G:H2'	55:DA:2157:G:H1	1.76	0.50
55:DA:31:C:O3'	55:DA:1238:G:H5''	2.12	0.50
28:DB:111:U:H2'	28:DB:112:G:C8	2.45	0.50
28:DB:1:U:H2'	28:DB:2:G:C8	2.46	0.50
29:DC:154:LEU:HD13	29:DC:176:LEU:HD21	1.94	0.50
32:DD:99:GLU:CG	32:DD:182:ALA:HB2	2.41	0.50
1:AA:1061:G:H1	1:AA:1195:C:H41	1.59	0.50
1:BA:1194:U:H5'	5:BE:27:GLY:CA	2.42	0.50
1:BA:407:U:H2'	1:BA:408:A:C8	2.47	0.50
19:BS:52:HIS:CD2	19:BS:54:GLY:H	2.30	0.50
31:CA:1720:U:H2'	31:CA:1721:G:O4'	2.11	0.50
31:CA:644:A:H2'	31:CA:645:C:O4'	2.12	0.50
52:CY:12:PRO:HB3	52:CY:30:LEU:HD23	1.93	0.50
55:DA:610:C:H5'	69:DA:3623:HOH:O	2.10	0.50
34:DF:103:LEU:HG	34:DF:108:VAL:HG23	1.94	0.50
43:DP:33:ARG:HD2	69:DB:319:HOH:O	2.10	0.50
52:DY:27:ARG:HD3	69:DY:101:HOH:O	2.10	0.50
23:C2:33:LYS:HA	23:C2:52:ALA:HB3	1.92	0.50
39:CL:101:GLY:O	39:CL:120:PRO:HD2	2.11	0.50
47:CT:59:GLU:HA	47:CT:64:ALA:HA	1.93	0.50
55:DA:825:A:OP1	59:DA:3223:PUT:H12	2.12	0.50
55:DA:581:C:H2'	55:DA:582:A:C8	2.46	0.50
41:DN:100:LYS:HD3	69:DN:320:HOH:O	2.10	0.50
1:AA:212:G:H2'	1:AA:213:G:C8	2.46	0.50
1:AA:490:C:H2'	1:AA:491:G:H8	1.75	0.50
7:AG:111:ARG:HB3	7:AG:119:ARG:HG2	1.94	0.50
20:AT:57:ILE:HD12	20:AT:60:ARG:HE	1.76	0.50
5:BE:82:GLN:HG2	5:BE:149:SER:HA	1.93	0.50
12:BL:30:LYS:O	12:BL:82:ILE:HG22	2.11	0.50
20:BT:57:ILE:HD12	20:BT:60:ARG:HE	1.77	0.50
31:CA:2845:U:H2'	31:CA:2846:G:O4'	2.12	0.50
53:CZ:39:GLN:HB3	53:CZ:41:HIS:HE1	1.77	0.50
55:DA:1181:U:H2'	55:DA:1182:G:C8	2.46	0.50
55:DA:2547:A:H2'	55:DA:2548:U:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1381:U:H1'	7:BG:78:ARG:HE	1.76	0.50
8:BH:102:ALA:HB3	8:BH:113:ASP:HB3	1.93	0.50
23:C2:19:HIS:HE1	23:C2:21:TYR:CE1	2.29	0.50
25:C4:54:ASP:HB3	40:CM:57:LEU:HD22	1.93	0.50
50:CW:72:VAL:HG12	50:CW:93:ARG:HA	1.92	0.50
55:DA:1975:G:N2	63:DA:3225:PGE:H22	2.19	0.50
40:DM:53:GLY:HA3	55:DA:826:U:O2'	2.12	0.50
53:DZ:39:GLN:HB3	53:DZ:41:HIS:HE1	1.77	0.50
1:AA:1232:U:H5''	9:AI:126:GLN:HB3	1.94	0.50
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	1.93	0.50
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.94	0.50
1:AA:1458:G:H5''	20:AT:26:SER:HB3	1.93	0.50
31:CA:1181:U:H2'	31:CA:1182:G:C8	2.46	0.50
31:CA:2095:A:H8	31:CA:2095:A:H5''	1.77	0.50
31:CA:284:U:H2'	31:CA:285:G:H8	1.77	0.50
69:D0:216:HOH:O	55:DA:927:A:H1'	2.11	0.50
34:DF:106:ILE:HD12	34:DF:139:PRO:HG2	1.94	0.50
54:DI:111:ALA:O	54:DI:118:ILE:HB	2.11	0.50
1:AA:429:U:H5''	4:AD:9:LEU:HD12	1.94	0.49
1:BA:1317:C:OP1	14:BN:57:PRO:HD2	2.12	0.49
26:C5:8:LYS:HE3	31:CA:1031:G:H5''	1.93	0.49
31:CA:1783:A:N1	31:CA:2587:A:H2'	2.26	0.49
29:CC:162:VAL:HG22	29:CC:176:LEU:HA	1.94	0.49
55:DA:2133:G:H21	55:DA:2158:A:N6	2.09	0.49
55:DA:881:G:H1	55:DA:895:U:H3	1.60	0.49
46:DS:73:LYS:NZ	58:DS:203:MPD:H53	2.26	0.49
1:BA:21:G:H2'	1:BA:22:G:C8	2.47	0.49
6:BF:3:HIS:HA	6:BF:65:GLU:HA	1.94	0.49
7:BG:111:ARG:HB3	7:BG:119:ARG:HG2	1.93	0.49
7:BG:70:ARG:HG2	7:BG:96:ARG:HG2	1.94	0.49
31:CA:396:G:H1'	52:CY:29:PHE:CD2	2.47	0.49
29:CC:160:THR:O	29:CC:195:VAL:HG13	2.12	0.49
30:CD:99:GLU:CG	30:CD:182:ALA:HB2	2.42	0.49
34:CF:8:TYR:HA	34:CF:12:VAL:HB	1.94	0.49
32:DD:13:ARG:HD3	32:DD:21:SER:OG	2.12	0.49
46:DS:58:VAL:HG12	46:DS:102:SER:HB2	1.94	0.49
1:AA:403:C:H2'	1:AA:404:G:O4'	2.12	0.49
1:BA:745:G:H2'	1:BA:746:A:C8	2.47	0.49
2:BB:100:MET:HA	2:BB:107:VAL:HG21	1.93	0.49
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.95	0.49
31:CA:17:G:H4'	45:CR:25:TYR:HE2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:281:C:H2'	31:CA:282:A:C8	2.47	0.49
28:CB:111:U:H2'	28:CB:112:G:C8	2.47	0.49
45:CR:112:LYS:HD3	46:CS:48:LYS:HE2	1.94	0.49
55:DA:1425:G:H2'	55:DA:1426:G:C8	2.47	0.49
55:DA:839:U:H2'	55:DA:840:C:C6	2.48	0.49
49:DV:17:LYS:HE3	49:DV:40:ASN:HA	1.94	0.49
2:AB:100:MET:HA	2:AB:107:VAL:HG21	1.93	0.49
3:AC:14:ILE:HG21	3:AC:178:LEU:HB3	1.93	0.49
31:CA:2788:C:H2'	31:CA:2789:C:C6	2.46	0.49
29:CC:210:ALA:HA	29:CC:213:TRP:NE1	2.26	0.49
55:DA:137:U:H3	55:DA:142:A:H61	1.60	0.49
55:DA:2577:A:H5''	55:DA:2578:G:H5'	1.93	0.49
55:DA:648:G:H5''	69:DA:6963:HOH:O	2.12	0.49
29:DC:162:VAL:HG22	29:DC:176:LEU:HA	1.94	0.49
33:DE:148:ILE:HB	33:DE:169:VAL:HG22	1.93	0.49
50:DW:64:VAL:HG22	50:DW:69:GLU:HG2	1.94	0.49
1:AA:745:G:H2'	1:AA:746:A:C8	2.48	0.49
12:AL:30:LYS:O	12:AL:82:ILE:HG22	2.11	0.49
31:CA:83:A:H2	31:CA:103:A:N7	2.09	0.49
31:CA:695:G:H4'	31:CA:1380:G:H5'	1.94	0.49
30:CD:35:THR:HG22	30:CD:73:VAL:HG21	1.94	0.49
36:CH:49:ALA:O	36:CH:53:GLU:HB2	2.13	0.49
43:CP:11:ALA:HB2	43:CP:96:GLY:N	2.27	0.49
38:CK:42:ALA:O	45:CR:64:ARG:HD3	2.12	0.49
55:DA:1436:G:N2	55:DA:1557:C:C2	2.81	0.49
29:DC:75:PRO:HG2	29:DC:97:LYS:HD3	1.95	0.49
1:AA:86:G:H21	1:AA:87:C:H41	1.61	0.49
7:AG:70:ARG:HG2	7:AG:96:ARG:HG2	1.94	0.49
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.43	0.49
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.93	0.49
55:DA:2258:C:H4'	55:DA:2259:U:OP2	2.12	0.49
45:DR:84:LYS:HG3	62:DA:3002:EDO:H22	1.94	0.49
37:DJ:103:ARG:HA	37:DJ:106:LEU:HD12	1.95	0.49
1:AA:1305:G:HO2'	1:AA:1306:A:H8	1.60	0.49
1:AA:643:C:H5'	8:AH:32:LEU:HD13	1.95	0.49
1:BA:1096:C:H2'	1:BA:1097:C:C6	2.48	0.49
6:BF:70:VAL:HA	6:BF:73:GLU:HG2	1.92	0.49
9:BI:31:ASN:HD21	9:BI:67:VAL:H	1.61	0.49
40:CM:57:LEU:HB2	40:CM:60:ARG:HH11	1.77	0.49
1:AA:1358:U:H3	1:AA:1363:A:H62	1.59	0.49
1:AA:17:U:H2'	1:AA:18:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:132:ASN:OD1	5:AE:134:ILE:HG22	2.13	0.49
1:BA:77:A:H2'	1:BA:78:A:C8	2.47	0.49
7:BG:130:ASN:HA	7:BG:135:VAL:HG11	1.95	0.49
31:CA:1380:G:H1'	31:CA:1569:A:N6	2.28	0.49
31:CA:1299:G:H2'	31:CA:1639:C:N4	2.27	0.49
29:CC:154:LEU:HD13	29:CC:176:LEU:HD21	1.95	0.49
25:D4:8:ARG:HD2	55:DA:245:G:O6	2.13	0.49
55:DA:388:G:N7	55:DA:390:U:H2'	2.27	0.49
55:DA:821:A:H1'	69:DA:3397:HOH:O	2.13	0.49
34:DF:8:TYR:HA	34:DF:12:VAL:HB	1.94	0.49
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.42	0.49
7:AG:130:ASN:HA	7:AG:135:VAL:HG11	1.95	0.49
1:AA:719:C:O2'	18:AR:38:LYS:HB3	2.13	0.49
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	1.94	0.49
5:BE:97:GLN:HE21	5:BE:124:LEU:HD13	1.76	0.49
26:C5:17:VAL:CG1	26:C5:26:ILE:HD12	2.42	0.49
31:CA:247:G:N7	31:CA:249:C:C2	2.81	0.49
55:DA:740:C:H5"	55:DA:1784:A:OP1	2.12	0.49
34:DF:158:THR:HG23	34:DF:160:ALA:N	2.25	0.49
46:DS:1:MET:HA	46:DS:42:ALA:O	2.13	0.49
52:DY:18:ARG:NH2	52:DY:24:ALA:HB2	2.27	0.49
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.94	0.49
35:CG:80:THR:CG2	35:CG:81:GLU:H	2.24	0.49
41:CN:3:GLN:HG3	41:CN:92:TRP:CD1	2.47	0.49
26:D5:16:ILE:CD1	26:D5:25:VAL:HG22	2.43	0.49
32:DD:146:ILE:HD12	32:DD:155:VAL:HG21	1.95	0.49
38:DK:47:HIS:HE1	69:DA:4185:HOH:O	1.96	0.49
1:AA:1096:C:H2'	1:AA:1097:C:C6	2.47	0.48
1:AA:1239:A:H62	1:AA:1299:A:H62	1.61	0.48
31:CA:1324:G:H1'	31:CA:1616:A:N6	2.28	0.48
55:DA:1014:A:H1'	69:DA:5823:HOH:O	2.12	0.48
55:DA:118:A:C8	55:DA:119:A:C8	3.01	0.48
55:DA:2343:U:H2'	55:DA:2344:U:C6	2.48	0.48
55:DA:2427:C:H5"	55:DA:2428:G:OP1	2.12	0.48
55:DA:284:U:H2'	55:DA:285:G:C8	2.48	0.48
9:AI:84:THR:HG21	9:AI:103:PHE:HB2	1.94	0.48
4:BD:147:GLU:HA	4:BD:150:LYS:HD2	1.95	0.48
1:BA:1216:A:H5"	14:BN:5:SER:HB3	1.96	0.48
31:CA:1783:A:H5'	31:CA:2608:G:H4'	1.95	0.48
31:CA:881:G:H1	31:CA:895:U:H3	1.60	0.48
34:CF:103:LEU:HG	34:CF:108:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C1:42:HIS:CD2	42:CO:101:GLY:H	2.31	0.48
55:DA:195:A:H61	55:DA:198:C:H3'	1.77	0.48
29:DC:162:VAL:CG1	29:DC:174:LEU:HD22	2.43	0.48
52:DY:12:PRO:HB3	52:DY:30:LEU:HD23	1.94	0.48
6:AF:74:LEU:O	6:AF:77:THR:HG22	2.13	0.48
16:AP:2:VAL:HG21	16:AP:33:ILE:HD11	1.95	0.48
19:AS:52:HIS:CD2	19:AS:54:GLY:H	2.31	0.48
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.49	0.48
1:BA:429:U:H1'	1:BA:430:A:H5''	1.95	0.48
1:BA:202:G:O2'	1:BA:468:A:H8	1.96	0.48
31:CA:2800:A:C2	31:CA:2895:G:H1'	2.48	0.48
44:DQ:6:LYS:O	44:DQ:10:GLN:HG2	2.14	0.48
14:AN:53:ARG:HH21	19:AS:37:ARG:HH22	1.61	0.48
1:BA:1152:A:H5'	10:BJ:15:HIS:HB2	1.95	0.48
1:BA:392:C:H2'	1:BA:393:A:C8	2.49	0.48
31:CA:1056:G:H4'	31:CA:1086:A:C8	2.48	0.48
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.47	0.48
31:CA:2350:C:H2'	31:CA:2351:G:O4'	2.13	0.48
31:CA:279:A:H61	31:CA:361:G:H1'	1.79	0.48
34:CF:33:LYS:HG3	34:CF:157:THR:HB	1.95	0.48
37:CJ:86:ILE:HG21	37:CJ:98:VAL:HB	1.96	0.48
31:CA:2393:U:H5''	40:CM:62:PRO:HB3	1.95	0.48
43:CP:27:VAL:HG21	43:CP:40:ILE:HD12	1.94	0.48
41:DN:123:LYS:HB3	55:DA:2484:G:H1'	1.95	0.48
28:DB:81:G:H1'	69:DB:339:HOH:O	2.13	0.48
19:BS:32:ARG:HE	19:BS:57:HIS:CD2	2.31	0.48
26:C5:16:ILE:CD1	26:C5:25:VAL:HG22	2.43	0.48
31:CA:1093:G:H1'	31:CA:1099:G:N2	2.27	0.48
31:CA:2030:6MZ:N3	31:CA:2499:C:H5''	2.28	0.48
1:AA:1216:A:H5''	14:AN:5:SER:HB3	1.95	0.48
1:AA:407:U:H2'	1:AA:408:A:C8	2.49	0.48
1:AA:601:G:H2'	1:AA:602:A:C8	2.49	0.48
1:BA:972:C:H4'	10:BJ:59:LYS:HG2	1.96	0.48
7:BG:72:THR:HG22	7:BG:96:ARG:HH12	1.77	0.48
1:BA:719:C:O2'	18:BR:38:LYS:HB3	2.13	0.48
31:CA:785:G:O2'	31:CA:1779:U:H5''	2.13	0.48
31:CA:818:G:H5'	31:CA:839:U:OP1	2.14	0.48
33:CE:126:VAL:HG21	33:CE:133:LEU:HB3	1.95	0.48
55:DA:1622:G:H1'	69:DA:6193:HOH:O	2.14	0.48
55:DA:1935:G:H1'	55:DA:1964:G:N2	2.28	0.48
55:DA:2018:G:H2'	55:DA:2019:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:DQ:29:LYS:HB3	44:DQ:40:LEU:HD12	1.96	0.48
1:AA:1152:A:H5'	10:AJ:15:HIS:HB2	1.96	0.48
1:AA:1239:A:H62	1:AA:1299:A:N6	2.12	0.48
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.49	0.48
1:AA:429:U:H1'	1:AA:430:A:H5''	1.95	0.48
4:AD:73:ARG:HG3	4:AD:204:TYR:CE1	2.48	0.48
1:AA:1298:U:H3	7:AG:114:LYS:HA	1.79	0.48
1:BA:1232:U:H5''	9:BI:126:GLN:HB3	1.96	0.48
31:CA:1310:G:H1'	31:CA:1611:C:H5''	1.96	0.48
31:CA:2271:G:OP1	51:CX:18:ALA:HB1	2.13	0.48
46:CS:46:GLU:CD	46:CS:46:GLU:H	2.16	0.48
55:DA:281:C:H2'	55:DA:282:A:C8	2.48	0.48
42:DO:85:PRO:HA	42:DO:88:ALA:HB2	1.95	0.48
9:AI:31:ASN:HD21	9:AI:67:VAL:H	1.61	0.48
1:BA:601:G:H2'	1:BA:602:A:C8	2.49	0.48
5:BE:18:VAL:HG11	5:BE:56:VAL:HG13	1.96	0.48
31:CA:2680:U:H2'	31:CA:2681:C:C6	2.48	0.48
31:CA:763:G:H2'	31:CA:765:C:OP2	2.12	0.48
38:DK:30:THR:HG22	55:DA:1006:C:O4'	2.14	0.48
55:DA:2887[A]:A:H2'	55:DA:2888[A]:C:C6	2.49	0.48
54:DI:58:THR:HB	55:DA:1046:A:H4'	1.95	0.48
43:DP:1:MET:HB3	43:DP:6:ALA:HB2	1.95	0.48
1:AA:412:A:H3'	1:AA:413:G:C5'	2.43	0.48
1:AA:662:U:H2'	1:AA:663:A:C8	2.49	0.48
12:AL:53:CYS:HB3	12:AL:67:ILE:HD11	1.96	0.48
31:CA:1141:U:H4'	31:CA:1142:A:O4'	2.14	0.48
31:CA:1405:U:H2'	31:CA:1406:U:C6	2.48	0.48
31:CA:2849:U:H4'	31:CA:2868:A:C2	2.48	0.48
31:CA:364:C:H2'	31:CA:365:U:C6	2.48	0.48
37:CJ:103:ARG:HA	37:CJ:106:LEU:HD12	1.95	0.48
31:CA:2364:C:H4'	51:CX:56:ASP:OD1	2.14	0.48
55:DA:1101:U:H2'	55:DA:1102:C:C6	2.49	0.48
55:DA:296:U:H2'	55:DA:297:G:H8	1.79	0.48
1:AA:1057:G:O3'	3:AC:197:GLY:HA3	2.14	0.48
13:BM:106:ALA:HB3	13:BM:110:LYS:HE3	1.96	0.48
31:CA:137:U:H3	31:CA:142:A:H61	1.62	0.48
34:CF:106:ILE:HD12	34:CF:139:PRO:HG2	1.95	0.48
55:DA:1441:G:H2'	55:DA:1442:U:C6	2.49	0.48
55:DA:1428:C:C5	55:DA:1569:A:H5''	2.49	0.48
37:DJ:86:ILE:HG21	37:DJ:98:VAL:HB	1.95	0.48
31:CA:1776:G:N2	31:CA:1789:A:H1'	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:831:G:O5'	31:CA:831:G:H8	1.96	0.47
35:CG:138:LYS:HA	35:CG:141:ILE:HG22	1.96	0.47
27:D0:12:SER:HB3	55:DA:988:A:P	2.54	0.47
55:DA:142:A:H2'	55:DA:143:C:C6	2.49	0.47
55:DA:622:G:H5''	55:DA:622:G:H8	1.79	0.47
24:D3:2:LYS:HE2	55:DA:687:C:H5''	1.96	0.47
38:DK:58:ASN:HA	38:DK:126:ALA:O	2.14	0.47
45:DR:104:VAL:HG11	46:DS:45:GLU:HA	1.96	0.47
1:BA:1239:A:H62	1:BA:1299:A:N6	2.13	0.47
1:BA:649:A:H2'	1:BA:650:G:O4'	2.14	0.47
1:BA:662:U:H2'	1:BA:663:A:C8	2.49	0.47
1:BA:714:G:H2'	1:BA:715:A:C8	2.49	0.47
13:BM:86:TYR:CZ	13:BM:90:ARG:HD2	2.49	0.47
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.49	0.47
31:CA:1999:C:H5''	31:CA:2723:C:O2'	2.15	0.47
31:CA:528:A:C8	31:CA:528:A:C3'	2.97	0.47
31:CA:942:G:H4'	31:CA:1190:G:H5'	1.96	0.47
49:CV:82:ARG:CB	49:CV:97:LYS:HG3	2.43	0.47
51:CX:37:ILE:HG21	51:CX:80:ILE:HG21	1.96	0.47
55:DA:21:A:H2'	55:DA:22:C:O4'	2.14	0.47
55:DA:364:C:H2'	55:DA:365:U:C6	2.49	0.47
1:AA:620:C:C2	4:AD:132:ILE:HG21	2.50	0.47
19:AS:51:VAL:HG21	19:AS:71:LEU:HB3	1.97	0.47
3:BC:14:ILE:HG21	3:BC:178:LEU:HB3	1.96	0.47
5:BE:13:GLU:HB3	5:BE:39:VAL:HG12	1.96	0.47
5:BE:90:THR:HG22	5:BE:91:GLY:H	1.79	0.47
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.29	0.47
46:CS:78:ARG:HB2	46:CS:83:TYR:HD1	1.79	0.47
55:DA:1746:A:H2'	55:DA:1747:U:C6	2.50	0.47
55:DA:2543:G:H2'	55:DA:2544:G:C8	2.49	0.47
44:DQ:95:ALA:HB3	69:DA:4560:HOH:O	2.13	0.47
6:AF:6:ILE:HG13	6:AF:89:VAL:HG23	1.95	0.47
4:BD:192:SER:HB3	4:BD:195:ILE:HD12	1.96	0.47
5:BE:157:ARG:HG2	5:BE:158:GLY:N	2.29	0.47
19:BS:30:PRO:HB2	19:BS:50:ALA:HB2	1.97	0.47
31:CA:980:A:C4	31:CA:1136:G:O4'	2.68	0.47
38:CK:58:ASN:HA	38:CK:126:ALA:O	2.15	0.47
49:CV:74:ASN:HD22	49:CV:77:THR:H	1.61	0.47
55:DA:1796:U:H2'	55:DA:1797:G:H8	1.78	0.47
29:DC:21:ASN:HB3	29:DC:24:LEU:HG	1.97	0.47
1:AA:714:G:H2'	1:AA:715:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1053:G:N7	1:BA:1200:C:H5''	2.30	0.47
1:BA:1239:A:H62	1:BA:1299:A:H62	1.61	0.47
9:BI:12:ARG:HG3	9:BI:107:ASP:HB3	1.96	0.47
31:CA:1998:A:H2'	31:CA:1999:C:O4'	2.14	0.47
28:DB:18:G:H1	28:DB:65:U:H3	1.62	0.47
39:DL:113:MET:HE1	39:DL:116:ILE:HD11	1.94	0.47
48:DU:58:VAL:HG22	48:DU:85:VAL:HG22	1.96	0.47
1:AA:202:G:O2'	1:AA:468:A:H8	1.96	0.47
31:CA:1441:G:H2'	31:CA:1442:U:C6	2.50	0.47
31:CA:688:U:H2'	31:CA:689:A:H8	1.80	0.47
44:DQ:31:TRP:CD2	44:DQ:40:LEU:HD21	2.49	0.47
1:AA:392:C:H2'	1:AA:393:A:C8	2.49	0.47
13:AM:86:TYR:CZ	13:AM:90:ARG:HD2	2.50	0.47
1:BA:429:U:C5'	4:BD:9:LEU:HD12	2.45	0.47
31:CA:142:A:H2'	31:CA:143:C:C6	2.50	0.47
31:CA:2189:U:O2'	31:CA:2190:G:H5'	2.15	0.47
31:CA:2520:C:H2'	31:CA:2521:C:H6	1.79	0.47
31:CA:460:A:H2'	31:CA:461:C:O4'	2.15	0.47
31:CA:736:C:O5'	31:CA:736:C:H6	1.98	0.47
31:CA:747:5MU:O2	31:CA:2014:A:H1'	2.15	0.47
31:CA:787:C:H5''	31:CA:788:A:H5'	1.97	0.47
31:CA:987:C:H2'	31:CA:988:A:O4'	2.14	0.47
55:DA:1590:A:H2'	55:DA:1591:A:C8	2.50	0.47
55:DA:2869:G:H2'	55:DA:2870:C:O4'	2.15	0.47
54:DI:93:ALA:O	54:DI:97:LYS:HG3	2.14	0.47
40:DM:62:PRO:HB3	55:DA:2393:U:H5''	1.96	0.47
42:DO:56:LYS:HE3	42:DO:94:TYR:OH	2.14	0.47
17:AQ:68:SER:OG	17:AQ:71:LYS:HB2	2.14	0.47
31:CA:1775:U:H2'	31:CA:1776:G:O4'	2.14	0.47
30:CD:150:GLN:NE2	31:CA:2032:G:H1'	2.29	0.47
31:CA:2190:G:H2'	31:CA:2191:A:H8	1.78	0.47
29:CC:147:LYS:HB2	29:CC:150:LYS:HD2	1.96	0.47
55:DA:1069:A:H5'	55:DA:1070:A:H8	1.80	0.47
55:DA:553:G:H2'	55:DA:554:U:O4'	2.14	0.47
38:DK:9:GLU:HG3	69:DA:5367:HOH:O	2.15	0.47
1:AA:1061:G:H1	1:AA:1195:C:N4	2.13	0.47
1:AA:649:A:H2'	1:AA:650:G:O4'	2.14	0.47
4:AD:147:GLU:HA	4:AD:150:LYS:HD2	1.96	0.47
5:AE:13:GLU:HB3	5:AE:39:VAL:HG12	1.96	0.47
5:AE:90:THR:HG22	5:AE:91:GLY:H	1.80	0.47
1:BA:1069:C:O2'	1:BA:1192:C:H1'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1463:U:H2'	1:BA:1464:U:C6	2.50	0.47
31:CA:1428:C:C5	31:CA:1569:A:H5''	2.49	0.47
31:CA:25:U:H2'	31:CA:26:G:O4'	2.15	0.47
31:CA:296:U:H2'	31:CA:297:G:H8	1.80	0.47
35:CG:24:ILE:HD12	35:CG:72:LEU:HD11	1.97	0.47
32:DD:150[A]:MEQ:OE1	55:DA:2032:G:H1'	2.15	0.47
55:DA:2723:C:H2'	55:DA:2724:U:O4'	2.15	0.47
44:DQ:6:LYS:HG3	61:DQ:201:PEG:H41	1.97	0.47
1:BA:1512:U:H2'	1:BA:1513:A:C8	2.50	0.47
7:BG:47:LEU:HD22	7:BG:58:GLU:HG2	1.96	0.47
31:CA:1343:G:H2'	31:CA:1344:U:C6	2.49	0.47
31:CA:2271:G:H2'	31:CA:2272:U:C6	2.50	0.47
31:CA:279:A:N6	31:CA:361:G:H1'	2.29	0.47
55:DA:1180:U:H5''	55:DA:1180:U:H6	1.80	0.47
55:DA:1182:G:H2'	55:DA:1183:U:O4'	2.15	0.47
55:DA:1278:C:H2'	55:DA:1279:G:H8	1.79	0.47
55:DA:1641:A:H2'	55:DA:1642:G:O4'	2.15	0.47
43:DP:100:HIS:CD2	28:DB:48:U:H4'	2.50	0.47
1:AA:1053:G:N7	1:AA:1200:C:H5''	2.30	0.47
1:AA:392:C:H2'	1:AA:393:A:H8	1.80	0.47
13:AM:85:CYS:HB3	19:AS:74:PHE:CE1	2.49	0.47
1:BA:784:A:H4'	31:CA:1837:C:OP1	2.14	0.47
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.50	0.47
30:CD:25:THR:HG21	30:CD:193:VAL:HG22	1.97	0.47
55:DA:279:A:N6	55:DA:361:G:H1'	2.30	0.47
40:DM:81:ASP:HA	40:DM:84:LYS:HD2	1.97	0.47
1:AA:620:C:H2'	1:AA:621:A:O4'	2.15	0.46
5:BE:106:ILE:HG13	5:BE:123:VAL:O	2.15	0.46
31:CA:2313:C:H5''	34:CF:88:LYS:HD3	1.98	0.46
31:CA:571:U:H1'	31:CA:573:U:C6	2.50	0.46
34:CF:36:LEU:HB2	34:CF:57:LEU:HD21	1.97	0.46
42:CO:54:LEU:HD23	42:CO:66:ALA:HB2	1.97	0.46
42:CO:72:ASP:OD2	42:CO:75:ILE:HG12	2.15	0.46
45:CR:58:ARG:HH11	45:CR:62:ILE:HD11	1.78	0.46
55:DA:2026:U:H2'	55:DA:2027:G:O4'	2.15	0.46
51:DX:37:ILE:HG21	51:DX:80:ILE:HG21	1.96	0.46
1:BA:532:A:H61	3:BC:193:TYR:HD2	1.62	0.46
5:BE:105:ILE:HA	5:BE:123:VAL:HG23	1.97	0.46
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.97	0.46
31:CA:1641:A:H2'	31:CA:1642:G:O4'	2.16	0.46
31:CA:1813:G:H2'	31:CA:1814:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:284:U:H2'	31:CA:285:G:C8	2.50	0.46
31:CA:372:G:H5''	52:CY:61:LYS:HD3	1.97	0.46
55:DA:1682:G:H3'	69:DA:4329:HOH:O	2.15	0.46
55:DA:2377:A:H2'	55:DA:2378:A:C8	2.50	0.46
55:DA:697:G:H2'	55:DA:698:C:C6	2.50	0.46
29:DC:147:LYS:HB2	29:DC:150:LYS:HD2	1.97	0.46
42:DO:72:ASP:OD2	42:DO:75:ILE:HG12	2.15	0.46
43:DP:41:ALA:HB2	43:DP:48:LEU:HD23	1.97	0.46
49:DV:14:LEU:HD11	49:DV:71:ALA:HB2	1.97	0.46
1:BA:735:C:H5'	18:BR:60:LYS:HD3	1.97	0.46
1:BA:1057:G:O3'	3:BC:197:GLY:HA3	2.15	0.46
11:BK:111:THR:HG23	21:BU:3:VAL:HG22	1.96	0.46
31:CA:1809:A:H2'	31:CA:1810:A:C8	2.50	0.46
31:CA:392:U:H2'	31:CA:393:C:H6	1.79	0.46
38:DK:35:ARG:HB3	38:DK:54:ILE:HD11	1.97	0.46
46:DS:37:GLU:HB3	46:DS:53:PHE:CE1	2.51	0.46
1:AA:1463:U:H2'	1:AA:1464:U:C6	2.51	0.46
1:AA:857:C:H2'	1:AA:858:G:O4'	2.15	0.46
7:AG:47:LEU:HD22	7:AG:58:GLU:HG2	1.98	0.46
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.81	0.46
1:BA:1026:G:H1	1:BA:1035:A:H2	1.62	0.46
1:BA:59:A:H5''	1:BA:387:U:H5''	1.97	0.46
1:BA:1298:U:H3	7:BG:114:LYS:HA	1.79	0.46
24:C3:24:THR:HG23	24:C3:27:GLY:HA3	1.97	0.46
31:CA:1754:A:H8	31:CA:1754:A:O5'	1.98	0.46
31:CA:569:U:H5''	31:CA:821:A:C2	2.50	0.46
55:DA:136:G:H1	55:DA:143:C:H42	1.62	0.46
55:DA:1424:G:H2'	55:DA:1425:G:O4'	2.15	0.46
55:DA:747:5MU:O2	55:DA:2014:A:H1'	2.16	0.46
55:DA:2402:U:C2'	55:DA:2403:C:H5'	2.45	0.46
55:DA:352:A:H8	55:DA:352:A:H5''	1.80	0.46
47:DT:17:VAL:HA	47:DT:43:ALA:HB1	1.96	0.46
1:AA:1141:C:O2'	1:AA:1142:G:H8	1.99	0.46
1:AA:34:C:H2'	1:AA:35:G:C8	2.50	0.46
16:AP:54:LEU:HA	16:AP:57:ILE:HD12	1.97	0.46
19:AS:30:PRO:HB2	19:AS:50:ALA:HB2	1.98	0.46
1:BA:1194:U:C5'	5:BE:27:GLY:HA2	2.45	0.46
6:BF:16:GLU:O	6:BF:19:PRO:HD2	2.15	0.46
16:BP:4:ILE:HD13	16:BP:57:ILE:HG23	1.97	0.46
19:BS:51:VAL:HG21	19:BS:71:LEU:HB3	1.98	0.46
31:CA:1430:G:H2'	31:CA:1431:A:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2233:U:H2'	31:CA:2234:G:C8	2.50	0.46
46:CS:49:ILE:HB	46:CS:51:VAL:O	2.15	0.46
54:DI:57:ASN:HB3	54:DI:76:PHE:HB3	1.96	0.46
42:DO:35:LYS:HB2	42:DO:112:TYR:CE1	2.51	0.46
46:DS:22:LEU:HA	69:DS:311:HOH:O	2.15	0.46
6:AF:16:GLU:O	6:AF:19:PRO:HD2	2.16	0.46
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	1.96	0.46
1:AA:735:C:H5'	18:AR:60:LYS:HD3	1.98	0.46
20:AT:48:GLN:HE21	20:AT:52:ASN:ND2	2.13	0.46
31:CA:355:U:H2'	31:CA:356:G:C8	2.51	0.46
55:DA:570:G:H2'	55:DA:2030:6MZ:N7	2.31	0.46
41:DN:16:ARG:HB3	28:DB:90:C:OP1	2.16	0.46
1:BA:1356:G:H2'	1:BA:1357:A:C8	2.50	0.46
1:BA:490:C:H2'	1:BA:491:G:C8	2.50	0.46
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.43	0.46
20:BT:44:LYS:HB3	20:BT:87:ALA:HB2	1.97	0.46
31:CA:1510:G:H2'	31:CA:1511:G:O4'	2.16	0.46
31:CA:1974:C:H2'	31:CA:1975:G:H8	1.81	0.46
31:CA:639:U:H2'	31:CA:640:C:C6	2.51	0.46
34:CF:44:ILE:HG21	34:CF:79:ILE:HG22	1.97	0.46
44:CQ:6:LYS:O	44:CQ:10:GLN:HG2	2.16	0.46
31:CA:2718:G:OP1	44:CQ:98:TYR:HD2	1.99	0.46
52:CY:18:ARG:NH2	52:CY:24:ALA:HB2	2.31	0.46
55:DA:2328:A:H2'	55:DA:2329:U:C6	2.51	0.46
55:DA:2626:C:H2'	55:DA:2627:G:O4'	2.16	0.46
55:DA:2849:U:H4'	55:DA:2868:A:C2	2.50	0.46
55:DA:639:U:H2'	55:DA:640:C:C6	2.51	0.46
34:DF:44:ILE:HG21	34:DF:79:ILE:HG22	1.98	0.46
1:AA:373:A:H61	1:AA:391:G:H1'	1.81	0.46
4:AD:54:GLN:HB3	4:AD:203:LEU:HD13	1.97	0.46
13:AM:93:ARG:HH12	19:AS:81:ARG:HH21	1.63	0.46
1:BA:392:C:H2'	1:BA:393:A:H8	1.79	0.46
28:CB:18:G:H1	28:CB:65:U:H3	1.62	0.46
29:CC:75:PRO:HG2	29:CC:97:LYS:HD3	1.97	0.46
41:CN:34:LYS:HE3	41:CN:131:VAL:HG11	1.98	0.46
55:DA:225:C:H2'	55:DA:226:A:O4'	2.16	0.46
55:DA:2461:A:H1'	55:DA:2492:U:C2	2.51	0.46
55:DA:279:A:H61	55:DA:361:G:H1'	1.79	0.46
55:DA:2830:C:H5'	69:DA:4054:HOH:O	2.16	0.46
54:DI:126:LEU:HA	54:DI:129:LEU:HD12	1.96	0.46
43:DP:31:THR:HG22	43:DP:33:ARG:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:73:C:O2'	1:BA:74:A:H8	1.99	0.46
7:BG:69:VAL:HG23	7:BG:100:ALA:HB1	1.97	0.46
16:BP:54:LEU:HA	16:BP:57:ILE:HD12	1.98	0.46
31:CA:1783:A:C2	31:CA:2588:G:O4'	2.69	0.46
31:CA:2328:A:H2'	31:CA:2329:U:C6	2.51	0.46
31:CA:2547:A:H2'	31:CA:2548:U:C6	2.51	0.46
31:CA:2688:G:H1'	31:CA:2721:A:N6	2.31	0.46
42:CO:85:PRO:HA	42:CO:88:ALA:HB2	1.97	0.46
55:DA:2609:U:C5	62:DA:3194:EDO:H12	2.51	0.46
34:DF:33:LYS:HG3	34:DF:157:THR:HB	1.96	0.46
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.51	0.46
13:AM:106:ALA:HB3	13:AM:110:LYS:HE3	1.98	0.46
1:BA:34:C:H2'	1:BA:35:G:C8	2.51	0.46
16:BP:20:VAL:HG13	16:BP:32:PHE:HB2	1.98	0.46
31:CA:2544:G:H5'	31:CA:2645:G:N2	2.31	0.46
31:CA:352:A:H5"	31:CA:352:A:H8	1.81	0.46
25:D4:45:ARG:HD3	55:DA:2418:A:OP1	2.16	0.46
55:DA:2065:C:H2'	55:DA:2066:C:O4'	2.16	0.46
55:DA:2097:A:C8	55:DA:2097:A:H5"	2.50	0.46
55:DA:2267:A:H5"	55:DA:2268:A:H5'	1.98	0.46
55:DA:2558:C:H2'	55:DA:2559:C:O4'	2.16	0.46
55:DA:2643:G:H2'	55:DA:2644:G:O4'	2.16	0.46
32:DD:129:THR:HG22	32:DD:141:ARG:HA	1.98	0.46
51:DX:38:VAL:HG12	51:DX:59:LEU:HB2	1.98	0.46
1:AA:579:A:H2'	1:AA:580:C:C6	2.51	0.45
1:AA:73:C:O2'	1:AA:74:A:H8	1.98	0.45
1:AA:429:U:C5'	4:AD:9:LEU:HD12	2.47	0.45
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.96	0.45
11:AK:21:ALA:HB2	11:AK:82:LEU:HD13	1.98	0.45
1:BA:1069:C:H4'	1:BA:1192:C:O2	2.16	0.45
1:BA:1103:C:H2'	1:BA:1104:G:O4'	2.16	0.45
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	1.97	0.45
31:CA:2461:A:H1'	31:CA:2492:U:C2	2.51	0.45
31:CA:2886:A:C2	31:CA:2887:A:H1'	2.51	0.45
38:CK:35:ARG:HB3	38:CK:54:ILE:HD11	1.98	0.45
55:DA:1532:A:C8	55:DA:1532:A:H5"	2.51	0.45
29:DC:8:PRO:O	55:DA:1695:G:H1'	2.16	0.45
55:DA:2141:G:H2'	55:DA:2142:A:C8	2.52	0.45
66:DA:3202:ACY:H2	69:DA:5043:HOH:O	2.15	0.45
55:DA:355:U:H2'	55:DA:356:G:C8	2.51	0.45
55:DA:455:C:N3	55:DA:472:A:H2'	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:634:C:H6	55:DA:634:C:O5'	1.99	0.45
33:DE:33:VAL:HG22	58:DA:3192:MPD:C1	2.39	0.45
47:DT:93:ALA:HB2	55:DA:1614:A:N1	2.31	0.45
1:AA:1003:G:H21	1:AA:1005:A:H5'	1.81	0.45
69:AA:1745:HOH:O	12:AL:115:SER:HB3	2.16	0.45
16:AP:4:ILE:HD13	16:AP:57:ILE:HG23	1.98	0.45
20:AT:39:ILE:HG23	20:AT:86:LEU:HD11	1.98	0.45
1:BA:1305:G:HO2'	1:BA:1306:A:H8	1.61	0.45
1:BA:857:C:H2'	1:BA:858:G:O4'	2.16	0.45
31:CA:2377:A:H2'	31:CA:2378:A:C8	2.50	0.45
31:CA:2845:U:H5''	44:CQ:52:ASN:O	2.15	0.45
43:CP:41:ALA:HB2	43:CP:48:LEU:HD23	1.97	0.45
35:DG:24:ILE:HD12	35:DG:72:LEU:HD11	1.97	0.45
45:DR:76:TYR:CZ	45:DR:80:ILE:HG13	2.50	0.45
49:DV:52:LEU:C	49:DV:54:GLN:H	2.18	0.45
1:AA:1026:G:H1	1:AA:1035:A:H2	1.63	0.45
1:AA:328:C:H2'	1:AA:328:C:O2	2.17	0.45
1:AA:623:C:H6	1:AA:623:C:O5'	2.00	0.45
6:AF:3:HIS:HA	6:AF:65:GLU:HA	1.98	0.45
1:BA:920:U:H2'	1:BA:921:U:C6	2.51	0.45
1:BA:502:A:OP1	12:BL:115:SER:HB2	2.17	0.45
31:CA:2822:G:H2'	31:CA:2823:A:H5''	1.98	0.45
46:CS:1:MET:HA	46:CS:42:ALA:O	2.16	0.45
49:CV:72:ILE:HG12	49:CV:83:VAL:HG23	1.99	0.45
55:DA:1426:G:O5'	55:DA:1426:G:H8	1.98	0.45
29:DC:50:THR:OG1	55:DA:1813:G:H1'	2.17	0.45
33:DE:58:LYS:HD2	55:DA:675:A:OP1	2.17	0.45
44:DQ:52:ASN:O	55:DA:2845:U:H5''	2.14	0.45
48:DU:33:LYS:HE2	63:DU:201:PGE:H32	1.98	0.45
1:AA:1069:C:H4'	1:AA:1192:C:O2	2.16	0.45
1:AA:920:U:H2'	1:AA:921:U:C6	2.51	0.45
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.99	0.45
1:BA:1141:C:O2'	1:BA:1142:G:H8	1.99	0.45
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	1.99	0.45
21:BU:11:PRO:HG2	21:BU:14:VAL:HB	1.98	0.45
23:C2:25:LYS:HD2	23:C2:52:ALA:HB1	1.97	0.45
31:CA:2182:U:H2'	31:CA:2183:A:C8	2.51	0.45
41:CN:40:ARG:HD3	41:CN:93:VAL:HG21	1.99	0.45
44:CQ:114:LEU:HD22	44:CQ:114:LEU:H	1.82	0.45
55:DA:1796:U:H2'	55:DA:1797:G:C8	2.52	0.45
55:DA:191:A:H2'	55:DA:192:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:DD:25:THR:HG21	32:DD:193:VAL:HG22	1.98	0.45
34:DF:122:PHE:CE2	34:DF:167:ARG:HD3	2.52	0.45
34:DF:88:LYS:HD3	55:DA:2313:C:H5''	1.99	0.45
46:DS:72:VAL:HG13	69:DS:346:HOH:O	2.16	0.45
5:BE:99:ALA:HB3	5:BE:122:ASN:HB3	1.97	0.45
7:BG:26:PHE:HA	7:BG:29:ILE:HD12	1.97	0.45
41:CN:121:ALA:HA	41:CN:124:LEU:HD12	1.98	0.45
55:DA:1237:A:H4'	55:DA:1238:G:OP1	2.16	0.45
23:D2:8:LYS:HE2	55:DA:2420:C:H5''	1.97	0.45
55:DA:2557:G:H2'	55:DA:2558:C:H6	1.82	0.45
41:DN:77:PRO:HG2	41:DN:80:VAL:HG21	1.97	0.45
45:DR:78:LYS:HG2	69:DA:6376:HOH:O	2.17	0.45
1:AA:167:A:H2'	1:AA:168:G:O4'	2.17	0.45
9:AI:12:ARG:HG3	9:AI:107:ASP:HB3	1.98	0.45
1:BA:1402:4OC:H2'	1:BA:1403:C:O4'	2.16	0.45
1:BA:212:G:H2'	1:BA:213:G:H8	1.80	0.45
31:CA:197:A:H2	31:CA:2434:A:N6	2.14	0.45
31:CA:2101:A:H2'	31:CA:2102:G:H8	1.81	0.45
22:C1:4:GLN:HA	31:CA:2615:U:C2	2.51	0.45
31:CA:2728:U:O2'	31:CA:2729:G:H8	1.99	0.45
24:D3:24:THR:HG23	24:D3:27:GLY:HA3	1.98	0.45
55:DA:2014:A:H2'	55:DA:2015:A:C8	2.51	0.45
55:DA:2047:C:C5	66:DA:3202:ACY:H3	2.51	0.45
42:DO:45:ARG:HD2	69:DA:5551:HOH:O	2.16	0.45
1:AA:1190:G:H5'	3:AC:176:HIS:CE1	2.51	0.45
5:BE:105:ILE:H	5:BE:123:VAL:H	1.65	0.45
5:BE:90:THR:HG22	5:BE:91:GLY:N	2.32	0.45
31:CA:1380:G:H1'	31:CA:1569:A:H61	1.81	0.45
31:CA:1590:A:H2'	31:CA:1591:A:C8	2.52	0.45
31:CA:2353:G:H2'	31:CA:2354:C:O4'	2.16	0.45
45:CR:76:TYR:CZ	45:CR:80:ILE:HG13	2.52	0.45
42:DO:54:LEU:HD23	42:DO:66:ALA:HB2	1.98	0.45
2:AB:207:ILE:HG13	2:AB:207:ILE:H	1.60	0.45
1:BA:123:U:H5''	1:BA:311:C:O2'	2.17	0.45
1:BA:729:A:H2'	1:BA:730:G:O4'	2.16	0.45
4:BD:88:GLU:HG2	4:BD:188:ARG:HD3	1.97	0.45
15:BO:64:ARG:HH12	15:BO:88:ARG:NH1	2.15	0.45
31:CA:136:G:H1	31:CA:143:C:H42	1.64	0.45
30:CD:13:ARG:HD3	30:CD:21:SER:OG	2.17	0.45
55:DA:1179:G:H2'	55:DA:1180:U:C6	2.51	0.45
55:DA:780:G:H2'	55:DA:782:A:N7	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:825:A:H2'	55:DA:826:U:O4'	2.17	0.45
32:DD:159:LYS:HE2	69:DA:4766:HOH:O	2.16	0.45
41:DN:19:GLY:O	41:DN:97:GLN:HB3	2.17	0.45
42:DO:29:VAL:HG13	42:DO:83:LEU:HD11	1.98	0.45
51:DX:57:HIS:N	51:DX:57:HIS:CD2	2.85	0.45
1:AA:843:U:H1'	1:AA:845:A:C6	2.52	0.45
5:AE:16:ILE:HD13	5:AE:137:VAL:HG11	1.99	0.45
5:AE:18:VAL:HG11	5:AE:56:VAL:HG13	1.99	0.45
7:AG:26:PHE:HA	7:AG:29:ILE:HD12	1.99	0.45
1:BA:1194:U:H5'	5:BE:27:GLY:HA2	1.97	0.45
1:BA:328:C:O2	1:BA:328:C:H2'	2.16	0.45
9:BI:84:THR:HG21	9:BI:103:PHE:CB	2.47	0.45
31:CA:1069:A:H5'	31:CA:1070:A:H8	1.81	0.45
31:CA:1121:C:H2'	31:CA:1122:G:O4'	2.17	0.45
31:CA:790:U:H3	31:CA:795:C:H5'	1.82	0.45
22:D1:3:VAL:HG22	22:D1:4:GLN:H	1.81	0.45
1:AA:1484:C:O2'	55:DA:1961:C:H5'	2.16	0.45
34:DF:61:SER:HB2	34:DF:91:LEU:HD21	1.99	0.45
54:DI:53:ARG:HD2	54:DI:55:VAL:HG23	1.97	0.45
38:DK:7:LYS:O	38:DK:11:VAL:HG23	2.17	0.45
46:DS:83:TYR:CE1	55:DA:1187:G:H5''	2.51	0.45
4:AD:88:GLU:HG2	4:AD:188:ARG:HD3	1.98	0.45
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.81	0.45
1:BA:1197:A:H3'	1:BA:1198:G:H5''	1.99	0.45
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.82	0.45
1:BA:82:G:N1	1:BA:84:U:H5	2.10	0.45
1:BA:1108:G:H5''	3:BC:176:HIS:CE1	2.52	0.45
13:BM:16:VAL:HG13	13:BM:34:LEU:HD12	1.98	0.45
1:BA:1329:A:H5''	13:BM:26:GLY:H	1.82	0.45
31:CA:206:U:H2'	31:CA:207:A:C8	2.37	0.45
31:CA:2364:C:OP1	51:CX:55:ARG:HD3	2.17	0.45
55:DA:2182:U:H2'	55:DA:2183:A:C8	2.52	0.45
55:DA:2345:G:N3	55:DA:2381:A:H2'	2.32	0.45
55:DA:2903:U:H3'	69:DA:6757:HOH:O	2.17	0.45
1:AA:1512:U:H2'	1:AA:1513:A:C8	2.52	0.44
1:AA:235:C:H2'	1:AA:236:A:C8	2.52	0.44
19:AS:53:ASN:HD22	19:AS:58:VAL:HG23	1.82	0.44
1:BA:32:A:H2'	1:BA:33:A:C8	2.52	0.44
1:BA:49:U:O2	1:BA:362:G:H1'	2.17	0.44
1:BA:373:A:H61	1:BA:391:G:H1'	1.82	0.44
12:BL:53:CYS:HB3	12:BL:67:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BS:53:ASN:HD22	19:BS:58:VAL:HG23	1.81	0.44
31:CA:1494:A:H2'	31:CA:1495:A:C8	2.52	0.44
31:CA:1532:A:C8	31:CA:1532:A:H5''	2.51	0.44
31:CA:2141:G:H2'	31:CA:2142:A:C8	2.53	0.44
31:CA:309:A:H4'	49:CV:16:GLY:HA2	1.99	0.44
22:C1:42:HIS:HD2	42:CO:101:GLY:H	1.63	0.44
27:D0:19:LYS:O	27:D0:22:ALA:HB3	2.17	0.44
55:DA:1401:G:H2'	55:DA:1402:U:C6	2.52	0.44
1:AA:1494:G:C8	55:DA:1913:A:C2	3.05	0.44
36:DH:29:PHE:HB2	55:DA:2198:A:C2	2.52	0.44
55:DA:2767:C:H2'	55:DA:2768:U:C6	2.52	0.44
55:DA:466:A:O4'	55:DA:683:U:H4'	2.16	0.44
1:AA:864:A:H4'	5:AE:90:THR:HG23	1.99	0.44
9:AI:6:TYR:HB2	9:AI:21:ILE:HB	1.99	0.44
1:BA:1063:C:H2'	1:BA:1064:G:C8	2.52	0.44
1:BA:591:U:H2'	1:BA:592:G:H8	1.83	0.44
2:BB:207:ILE:HG13	2:BB:207:ILE:H	1.61	0.44
5:BE:13:GLU:CB	5:BE:39:VAL:HG12	2.47	0.44
7:BG:138:ARG:HE	7:BG:138:ARG:HB3	1.62	0.44
31:CA:225:C:H2'	31:CA:226:A:O4'	2.17	0.44
31:CA:2261:C:H1'	31:CA:2388:A:N3	2.32	0.44
31:CA:593:U:H2'	31:CA:594:U:C6	2.53	0.44
31:CA:686:U:H2'	31:CA:788:A:N1	2.32	0.44
28:CB:29:A:H2'	28:CB:30:C:C6	2.53	0.44
55:DA:1171:G:H1'	55:DA:1179:G:N2	2.32	0.44
55:DA:1510:G:H2'	55:DA:1511:G:O4'	2.16	0.44
55:DA:1979:U:OP1	59:DA:3212:PUT:H32	2.17	0.44
55:DA:739:A:H2'	69:DA:7494:HOH:O	2.18	0.44
1:AA:1329:A:H5''	13:AM:26:GLY:H	1.82	0.44
1:BA:1238:A:H5'	1:BA:1336:C:H41	1.82	0.44
6:AF:16:GLU:HB3	4:BD:189:SER:HA	1.98	0.44
13:BM:93:ARG:HH12	19:BS:81:ARG:HH21	1.66	0.44
20:BT:5:LYS:HB3	20:BT:7:ALA:H	1.83	0.44
31:CA:2428:G:H21	40:CM:60:ARG:HD3	1.83	0.44
29:CC:107:PRO:HB3	29:CC:142:HIS:NE2	2.32	0.44
29:CC:271:ARG:HD3	31:CA:1819:A:H2	1.83	0.44
42:CO:8:ARG:HE	42:CO:43:GLU:HG2	1.83	0.44
47:CT:86:MET:HB2	47:CT:96:ILE:HD11	2.00	0.44
55:DA:2184:A:H8	55:DA:2184:A:O5'	2.01	0.44
55:DA:2578:G:OP2	55:DA:2578:G:H4'	2.17	0.44
55:DA:278:A:H2'	55:DA:278:A:N3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D4:4:ILE:HD11	55:DA:592:A:N3	2.33	0.44
36:DH:41:LYS:HA	36:DH:44:ILE:HG12	1.99	0.44
17:AQ:77:ARG:NH2	17:AQ:79:VAL:HG22	2.33	0.44
11:AK:111:THR:HG23	21:AU:3:VAL:HG22	2.00	0.44
1:BA:623:C:H6	1:BA:623:C:O5'	2.01	0.44
11:BK:21:ALA:HB2	11:BK:82:LEU:HD13	1.99	0.44
31:CA:392:U:H2'	31:CA:393:C:C6	2.53	0.44
42:CO:95:THR:HG21	42:CO:113:ILE:HD11	1.99	0.44
43:CP:16:ARG:HD2	43:CP:16:ARG:HA	1.81	0.44
55:DA:128:C:H2'	55:DA:129:C:C6	2.53	0.44
55:DA:757:G:H5''	69:DA:3996:HOH:O	2.18	0.44
55:DA:78:U:H2'	55:DA:79:C:C6	2.53	0.44
55:DA:96:C:H2'	55:DA:97:C:H6	1.83	0.44
34:DF:36:LEU:HB2	34:DF:57:LEU:HD21	1.99	0.44
46:DS:76:LYS:O	46:DS:84:ARG:HA	2.17	0.44
51:DX:39:ARG:HD3	69:DX:117:HOH:O	2.16	0.44
1:AA:123:U:H5''	1:AA:311:C:O2'	2.18	0.44
1:AA:1402:4OC:H2'	1:AA:1403:C:O4'	2.17	0.44
1:AA:212:G:H2'	1:AA:213:G:H8	1.81	0.44
1:AA:946:A:H2'	1:AA:947:G:C8	2.53	0.44
18:AR:52:GLN:HA	18:AR:55:LEU:HD12	1.98	0.44
1:BA:243:A:C2	1:BA:245:U:C2	3.05	0.44
31:CA:128:C:H2'	31:CA:129:C:C6	2.52	0.44
31:CA:1344:U:O2'	31:CA:1384:A:H2'	2.17	0.44
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.52	0.44
31:CA:2014:A:H2'	31:CA:2015:A:C8	2.52	0.44
37:CJ:55:ILE:HD12	37:CJ:74:PRO:HD3	1.99	0.44
40:CM:82:LEU:HD11	40:CM:116:VAL:HG23	1.99	0.44
41:CN:77:PRO:HG2	41:CN:80:VAL:HG21	2.00	0.44
45:DR:40:ILE:HG12	58:DS:203:MPD:H31	2.00	0.44
49:DV:25:VAL:HA	49:DV:36:VAL:HG22	1.98	0.44
5:AE:90:THR:HG22	5:AE:91:GLY:N	2.33	0.44
31:CA:2641:G:H2'	31:CA:2642:G:H8	1.83	0.44
31:CA:96:C:H2'	31:CA:97:C:H6	1.82	0.44
29:CC:145:GLU:HB2	29:CC:188:CYS:HB3	1.99	0.44
50:CW:77:VAL:HG23	50:CW:89:ILE:HG12	2.00	0.44
55:DA:1278:C:H2'	55:DA:1279:G:C8	2.53	0.44
25:D4:19:LYS:HB2	55:DA:651:G:OP1	2.18	0.44
35:DG:17:VAL:HG11	35:DG:50:LEU:HD21	2.00	0.44
40:DM:19:LEU:HD12	55:DA:587:C:O2'	2.18	0.44
1:AA:411:A:P	4:AD:26:ARG:HH12	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:50:LEU:HD22	7:AG:124:LEU:HD13	1.99	0.44
1:BA:532:A:N1	3:BC:193:TYR:HB3	2.33	0.44
1:BA:935:A:H2'	1:BA:936:C:C6	2.53	0.44
1:BA:522:C:H41	12:BL:50:ARG:NH2	2.15	0.44
31:CA:278:A:N3	31:CA:278:A:H2'	2.33	0.44
31:CA:576:U:H2'	31:CA:577:G:C8	2.52	0.44
31:CA:78:U:H2'	31:CA:79:C:C6	2.53	0.44
30:CD:104:VAL:HG23	30:CD:177:VAL:HG21	2.00	0.44
55:DA:1442:U:H2'	55:DA:1443:U:C6	2.52	0.44
55:DA:1965:C:OP1	55:DA:1966:A:C2'	2.66	0.44
55:DA:2607:G:H2'	55:DA:2608:G:O4'	2.17	0.44
55:DA:2681:C:C2	55:DA:2724:U:O4	2.71	0.44
47:DT:6:LYS:HA	47:DT:103:ILE:O	2.18	0.44
48:DU:15:HIS:HB3	48:DU:31:VAL:HG12	2.00	0.44
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.83	0.44
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.81	0.44
1:BA:407:U:H2'	1:BA:408:A:H8	1.83	0.44
18:BR:20:GLU:HA	18:BR:55:LEU:HD23	2.00	0.44
22:C1:2:ALA:N	31:CA:2577:A:H2	2.16	0.44
31:CA:1401:G:H2'	31:CA:1402:U:C6	2.53	0.44
28:CB:89:U:C6	31:CA:958:U:H2'	2.53	0.44
43:CP:31:THR:HG22	43:CP:33:ARG:H	1.83	0.44
48:CU:15:HIS:HB3	48:CU:31:VAL:HG12	1.99	0.44
48:CU:58:VAL:HG22	48:CU:85:VAL:HG22	1.98	0.44
33:DE:23:PHE:HE2	33:DE:25:GLU:HG3	1.82	0.44
54:DI:50:VAL:CG1	54:DI:92:ALA:HB2	2.48	0.44
41:DN:34:LYS:HE3	41:DN:131:VAL:HG11	1.98	0.44
51:DX:47:ALA:HB1	51:DX:51:VAL:O	2.17	0.44
51:DX:59:LEU:HD12	51:DX:80:ILE:HD12	1.99	0.44
1:AA:1486:G:H2'	1:AA:1487:G:O4'	2.18	0.44
6:AF:93:LYS:HE2	6:AF:93:LYS:H	1.82	0.44
10:AJ:46:LYS:HG2	10:AJ:68:ARG:HG2	1.99	0.44
12:AL:5:ASN:O	12:AL:9:ARG:HD2	2.18	0.44
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	2.00	0.44
17:BQ:9:GLN:O	17:BQ:25:ILE:HG23	2.18	0.44
23:C2:39:PHE:HB2	23:C2:46:HIS:CE1	2.53	0.44
1:BA:1517:G:H1'	31:CA:1919:A:O3'	2.17	0.44
31:CA:571:U:H1'	31:CA:573:U:H6	1.82	0.44
36:CH:21:VAL:HG21	36:CH:25:TYR:HD2	1.82	0.44
55:DA:2849:U:N3	55:DA:2867:G:O4'	2.50	0.44
55:DA:577:G:H1'	69:DA:3571:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DI:120:ALA:HA	54:DI:123:ILE:HD11	2.00	0.44
37:DJ:19:ASN:N	37:DJ:20:PRO:HD2	2.33	0.44
37:DJ:55:ILE:HD12	37:DJ:74:PRO:HD3	1.99	0.44
42:DO:8:ARG:HE	42:DO:43:GLU:HG2	1.83	0.44
1:BA:235:C:H2'	1:BA:236:A:C8	2.53	0.43
1:BA:946:A:H2'	1:BA:947:G:C8	2.53	0.43
6:BF:38:ARG:HH12	6:BF:99:ALA:HB3	1.82	0.43
7:BG:116:MET:HA	7:BG:119:ARG:HB2	2.00	0.43
10:BJ:46:LYS:HG2	10:BJ:68:ARG:HG2	1.99	0.43
31:CA:1024:G:H3'	31:CA:1025:G:H2'	1.99	0.43
31:CA:12:U:O2	31:CA:12:U:H2'	2.17	0.43
31:CA:1791:A:N6	31:CA:1828:G:O2'	2.51	0.43
30:CD:118:PHE:HZ	31:CA:2048:G:H21	1.66	0.43
47:CT:6:LYS:HG2	47:CT:104:THR:HG23	2.00	0.43
55:DA:320:A:H4'	55:DA:322:A:C8	2.53	0.43
55:DA:492:A:H2'	55:DA:493:G:O4'	2.18	0.43
55:DA:729:G:H2'	55:DA:1775:U:H1'	2.00	0.43
55:DA:739:A:H1'	55:DA:740:C:H5	1.83	0.43
34:DF:14:LYS:O	34:DF:18:THR:HG22	2.18	0.43
44:DQ:113:ARG:HG2	44:DQ:115:ASN:HD21	1.83	0.43
1:AA:490:C:H2'	1:AA:491:G:C8	2.52	0.43
5:AE:13:GLU:CB	5:AE:39:VAL:HG12	2.47	0.43
21:AU:11:PRO:HG2	21:AU:14:VAL:HB	1.99	0.43
1:BA:363:A:H2'	1:BA:364:A:O4'	2.18	0.43
1:BA:604:G:H2'	1:BA:605:U:O4'	2.18	0.43
12:BL:90:LEU:HD23	12:BL:93:VAL:HG21	2.00	0.43
27:C0:46:GLY:HA3	31:CA:851:C:O2'	2.19	0.43
31:CA:2006:C:H2'	31:CA:2007:U:C6	2.53	0.43
31:CA:2582:G:C2	31:CA:2583:G:C8	3.06	0.43
31:CA:727:A:H2'	31:CA:728:G:C8	2.53	0.43
55:DA:521:U:H2'	55:DA:522:A:C8	2.53	0.43
33:DE:145:ASP:HA	33:DE:166:LYS:HB3	2.01	0.43
50:DW:77:VAL:HG23	50:DW:89:ILE:HG12	2.01	0.43
1:AA:756:C:H2'	1:AA:757:U:O4'	2.19	0.43
9:AI:84:THR:HG21	9:AI:103:PHE:CB	2.47	0.43
1:BA:994:A:N1	1:BA:1047:G:H4'	2.33	0.43
20:BT:22:ALA:O	20:BT:26:SER:HB2	2.18	0.43
31:CA:1280:G:H1	31:CA:1290:C:H42	1.67	0.43
31:CA:197:A:C2	31:CA:2434:A:N6	2.84	0.43
31:CA:2771:C:H2'	31:CA:2772:C:H6	1.83	0.43
33:CE:108:ILE:HG21	33:CE:181:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:CO:29:VAL:HG13	42:CO:83:LEU:HD11	2.00	0.43
44:CQ:113:ARG:HG2	44:CQ:115:ASN:HD21	1.82	0.43
49:CV:72:ILE:H	49:CV:72:ILE:HG13	1.64	0.43
27:D0:24:LEU:HD11	27:D0:54:MET:CE	2.48	0.43
55:DA:1354:A:H2'	55:DA:1355:G:O4'	2.18	0.43
55:DA:1485:U:H2'	55:DA:1486:U:C6	2.53	0.43
55:DA:2123:G:H2'	55:DA:2124:G:H8	1.82	0.43
32:DD:119:ALA:HB3	32:DD:165:MET:HB2	1.99	0.43
36:DH:116:ARG:HH21	36:DH:133:GLN:HB2	1.83	0.43
1:AA:729:A:H2'	1:AA:730:G:O4'	2.17	0.43
1:AA:855:U:H2'	1:AA:856:C:C6	2.53	0.43
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	2.00	0.43
1:BA:1478:U:H2'	1:BA:1479:C:C6	2.54	0.43
1:BA:167:A:H2'	1:BA:168:G:O4'	2.18	0.43
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.82	0.43
22:C1:19:HIS:CE1	31:CA:2624:G:H1'	2.53	0.43
31:CA:1826:G:C6	31:CA:1827:U:C4	3.06	0.43
31:CA:2840:C:H5''	42:CO:53:THR:HG21	1.99	0.43
31:CA:609:A:H2'	31:CA:610:C:O4'	2.19	0.43
29:CC:208:ALA:HB2	31:CA:1790:C:O2'	2.19	0.43
34:CF:61:SER:HB2	34:CF:91:LEU:HD21	2.00	0.43
36:CH:41:LYS:HA	36:CH:44:ILE:HG12	2.00	0.43
38:CK:7:LYS:O	38:CK:11:VAL:HG23	2.19	0.43
31:CA:492:A:H2	47:CT:7:HIS:NE2	2.16	0.43
55:DA:2101:A:H2'	55:DA:2102:G:H8	1.83	0.43
35:DG:155:GLU:HG2	35:DG:157:TYR:H	1.84	0.43
43:DP:30:ARG:HG3	43:DP:35:ILE:HD12	2.00	0.43
47:DT:6:LYS:HG2	47:DT:104:THR:HG23	2.00	0.43
1:AA:1478:U:H2'	1:AA:1479:C:C6	2.53	0.43
1:AA:682:G:H2'	1:AA:683:G:H8	1.83	0.43
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	2.01	0.43
3:AC:180:ALA:HA	3:AC:206:GLU:HA	2.01	0.43
8:AH:64:LYS:HB3	8:AH:71:VAL:HG21	2.01	0.43
12:AL:33:VAL:HG22	12:AL:79:VAL:HG22	2.00	0.43
1:BA:1417:G:C6	1:BA:1482:G:C6	3.07	0.43
13:BM:23:TYR:HB3	13:BM:66:GLU:HA	2.00	0.43
31:CA:1274:A:N3	31:CA:1297:C:H1'	2.33	0.43
31:CA:1447:C:H2'	31:CA:1448:G:H8	1.84	0.43
31:CA:521:U:H2'	31:CA:522:A:C8	2.53	0.43
31:CA:56:A:H61	31:CA:114:U:H3	1.66	0.43
35:CG:17:VAL:HG11	35:CG:50:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:CN:41:LEU:HD21	41:CN:124:LEU:HD22	2.01	0.43
47:CT:17:VAL:HA	47:CT:43:ALA:HB1	2.00	0.43
47:CT:62:ASP:HB3	47:CT:63:GLY:H	1.73	0.43
47:CT:95:ARG:CZ	47:CT:97:LEU:HD21	2.49	0.43
55:DA:861:A:C2	55:DA:917:A:C4	3.06	0.43
34:DF:40:VAL:HG23	34:DF:86:GLY:HA2	2.00	0.43
1:AA:1500:A:H5''	1:AA:1508:A:H5''	2.01	0.43
4:AD:102:VAL:HG13	4:AD:107:PHE:HB2	2.00	0.43
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	2.01	0.43
8:AH:76:GLN:O	8:AH:127:CYS:HB2	2.19	0.43
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.99	0.43
12:AL:80:ILE:HG22	12:AL:104:CYS:HB2	2.00	0.43
1:BA:9:G:OP2	5:BE:126:LYS:HE2	2.19	0.43
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.99	0.43
6:BF:3:HIS:CD2	6:BF:92:THR:HG23	2.53	0.43
24:C3:10:LEU:O	24:C3:14:ARG:HB2	2.18	0.43
31:CA:2027:G:C6	31:CA:2028:U:C4	3.07	0.43
31:CA:2781:A:H5''	31:CA:2782:G:H5'	2.01	0.43
31:CA:685:A:H1'	31:CA:688:U:O4	2.18	0.43
30:CD:172:VAL:HG12	30:CD:175:LEU:HD21	2.01	0.43
47:CT:6:LYS:HA	47:CT:103:ILE:O	2.18	0.43
22:D1:40:ARG:HH22	55:DA:2884[B]:U:H2'	1.84	0.43
55:DA:738:G:C6	55:DA:739:A:C6	3.07	0.43
32:DD:105:LYS:HD3	32:DD:106:LYS:HG3	1.99	0.43
52:DY:10:LYS:HD3	55:DA:397:U:OP2	2.19	0.43
1:AA:994:A:N1	1:AA:1047:G:H4'	2.34	0.43
1:AA:1373:G:C5'	7:AG:36:LYS:HB2	2.48	0.43
20:AT:31:PHE:HA	20:AT:34:LYS:HD2	2.00	0.43
1:BA:1486:G:H2'	1:BA:1487:G:O4'	2.17	0.43
1:BA:601:G:H2'	1:BA:602:A:H8	1.84	0.43
4:BD:105:MET:HE2	4:BD:171:LEU:HD22	2.01	0.43
9:BI:6:TYR:HB2	9:BI:21:ILE:HB	1.99	0.43
15:BO:64:ARG:HH22	15:BO:88:ARG:NH2	2.17	0.43
31:CA:1484:U:H2'	31:CA:1485:U:C6	2.54	0.43
31:CA:1485:U:H2'	31:CA:1486:U:C6	2.53	0.43
31:CA:184:C:H2'	31:CA:185:G:C8	2.54	0.43
31:CA:2179:C:H2'	31:CA:2180:U:C6	2.53	0.43
31:CA:2607:G:H2'	31:CA:2608:G:O4'	2.18	0.43
31:CA:2636:C:H2'	31:CA:2637:U:H6	1.82	0.43
31:CA:357:C:H2'	31:CA:358:U:C6	2.54	0.43
25:C4:2:PRO:N	31:CA:591:U:H1'	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:21:ASN:HB3	29:CC:24:LEU:HG	2.00	0.43
55:DA:1759:A:H4'	55:DA:2715:C:O4'	2.18	0.43
55:DA:307:G:N2	55:DA:309:A:H3'	2.33	0.43
55:DA:831:G:C6	55:DA:832:U:C4	3.07	0.43
46:DS:53:PHE:HB3	69:DS:301:HOH:O	2.18	0.43
1:AA:1387:G:H2'	1:AA:1388:C:C6	2.53	0.43
1:AA:363:A:H2'	1:AA:364:A:O4'	2.18	0.43
1:AA:409:U:H2'	1:AA:410:G:O4'	2.19	0.43
1:AA:601:G:H2'	1:AA:602:A:H8	1.84	0.43
1:AA:865:A:H8	1:AA:865:A:O5'	2.02	0.43
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	2.01	0.43
1:AA:502:A:OP1	12:AL:115:SER:HB2	2.19	0.43
1:BA:855:U:H2'	1:BA:856:C:C6	2.54	0.43
1:BA:864:A:H4'	5:BE:90:THR:HG23	2.00	0.43
31:CA:1170:C:H42	31:CA:1178:C:N4	2.16	0.43
31:CA:1231:U:H2'	31:CA:1232:G:H8	1.83	0.43
31:CA:1442:U:H2'	31:CA:1443:U:C6	2.53	0.43
31:CA:1939:5MU:H3'	69:CA:3666:HOH:O	2.17	0.43
31:CA:2024:G:C4	31:CA:2040:G:N2	2.87	0.43
38:CK:89:PHE:CE2	38:CK:100:VAL:HG11	2.54	0.43
43:CP:30:ARG:HG3	43:CP:35:ILE:HD12	2.00	0.43
55:DA:357:C:H2'	55:DA:358:U:C6	2.54	0.43
33:DE:72:SER:HB2	69:DE:449:HOH:O	2.19	0.43
36:DH:57:LYS:HA	36:DH:60:GLU:HG2	2.00	0.43
40:DM:109:LYS:HA	40:DM:126:ARG:O	2.18	0.43
45:DR:51:ARG:HH22	55:DA:993:G:P	2.42	0.43
46:DS:45:GLU:HG3	46:DS:46:GLU:OE2	2.18	0.43
1:AA:591:U:H2'	1:AA:592:G:H8	1.84	0.43
1:AA:59:A:H5''	1:AA:387:U:H5''	2.00	0.43
1:AA:81:A:H2	1:AA:88:U:H3	1.66	0.43
1:BA:409:U:H2'	1:BA:410:G:O4'	2.19	0.43
9:BI:51:PRO:HB3	9:BI:84:THR:HG23	2.00	0.43
31:CA:2185:U:H2'	31:CA:2186:G:C8	2.53	0.43
31:CA:825:A:H2'	31:CA:826:U:O4'	2.19	0.43
30:CD:157:LYS:CG	31:CA:2619:C:H5''	2.48	0.43
33:CE:145:ASP:HA	33:CE:166:LYS:HB3	2.01	0.43
40:CM:21:ARG:HA	40:CM:21:ARG:HD3	1.77	0.43
53:CZ:21:LEU:HB3	53:CZ:50:VAL:HG22	2.01	0.43
55:DA:1484:U:H2'	55:DA:1485:U:C6	2.54	0.43
55:DA:2243:U:O2	55:DA:2434:A:C2	2.72	0.43
55:DA:834:G:H2'	55:DA:835:C:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DC:233:GLY:HA3	69:DC:347:HOH:O	2.19	0.43
1:AA:49:U:O2	1:AA:362:G:H1'	2.19	0.43
1:AA:935:A:H2'	1:AA:936:C:C6	2.54	0.43
20:AT:36:TYR:CE2	20:AT:79:LEU:HD21	2.54	0.43
1:BA:214:C:H2'	1:BA:215:C:H6	1.83	0.43
1:BA:299:G:H2'	1:BA:300:A:C8	2.54	0.43
8:BH:22:LYS:O	8:BH:63:LEU:HD12	2.19	0.43
15:BO:26:GLU:HG3	15:BO:81:LEU:HD22	2.01	0.43
15:BO:78:TYR:HE1	15:BO:88:ARG:HH21	1.67	0.43
20:BT:67:ILE:O	20:BT:68:HIS:HB2	2.19	0.43
29:CC:18:LYS:HE3	31:CA:1565:C:H5'	2.01	0.43
31:CA:2123:G:O5'	31:CA:2123:G:H8	2.02	0.43
31:CA:2747:G:O6	31:CA:2755:C:H5''	2.18	0.43
34:CF:40:VAL:HG23	34:CF:86:GLY:HA2	1.99	0.43
55:DA:1001:A:O5'	55:DA:1001:A:H8	2.01	0.43
55:DA:1093:G:H1'	55:DA:1099:G:N2	2.34	0.43
55:DA:1494:A:H2'	55:DA:1495:A:C8	2.53	0.43
41:DN:18[B]:ARG:HG3	28:DB:90:C:C5'	2.49	0.43
53:DZ:18:LEU:HB2	53:DZ:53:VAL:HG11	2.01	0.43
13:AM:23:TYR:HB3	13:AM:66:GLU:HA	2.00	0.42
4:BD:102:VAL:HG13	4:BD:107:PHE:HB2	2.00	0.42
30:CD:104:VAL:CG2	30:CD:177:VAL:HG21	2.48	0.42
36:CH:48:GLU:HA	36:CH:51:ARG:HB3	2.00	0.42
55:DA:184:C:H2'	55:DA:185:G:C8	2.54	0.42
29:DC:145:GLU:HB2	29:DC:188:CYS:HB3	2.00	0.42
29:DC:35:GLU:HG3	29:DC:64:ILE:HD11	2.00	0.42
33:DE:28:VAL:O	33:DE:32:VAL:HG23	2.19	0.42
41:DN:121:ALA:HA	41:DN:124:LEU:HD12	2.01	0.42
1:AA:604:G:H2'	1:AA:605:U:O4'	2.18	0.42
1:BA:8:A:C6	4:BD:206:LYS:HB3	2.54	0.42
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	2.01	0.42
3:BC:47:LEU:HD22	3:BC:76:VAL:HG22	2.01	0.42
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	2.00	0.42
31:CA:935:C:H2'	31:CA:936:A:C8	2.54	0.42
31:CA:95:A:H4'	53:CZ:38:GLN:O	2.19	0.42
27:C0:12:SER:HB3	31:CA:988:A:P	2.59	0.42
24:D3:10:LEU:O	24:D3:14:ARG:HB2	2.19	0.42
25:D4:39:LYS:HB3	69:D4:133:HOH:O	2.18	0.42
55:DA:1183:U:H2'	55:DA:1184:U:C6	2.54	0.42
55:DA:1847:A:O5'	55:DA:1847:A:H8	2.01	0.42
55:DA:2609:U:H5	62:DA:3194:EDO:H12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2747:G:O6	55:DA:2755:C:H5''	2.19	0.42
55:DA:2848:G:H1'	55:DA:2867:G:N2	2.33	0.42
55:DA:720:U:H2'	55:DA:721:A:C8	2.55	0.42
34:DF:118:SER:OG	34:DF:120:LYS:HG3	2.19	0.42
34:DF:131:GLY:HA3	55:DA:2305:U:H5''	2.01	0.42
1:AA:1293:C:H2'	1:AA:1294:G:C8	2.54	0.42
19:AS:64:ASP:HB3	34:DF:115:ARG:HH21	1.83	0.42
1:BA:1387:G:H2'	1:BA:1388:C:C6	2.54	0.42
26:C5:17:VAL:HG11	26:C5:26:ILE:HD12	2.01	0.42
31:CA:1562:U:H2'	31:CA:1563:U:O4'	2.19	0.42
31:CA:1825:U:H6	31:CA:1825:U:O5'	2.02	0.42
31:CA:459:U:H2'	31:CA:460:A:C8	2.50	0.42
31:CA:540:C:H2'	31:CA:541:A:H8	1.84	0.42
31:CA:622:G:H2'	31:CA:623:C:C6	2.54	0.42
31:CA:720:U:H2'	31:CA:721:A:C8	2.54	0.42
30:CD:101:PHE:HA	30:CD:104:VAL:HG13	2.01	0.42
55:DA:2133:G:H2'	55:DA:2157:G:H22	1.83	0.42
55:DA:2105:U:O4	55:DA:2184:A:C2	2.71	0.42
55:DA:2621:G:H5''	69:DA:4246:HOH:O	2.19	0.42
55:DA:2721:A:H2'	55:DA:2722:G:O4'	2.18	0.42
55:DA:2852:G:H4'	69:DA:5849:HOH:O	2.19	0.42
52:DY:66:THR:O	52:DY:69:ALA:HB3	2.19	0.42
7:AG:56:LYS:HB3	7:AG:57:SER:H	1.63	0.42
1:BA:1293:C:H2'	1:BA:1294:G:C8	2.55	0.42
1:BA:1373:G:C5'	7:BG:36:LYS:HB2	2.49	0.42
1:BA:631:C:H6	1:BA:631:C:O5'	2.02	0.42
1:BA:756:C:H2'	1:BA:757:U:O4'	2.19	0.42
22:C1:8:PRO:HG2	31:CA:1264:A:H5'	2.01	0.42
31:CA:70:G:H5''	31:CA:112:U:O2	2.19	0.42
31:CA:2282:G:OP1	31:CA:2283:C:H1'	2.19	0.42
31:CA:2341:G:H2'	31:CA:2342:C:O4'	2.19	0.42
31:CA:328:U:O3'	49:CV:66:GLN:HG3	2.18	0.42
31:CA:39:G:H2'	31:CA:40:U:C6	2.54	0.42
28:CB:90:C:H5'	41:CN:18:ARG:HA	2.02	0.42
46:CS:24:LYS:HA	46:CS:94:THR:OG1	2.20	0.42
52:CY:51:VAL:HG22	52:CY:52:SER:O	2.18	0.42
55:DA:1231:U:H2'	55:DA:1232:G:H8	1.84	0.42
55:DA:1976:U:H1'	63:DA:3225:PGE:H2	2.01	0.42
55:DA:2741:A:H2'	55:DA:2742:G:O4'	2.19	0.42
55:DA:2845:U:H2'	55:DA:2846:G:O4'	2.20	0.42
35:DG:145:ALA:HB1	35:DG:164:TYR:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DI:65:GLU:HA	54:DI:70:GLU:HG3	2.00	0.42
38:DK:3:THR:HA	69:DR:307:HOH:O	2.19	0.42
46:DS:73:LYS:HZ2	58:DS:203:MPD:C5	2.28	0.42
1:AA:21:G:H2'	1:AA:22:G:C8	2.54	0.42
1:BA:1491:G:H2'	1:BA:1492:A:C8	2.55	0.42
10:BJ:29:ALA:HB2	10:BJ:87:LEU:HD11	2.02	0.42
31:CA:1677:A:C8	31:CA:1677:A:H5''	2.55	0.42
31:CA:2494:G:O3'	41:CN:79:ALA:HA	2.18	0.42
31:CA:608:A:H2'	31:CA:609:A:C8	2.54	0.42
31:CA:740:C:H5'	31:CA:1784:A:H3'	2.02	0.42
55:DA:1446:C:H2'	55:DA:1447:C:C6	2.54	0.42
55:DA:2064:C:H2'	55:DA:2065:C:C6	2.55	0.42
55:DA:2341:G:H2'	55:DA:2342:C:O4'	2.20	0.42
55:DA:2636:C:H2'	55:DA:2637:U:H6	1.82	0.42
55:DA:609:A:H2'	55:DA:610:C:O4'	2.20	0.42
32:DD:143:PRO:HA	69:DD:410:HOH:O	2.20	0.42
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	2.01	0.42
1:BA:682:G:H2'	1:BA:683:G:H8	1.84	0.42
5:BE:47:GLY:HA3	5:BE:71:MET:HG2	2.01	0.42
31:CA:2520:C:H2'	31:CA:2521:C:C6	2.55	0.42
31:CA:2569:G:H5''	31:CA:2569:G:C8	2.55	0.42
31:CA:2641:G:H2'	31:CA:2642:G:C8	2.55	0.42
31:CA:396:G:H1'	52:CY:29:PHE:HD2	1.83	0.42
31:CA:374:A:C2	31:CA:401:A:C4	3.08	0.42
31:CA:740:C:H42	31:CA:757:G:H1	1.66	0.42
31:CA:998:C:OP2	45:CR:58:ARG:NH2	2.52	0.42
33:CE:126:VAL:HG23	33:CE:133:LEU:HB3	1.98	0.42
37:CJ:37:GLU:HB3	37:CJ:67:PHE:HZ	1.84	0.42
50:CW:31:TYR:O	50:CW:92:VAL:HA	2.20	0.42
51:CX:47:ALA:HB1	51:CX:51:VAL:O	2.19	0.42
55:DA:1028:A:H61	55:DA:1125:G:H2'	1.81	0.42
55:DA:1604:C:H5'	69:DA:3982:HOH:O	2.18	0.42
55:DA:348:A:H2'	55:DA:349:U:O4'	2.20	0.42
40:DM:36:LYS:HB3	69:DA:4844:HOH:O	2.20	0.42
41:DN:42:THR:HG22	41:DN:93:VAL:HG12	2.02	0.42
53:DZ:21:LEU:HB3	53:DZ:50:VAL:HG22	2.01	0.42
1:AA:486:U:H2'	1:AA:487:A:H8	1.85	0.42
7:AG:116:MET:HA	7:AG:119:ARG:HB2	2.00	0.42
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	2.01	0.42
1:BA:1508:A:H2'	1:BA:1509:C:O4'	2.19	0.42
1:BA:322:C:H41	1:BA:328:C:H6	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:211:THR:HA	2:BB:214:LEU:HB2	2.01	0.42
3:BC:180:ALA:HA	3:BC:206:GLU:HA	2.01	0.42
11:BK:31:ILE:HA	11:BK:46:THR:HG22	2.02	0.42
31:CA:1093:G:H1'	31:CA:1099:G:H22	1.84	0.42
31:CA:1635:A:H2'	31:CA:1636:U:O4'	2.19	0.42
35:CG:145:ALA:HB1	35:CG:164:TYR:HE1	1.85	0.42
49:CV:14:LEU:HD11	49:CV:71:ALA:HB2	2.01	0.42
32:DD:145:SER:O	55:DA:2512:C:H1'	2.19	0.42
55:DA:2824:C:C4	55:DA:2825:G:C5	3.07	0.42
55:DA:28:A:H1'	55:DA:513:A:C2	2.55	0.42
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	2.01	0.42
19:AS:11:ILE:HG12	19:AS:16:LEU:HD13	2.02	0.42
20:BT:35:VAL:HG21	20:BT:54:MET:HG2	2.01	0.42
11:BK:123:PRO:HD2	21:BU:38:TYR:HB2	2.01	0.42
31:CA:2207:C:H2'	31:CA:2208:C:C6	2.55	0.42
31:CA:300:A:H1'	31:CA:319:G:H1'	2.02	0.42
31:CA:19:A:O2'	31:CA:553:G:H4'	2.19	0.42
31:CA:668:A:H2'	31:CA:670:A:H62	1.85	0.42
34:CF:29:PRO:HB2	34:CF:169:LEU:HD22	2.02	0.42
48:CU:45:ALA:O	48:CU:49:LYS:HG2	2.19	0.42
55:DA:1313:U:O2	55:DA:1313:U:H2'	2.19	0.42
55:DA:1446:C:O5'	55:DA:1446:C:H6	2.02	0.42
28:DB:29:A:H2'	28:DB:30:C:C6	2.54	0.42
32:DD:146:ILE:HD12	32:DD:155:VAL:CG2	2.50	0.42
1:AA:299:G:H2'	1:AA:300:A:C8	2.54	0.42
10:AJ:29:ALA:HB2	10:AJ:87:LEU:HD11	2.02	0.42
20:AT:28:MET:HG2	20:AT:32:ILE:HD11	2.02	0.42
1:BA:1426:G:H2'	1:BA:1427:C:O4'	2.20	0.42
1:BA:413:G:H1'	1:BA:428:G:H21	1.84	0.42
1:BA:580:C:H2'	1:BA:581:G:O4'	2.19	0.42
8:BH:105:SER:HB2	8:BH:126:ILE:HD11	2.02	0.42
31:CA:1376:C:H2'	31:CA:1377:G:O4'	2.20	0.42
31:CA:573:U:N3	31:CA:2030:6MZ:H3'	2.34	0.42
31:CA:956:G:H5''	41:CN:76:LYS:HG3	2.02	0.42
48:CU:54:GLU:HB3	48:CU:88:LYS:HD2	2.02	0.42
32:DD:133:THR:HG21	55:DA:1676:A:H1'	2.02	0.42
55:DA:2813:A:H2	55:DA:2887[A]:A:N1	2.18	0.42
55:DA:2887[A]:A:H2'	55:DA:2888[A]:C:H6	1.85	0.42
55:DA:593:U:H2'	55:DA:594:U:C6	2.55	0.42
55:DA:686:U:H2'	55:DA:788:A:N1	2.34	0.42
29:DC:107:PRO:HB3	29:DC:142:HIS:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DH:21:VAL:HG21	36:DH:25:TYR:HD2	1.85	0.42
38:DK:114:LEU:O	38:DK:117:ALA:HB3	2.19	0.42
41:DN:5:LYS:HE2	69:DA:6106:HOH:O	2.20	0.42
46:DS:3:ALA:HB3	46:DS:101:ILE:HD12	2.02	0.42
46:DS:24:LYS:HA	46:DS:94:THR:OG1	2.19	0.42
48:DU:3:ARG:HD3	48:DU:5:GLU:H	1.85	0.42
50:DW:31:TYR:O	50:DW:92:VAL:HA	2.20	0.42
1:AA:227:G:H2'	1:AA:228:A:O4'	2.20	0.42
9:AI:51:PRO:HB3	9:AI:84:THR:HG23	2.00	0.42
1:BA:131:A:H2'	1:BA:132:C:C6	2.54	0.42
1:BA:382:A:H2'	1:BA:383:A:C8	2.54	0.42
20:BT:31:PHE:HA	20:BT:34:LYS:HD2	2.01	0.42
22:C1:6:ASN:ND2	31:CA:2020:A:H62	2.18	0.42
31:CA:1847:A:H8	31:CA:1847:A:O5'	2.03	0.42
22:C1:2:ALA:N	31:CA:2577:A:C2	2.88	0.42
31:CA:745:1MG:O2'	31:CA:748:G:H1'	2.19	0.42
38:CK:114:LEU:O	38:CK:117:ALA:HB3	2.20	0.42
45:CR:83:LEU:HB3	45:CR:88:VAL:HB	2.01	0.42
55:DA:121:G:H2'	55:DA:122:G:H8	1.85	0.42
55:DA:2706:A:O5'	55:DA:2706:A:H8	2.03	0.42
32:DD:172:VAL:HG12	32:DD:175:LEU:HD21	2.01	0.42
41:DN:57:VAL:HA	41:DN:112:LEU:HD21	2.02	0.42
45:DR:92:ARG:HB2	55:DA:997:G:OP1	2.20	0.42
20:AT:22:ALA:O	20:AT:26:SER:HB2	2.20	0.41
20:AT:43:ASP:HB3	20:AT:46:ALA:HB3	2.01	0.41
1:BA:374:A:OP1	1:BA:452:A:N1	2.53	0.41
1:BA:517:G:O2'	1:BA:530:G:H4'	2.20	0.41
1:BA:827:U:H2'	1:BA:870:U:O4	2.19	0.41
6:BF:38:ARG:NH1	6:BF:99:ALA:HB3	2.35	0.41
12:BL:33:VAL:HG22	12:BL:79:VAL:HG22	2.02	0.41
25:C4:57:LEU:HD11	31:CA:834:G:H5'	2.02	0.41
29:CC:35:GLU:HG3	29:CC:64:ILE:HD11	2.02	0.41
30:CD:141:ARG:HB2	31:CA:1656:C:H5''	2.02	0.41
46:CS:3:ALA:HB3	46:CS:101:ILE:HD12	2.02	0.41
22:D1:12:LYS:HD2	22:D1:12:LYS:HA	1.72	0.41
23:D2:39:PHE:HB2	23:D2:46:HIS:CE1	2.55	0.41
55:DA:2243:U:O2	55:DA:2434:A:H2	2.02	0.41
55:DA:39:G:H2'	55:DA:40:U:C6	2.55	0.41
55:DA:543:G:H5''	55:DA:543:G:H8	1.85	0.41
37:DJ:37:GLU:HB3	37:DJ:67:PHE:HZ	1.84	0.41
45:DR:13:ARG:HD2	69:DA:3914:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:116:MET:O	7:AG:120:LEU:HB2	2.19	0.41
2:BB:90:PHE:HB3	2:BB:151:ILE:HG22	2.02	0.41
5:BE:15:LEU:HD11	5:BE:18:VAL:HG23	2.02	0.41
22:C1:53:LYS:HE3	22:C1:56:ALA:HA	2.02	0.41
31:CA:2544:G:H5'	31:CA:2645:G:C2	2.55	0.41
31:CA:787:C:H3'	31:CA:791:C:H41	1.85	0.41
40:CM:109:LYS:HA	40:CM:126:ARG:O	2.20	0.41
33:DE:66:GLY:HA2	55:DA:2060:A:OP2	2.20	0.41
55:DA:2740:A:C6	55:DA:2764:A:C8	3.08	0.41
55:DA:612:G:H2'	55:DA:614:A:C8	2.55	0.41
38:DK:118:MET:HA	38:DK:121:LYS:NZ	2.35	0.41
1:AA:1426:G:H2'	1:AA:1427:C:O4'	2.20	0.41
1:AA:1533:C:H5'	1:AA:1534:A:OP1	2.20	0.41
17:AQ:21:ILE:HD12	17:AQ:23:VAL:CG2	2.50	0.41
9:BI:46:MET:HA	9:BI:49:ARG:HD2	2.02	0.41
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	2.02	0.41
3:BC:33:LEU:HD21	14:BN:93:ILE:HG12	2.02	0.41
31:CA:1190:G:H5''	40:CM:32:GLY:HA2	2.02	0.41
31:CA:1259:G:H2'	31:CA:1260:A:C8	2.55	0.41
31:CA:1638:C:H5''	31:CA:2710:C:O2'	2.19	0.41
30:CD:133:THR:CG2	31:CA:1993:U:H4'	2.39	0.41
31:CA:2428:G:N2	40:CM:60:ARG:NH2	2.58	0.41
31:CA:2198:A:C2	36:CH:29:PHE:HB2	2.55	0.41
52:CY:66:THR:O	52:CY:69:ALA:HB3	2.20	0.41
22:D1:27:SER:HA	69:DA:4108:HOH:O	2.20	0.41
55:DA:1450:G:C6	55:DA:1451:C:N4	2.88	0.41
55:DA:1562:U:H2'	55:DA:1563:U:O4'	2.20	0.41
55:DA:179:C:H2'	55:DA:180:G:O4'	2.21	0.41
55:DA:2005:A:H5''	69:DA:4377:HOH:O	2.20	0.41
55:DA:565:C:H2'	55:DA:566:U:O4'	2.20	0.41
54:DI:29:ASP:HB3	54:DI:106:PHE:HB2	2.00	0.41
1:AA:636:U:H2'	1:AA:637:C:C6	2.55	0.41
8:AH:41:LYS:HD2	8:AH:48:ASP:HA	2.02	0.41
1:BA:1062:U:H2'	1:BA:1063:C:C6	2.55	0.41
1:BA:1190:G:H5'	3:BC:176:HIS:CE1	2.55	0.41
35:CG:155:GLU:HG2	35:CG:157:TYR:H	1.85	0.41
31:CA:2849:U:P	44:CQ:93:ARG:HH21	2.43	0.41
49:CV:11:VAL:HG12	49:CV:72:ILE:HA	2.01	0.41
55:DA:1482:G:H1'	55:DA:1509:A:H61	1.85	0.41
55:DA:1554:U:H1'	59:DA:3219:PUT:H32	2.03	0.41
55:DA:198:C:O5'	55:DA:198:C:H6	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:DX:62:LYS:HE3	55:DA:2366:A:H4'	2.01	0.41
55:DA:2822:G:H2'	55:DA:2823:A:H5''	2.03	0.41
55:DA:300:A:H1'	55:DA:319:G:H1'	2.02	0.41
32:DD:38:LYS:O	32:DD:46:ARG:HA	2.20	0.41
54:DI:91:ALA:O	54:DI:95:LEU:HB2	2.20	0.41
45:DR:83:LEU:HB3	45:DR:88:VAL:HB	2.01	0.41
51:DX:39:ARG:HA	69:DX:110:HOH:O	2.19	0.41
1:AA:1017:U:H2'	1:AA:1018:G:H8	1.86	0.41
1:AA:1417:G:C6	1:AA:1482:G:C6	3.08	0.41
1:AA:262:A:H5'	20:AT:68:HIS:HB3	2.03	0.41
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.53	0.41
8:BH:38:ASN:O	8:BH:42:GLU:HG3	2.21	0.41
31:CA:1:G:H1	31:CA:2902:C:H42	1.68	0.41
31:CA:708:G:N2	31:CA:724:U:H1'	2.36	0.41
31:CA:984:A:H2'	31:CA:984:A:N3	2.35	0.41
46:CS:38:VAL:CG2	46:CS:57:GLY:HA3	2.50	0.41
24:D3:19:ARG:HD3	55:DA:125:A:OP2	2.21	0.41
55:DA:1093:G:H1'	55:DA:1099:G:H22	1.85	0.41
55:DA:1195:G:N3	55:DA:1226:A:H2	2.19	0.41
55:DA:1286:A:C6	55:DA:1329:U:C2	3.08	0.41
55:DA:1664:A:O5'	55:DA:1664:A:C8	2.73	0.41
55:DA:189:G:H2'	55:DA:205:G:N2	2.36	0.41
55:DA:2714:G:O2'	55:DA:2715:C:H5'	2.20	0.41
55:DA:622:G:C8	55:DA:622:G:H5''	2.55	0.41
28:DB:1:U:H2'	28:DB:2:G:H8	1.83	0.41
54:DI:132:TYR:HD2	54:DI:133:GLU:HG2	1.84	0.41
38:DK:89:PHE:CE2	38:DK:100:VAL:HG11	2.55	0.41
42:DO:31:HIS:C	42:DO:33:ILE:H	2.24	0.41
52:DY:18:ARG:HH21	52:DY:24:ALA:HB2	1.85	0.41
1:AA:827:U:H2'	1:AA:870:U:O4	2.20	0.41
15:AO:66:LEU:H	15:AO:66:LEU:HG	1.71	0.41
1:BA:562:U:H5	12:BL:15:LYS:HE2	1.85	0.41
31:CA:323:C:H6	31:CA:1205:A:N1	2.18	0.41
31:CA:5:A:C2	31:CA:2899:A:C2	3.09	0.41
31:CA:871:U:H2'	31:CA:872:U:C6	2.55	0.41
51:CX:59:LEU:HD12	51:CX:80:ILE:HD12	2.01	0.41
26:D5:11:CYS:HB3	26:D5:33:HIS:HE1	1.85	0.41
55:DA:1189:A:H2'	55:DA:1190:G:O4'	2.21	0.41
55:DA:2057:G:H5'	69:DA:5229:HOH:O	2.20	0.41
62:DA:3194:EDO:H22	69:DA:7234:HOH:O	2.19	0.41
34:DF:104:ILE:HD11	34:DF:175:PHE:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:DO:51:LEU:HA	42:DO:51:LEU:HD23	1.87	0.41
1:AA:517:G:O2'	1:AA:530:G:H4'	2.21	0.41
2:BB:117:LEU:HA	2:BB:120:GLN:HG2	2.01	0.41
6:BF:64:VAL:HG12	6:BF:65:GLU:N	2.36	0.41
12:BL:80:ILE:HG22	12:BL:104:CYS:HB2	2.01	0.41
12:BL:3:THR:HB	12:BL:6:GLN:HB2	2.03	0.41
16:BP:20:VAL:HG11	16:BP:32:PHE:HB2	2.02	0.41
18:BR:27:ALA:O	18:BR:30:LYS:HG2	2.21	0.41
31:CA:348:A:H2'	31:CA:349:U:O4'	2.20	0.41
30:CD:130:GLN:NE2	30:CD:142:VAL:HG23	2.35	0.41
40:CM:28:GLY:O	40:CM:29:LYS:C	2.58	0.41
31:CA:2250:G:N7	41:CN:82:MET:HB2	2.34	0.41
46:CS:3:ALA:HA	46:CS:40:MET:O	2.21	0.41
47:CT:20:VAL:O	47:CT:23:LEU:HB2	2.21	0.41
48:CU:47:VAL:HG11	48:CU:85:VAL:HG11	2.02	0.41
55:DA:1832:C:N4	55:DA:1833:C:C4	2.89	0.41
51:DX:41[A]:ARG:HG3	55:DA:2386:A:C2	2.55	0.41
55:DA:2438:U:O2'	55:DA:2439:A:H5''	2.21	0.41
55:DA:2695:U:H3'	69:DA:4531:HOH:O	2.21	0.41
33:DE:163:ASN:HB2	55:DA:322:A:OP2	2.20	0.41
55:DA:323:C:H6	55:DA:1205:A:N1	2.19	0.41
55:DA:819:A:C4	55:DA:1189:A:C2	3.09	0.41
55:DA:83:A:H2'	55:DA:84:A:C8	2.56	0.41
34:DF:162:SER:HB2	69:DF:207:HOH:O	2.20	0.41
54:DI:50:VAL:HG13	54:DI:85:VAL:HG22	2.03	0.41
47:DT:20:VAL:O	47:DT:23:LEU:HB2	2.20	0.41
48:DU:48:GLN:HG2	48:DU:53:VAL:O	2.20	0.41
48:DU:47:VAL:HG11	48:DU:85:VAL:HG11	2.02	0.41
52:DY:37:ARG:HG3	52:DY:48:THR:HG23	2.03	0.41
1:AA:631:C:O5'	1:AA:631:C:H6	2.04	0.41
1:AA:746:A:H2'	1:AA:747:A:C8	2.55	0.41
2:AB:90:PHE:HB3	2:AB:151:ILE:HG22	2.02	0.41
7:AG:107:ALA:HB1	7:AG:133:THR:HB	2.03	0.41
11:AK:36:ASP:OD2	11:AK:40:ASN:HB2	2.21	0.41
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	2.03	0.41
1:BA:1017:U:H2'	1:BA:1018:G:H8	1.85	0.41
1:BA:126:G:H2'	1:BA:127:G:O4'	2.21	0.41
1:BA:202:G:H1	1:BA:215:C:H42	1.69	0.41
2:BB:12:ALA:HB2	2:BB:212:LEU:HD13	2.01	0.41
31:CA:2660:A:H2'	31:CA:2661:G:C8	2.56	0.41
31:CA:287:G:H2'	31:CA:288:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:214:ARG:NH1	31:CA:1566:A:H5'	2.36	0.41
33:CE:19:PHE:HB3	33:CE:113:VAL:HG21	2.03	0.41
55:DA:1585:C:H2'	55:DA:1586:A:O4'	2.21	0.41
55:DA:2019:A:H2	55:DA:2035:G:H22	1.69	0.41
55:DA:2273:A:H2'	55:DA:2274:A:C8	2.55	0.41
55:DA:2519:U:C6	55:DA:2542:A:N6	2.89	0.41
35:DG:109:PHE:CD1	55:DA:2667:C:H1'	2.55	0.41
55:DA:302:C:H2'	55:DA:303:G:H8	1.86	0.41
45:DR:92:ARG:NH1	55:DA:997:G:H5''	2.36	0.41
34:DF:40:VAL:HG21	34:DF:50:LEU:HD12	2.03	0.41
36:DH:135:HIS:CG	36:DH:136:SER:H	2.39	0.41
1:AA:131:A:H2'	1:AA:132:C:C6	2.55	0.41
2:AB:12:ALA:HB2	2:AB:212:LEU:HD13	2.02	0.41
9:AI:46:MET:HA	9:AI:49:ARG:HD2	2.02	0.41
1:BA:240:G:H5''	1:BA:240:G:C8	2.56	0.41
1:BA:486:U:H2'	1:BA:487:A:H8	1.85	0.41
15:BO:24:SER:HB3	15:BO:27:VAL:HG23	2.03	0.41
31:CA:1676:A:H2'	31:CA:1677:A:O4'	2.20	0.41
31:CA:2146:C:H4'	31:CA:2147:A:O5'	2.21	0.41
30:CD:117:GLY:HA2	30:CD:164:GLN:HE22	1.85	0.41
39:CL:119:ALA:HA	39:CL:120:PRO:HD3	1.91	0.41
27:D0:18:PRO:HD2	69:D0:206:HOH:O	2.21	0.41
55:DA:1356:G:C2	55:DA:1376:C:O2	2.74	0.41
55:DA:1782:U:H2'	55:DA:1783:A:H5'	2.03	0.41
55:DA:2082:A:H2'	55:DA:2083:G:O4'	2.20	0.41
55:DA:2660:A:H2'	55:DA:2661:G:C8	2.56	0.41
33:DE:45:ALA:HB3	55:DA:38:A:H5'	2.02	0.41
1:AA:382:A:H2'	1:AA:383:A:C8	2.56	0.41
1:AA:580:C:H2'	1:AA:581:G:O4'	2.21	0.41
1:AA:845:A:O4'	1:AA:845:A:P	2.79	0.41
2:AB:211:THR:HA	2:AB:214:LEU:HB2	2.01	0.41
11:AK:31:ILE:HA	11:AK:46:THR:HG22	2.02	0.41
1:BA:536:C:OP1	69:BA:1701:HOH:O	2.22	0.41
7:BG:116:MET:O	7:BG:120:LEU:HB2	2.20	0.41
15:BO:66:LEU:H	15:BO:66:LEU:HG	1.71	0.41
47:CT:82:MET:HB2	47:CT:98:LYS:HB2	2.02	0.41
55:DA:287:G:H2'	55:DA:288:U:C6	2.56	0.41
37:DJ:55:ILE:HA	37:DJ:56:PRO:HD3	2.00	0.41
47:DT:100:THR:HG21	69:DT:346:HOH:O	2.21	0.41
47:DT:20:VAL:HG11	47:DT:44:ALA:HA	2.02	0.41
51:DX:41[B]:ARG:HA	51:DX:41[B]:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1088:G:H21	1:AA:1167:A:H62	1.69	0.41
1:AA:1508:A:H2'	1:AA:1509:C:O4'	2.21	0.41
1:AA:845:A:H2'	1:AA:846:G:O4'	2.21	0.41
17:AQ:12:VAL:HG12	17:AQ:55:ILE:HA	2.03	0.41
1:BA:1048:G:H4'	14:BN:3:LYS:HE2	2.03	0.41
1:BA:1171:A:H2'	1:BA:1172:C:C6	2.55	0.41
1:BA:1411:C:H2'	1:BA:1412:C:H6	1.85	0.41
1:BA:368:U:O4	36:DH:83:LYS:HB2	2.21	0.41
1:BA:577:G:C1'	1:BA:816:A:H2'	2.51	0.41
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	2.02	0.41
5:BE:57:PRO:HA	5:BE:60:ILE:HG13	2.02	0.41
12:BL:82:ILE:HD11	12:BL:95:TYR:HB2	2.03	0.41
19:BS:11:ILE:HG12	19:BS:16:LEU:HD13	2.02	0.41
31:CA:172:A:H2'	31:CA:173:A:C8	2.56	0.41
31:CA:379:G:O4'	31:CA:2232:C:H5''	2.21	0.41
31:CA:297:G:H5''	49:CV:85:PHE:HB2	2.02	0.41
46:CS:76:LYS:O	46:CS:84:ARG:HA	2.21	0.41
55:DA:1782:U:H3'	69:DA:4190:HOH:O	2.21	0.41
55:DA:665:U:H2'	55:DA:666:A:H8	1.85	0.41
46:DS:3:ALA:HA	46:DS:40:MET:O	2.21	0.41
47:DT:20:VAL:HA	47:DT:23:LEU:HD12	2.03	0.41
1:AA:9:G:OP2	5:AE:126:LYS:HE2	2.21	0.40
11:AK:52:PHE:CE2	11:AK:65:VAL:HG21	2.56	0.40
14:AN:46:LEU:HA	14:AN:49:GLN:HE21	1.85	0.40
1:BA:1068:G:N7	1:BA:1094:G:H2'	2.36	0.40
1:BA:377:G:H2'	1:BA:378:G:H8	1.86	0.40
22:C1:12:LYS:HA	22:C1:12:LYS:HD2	1.70	0.40
31:CA:528:A:N1	31:CA:2042:A:H2'	2.36	0.40
31:CA:2598:A:C8	31:CA:2599:G:H1'	2.56	0.40
31:CA:65:U:H2'	31:CA:66:C:C6	2.56	0.40
28:CB:24:G:H1'	28:CB:27:C:N4	2.36	0.40
42:CO:92:GLY:HA2	42:CO:94:TYR:CZ	2.56	0.40
43:CP:39:VAL:HG11	43:CP:87:ILE:HG21	2.03	0.40
27:D0:26:GLY:O	55:DA:929:U:H1'	2.21	0.40
55:DA:2261:C:H1'	55:DA:2388:A:N3	2.35	0.40
55:DA:65:U:H2'	55:DA:66:C:C6	2.56	0.40
54:DI:64:VAL:CG2	54:DI:69:PHE:HB2	2.50	0.40
49:DV:15:THR:HG23	55:DA:310:A:H5''	2.03	0.40
11:AK:123:PRO:HD2	21:AU:38:TYR:HB2	2.03	0.40
20:AT:44:LYS:HG3	20:AT:44:LYS:H	1.48	0.40
21:AU:40:LYS:HB2	21:AU:43:THR:OG1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:562:U:H4'	1:BA:563:A:O5'	2.21	0.40
11:BK:52:PHE:HE2	11:BK:65:VAL:HG21	1.86	0.40
31:CA:189:G:H2'	31:CA:205:G:N2	2.37	0.40
31:CA:1940:U:H5''	31:CA:1965:C:C5	2.55	0.40
31:CA:2538:C:H2'	31:CA:2539:C:C6	2.56	0.40
31:CA:244:A:H62	31:CA:254:G:H21	1.70	0.40
31:CA:304:U:H2'	31:CA:305:C:C6	2.56	0.40
33:CE:196:VAL:HG13	33:CE:200:LEU:HD13	2.03	0.40
39:CL:35:VAL:HB	39:CL:36:GLY:H	1.66	0.40
55:DA:2042:A:H2	69:DA:7342:HOH:O	2.04	0.40
36:DH:117:LEU:HA	36:DH:118:PRO:HD3	2.00	0.40
5:AE:80:THR:HB	5:AE:122:ASN:HB2	2.03	0.40
9:AI:98:LEU:HB3	9:AI:104:VAL:HG13	2.02	0.40
3:AC:33:LEU:HD21	14:AN:93:ILE:HG12	2.02	0.40
2:BB:83:ALA:HB3	2:BB:214:LEU:HD22	2.02	0.40
8:BH:76:GLN:O	8:BH:127:CYS:HB2	2.21	0.40
31:CA:2328:A:H8	31:CA:2328:A:O5'	2.04	0.40
31:CA:2464:G:C2	31:CA:2465:C:H1'	2.57	0.40
31:CA:2693:G:H2'	31:CA:2694:G:H8	1.85	0.40
31:CA:302:C:H2'	31:CA:303:G:H8	1.85	0.40
34:CF:40:VAL:HG21	34:CF:50:LEU:HD12	2.04	0.40
34:CF:8:TYR:HB2	34:CF:173:PHE:CZ	2.55	0.40
39:CL:15:GLY:HA2	39:CL:47:ILE:HG12	2.03	0.40
25:D4:26:HIS:NE2	25:D4:48:ALA:HB2	2.36	0.40
44:DQ:94:LYS:HE2	55:DA:1754:A:C8	2.56	0.40
55:DA:638:G:H2'	55:DA:639:U:C6	2.57	0.40
29:DC:53:HIS:NE2	29:DC:219:THR:HG23	2.37	0.40
32:DD:175:LEU:HA	69:DD:435:HOH:O	2.22	0.40
1:AA:1235:U:H2'	1:AA:1236:A:O4'	2.22	0.40
1:AA:377:G:H2'	1:AA:378:G:H8	1.87	0.40
1:AA:511:C:H5'	4:AD:44:ARG:CZ	2.52	0.40
2:AB:117:LEU:HA	2:AB:120:GLN:HG2	2.03	0.40
2:AB:20:THR:HA	2:AB:39:HIS:CE1	2.56	0.40
15:AO:24:SER:HB3	15:AO:27:VAL:HG23	2.04	0.40
1:BA:1235:U:H2'	1:BA:1236:A:O4'	2.22	0.40
10:BJ:59:LYS:H	10:BJ:59:LYS:HG3	1.66	0.40
11:BK:52:PHE:CE2	11:BK:65:VAL:HG21	2.56	0.40
13:BM:4:ILE:HA	13:BM:57:ARG:HG2	2.04	0.40
31:CA:1101:U:H2'	31:CA:1102:C:H6	1.86	0.40
31:CA:1313:U:H5'	69:CA:3366:HOH:O	2.21	0.40
31:CA:179:C:H2'	31:CA:180:G:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:7:G:H4'	38:CK:15:TRP:CZ2	2.56	0.40
31:CA:2547:A:H4'	39:CL:29:HIS:NE2	2.36	0.40
47:CT:29:VAL:O	47:CT:33:LEU:HD12	2.21	0.40
55:DA:2498:OMC:HM23	55:DA:2498:OMC:H1'	1.95	0.40
55:DA:2538:C:H2'	55:DA:2539:C:C6	2.57	0.40
34:DF:138:PHE:HA	34:DF:139:PRO:HD3	1.93	0.40
34:DF:175:PHE:HA	34:DF:176:PRO:HD3	1.95	0.40
43:DP:53:THR:HB	43:DP:65:THR:HG22	2.04	0.40
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.57	0.40
1:AA:407:U:H2'	1:AA:408:A:H8	1.86	0.40
8:AH:87:LYS:HB2	8:AH:125:ILE:CD1	2.50	0.40
1:AA:562:U:H5	12:AL:15:LYS:HE2	1.86	0.40
1:BA:110:C:H1'	69:BA:1786:HOH:O	2.21	0.40
1:BA:227:G:H2'	1:BA:228:A:O4'	2.20	0.40
1:BA:240:G:OP1	1:BA:240:G:H4'	2.22	0.40
10:BJ:12:ALA:HB3	10:BJ:18:ILE:HB	2.03	0.40
12:BL:44:LYS:HB2	12:BL:45:PRO:HD3	2.03	0.40
31:CA:2066:C:O2'	31:CA:2067:G:H5'	2.22	0.40
31:CA:4:U:H2'	31:CA:5:A:C8	2.57	0.40
31:CA:963:U:H2'	31:CA:964:C:C6	2.56	0.40
48:CU:30:ILE:HG22	48:CU:85:VAL:HB	2.02	0.40
49:CV:26:LYS:HB2	49:CV:35:ILE:HG22	2.04	0.40
24:D3:3:ARG:HB2	55:DA:1612:C:O2'	2.21	0.40
55:DA:192:C:O2'	55:DA:802:A:H1'	2.21	0.40
55:DA:2521:C:H2'	55:DA:2522:U:C6	2.57	0.40
55:DA:2844:G:H2'	55:DA:2845:U:O4'	2.22	0.40
33:DE:132:LYS:HD2	55:DA:320:A:OP2	2.21	0.40
33:DE:19:PHE:HB3	33:DE:113:VAL:HG21	2.03	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%)	203 (91%)	14 (6%)	5 (2%)	6	30
2	BB	222/224 (99%)	203 (91%)	14 (6%)	5 (2%)	6	30
3	AC	204/206 (99%)	193 (95%)	9 (4%)	2 (1%)	15	47
3	BC	204/206 (99%)	193 (95%)	8 (4%)	3 (2%)	10	38
4	AD	203/205 (99%)	191 (94%)	12 (6%)	0	100	100
4	BD	203/205 (99%)	192 (95%)	11 (5%)	0	100	100
5	AE	153/155 (99%)	139 (91%)	12 (8%)	2 (1%)	12	40
5	BE	148/155 (96%)	126 (85%)	17 (12%)	5 (3%)	3	23
6	AF	104/106 (98%)	95 (91%)	8 (8%)	1 (1%)	15	47
6	BF	98/106 (92%)	83 (85%)	12 (12%)	3 (3%)	4	24
7	AG	149/151 (99%)	137 (92%)	10 (7%)	2 (1%)	12	40
7	BG	149/151 (99%)	140 (94%)	7 (5%)	2 (1%)	12	40
8	AH	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	9	37
8	BH	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	51
9	AI	125/127 (98%)	109 (87%)	16 (13%)	0	100	100
9	BI	125/127 (98%)	109 (87%)	16 (13%)	0	100	100
10	AJ	97/99 (98%)	86 (89%)	8 (8%)	3 (3%)	4	24
10	BJ	96/99 (97%)	78 (81%)	14 (15%)	4 (4%)	3	18
11	AK	115/129 (89%)	104 (90%)	10 (9%)	1 (1%)	17	49
11	BK	115/129 (89%)	101 (88%)	13 (11%)	1 (1%)	17	49
12	AL	120/123 (98%)	110 (92%)	8 (7%)	2 (2%)	9	36
12	BL	120/123 (98%)	109 (91%)	9 (8%)	2 (2%)	9	36
13	AM	112/114 (98%)	99 (88%)	9 (8%)	4 (4%)	3	22
13	BM	112/114 (98%)	96 (86%)	10 (9%)	6 (5%)	2	13
14	AN	98/100 (98%)	89 (91%)	8 (8%)	1 (1%)	15	47
14	BN	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	15	47
15	AO	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
15	BO	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	13	43
16	AP	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	5	28
16	BP	80/82 (98%)	67 (84%)	10 (12%)	3 (4%)	3	20
17	AQ	78/80 (98%)	70 (90%)	5 (6%)	3 (4%)	3	20
17	BQ	78/80 (98%)	69 (88%)	5 (6%)	4 (5%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	68 (88%)	6 (8%)	3 (4%)	3	20
19	BS	77/79 (98%)	68 (88%)	7 (9%)	2 (3%)	5	28
20	AT	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
20	BT	83/86 (96%)	78 (94%)	4 (5%)	1 (1%)	13	43
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%)	45 (83%)	6 (11%)	3 (6%)	2	12
22	D1	54/56 (96%)	54 (100%)	0	0	100	100
23	C2	48/51 (94%)	43 (90%)	4 (8%)	1 (2%)	7	32
23	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	6	30
24	D3	44/46 (96%)	44 (100%)	0	0	100	100
25	C4	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	9	37
25	D4	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	9	37
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%)	51 (91%)	3 (5%)	2 (4%)	3	22
27	D0	57/58 (98%)	52 (91%)	5 (9%)	0	100	100
29	CC	269/272 (99%)	243 (90%)	21 (8%)	5 (2%)	8	34
29	DC	269/272 (99%)	245 (91%)	19 (7%)	5 (2%)	8	34
30	CD	207/209 (99%)	193 (93%)	11 (5%)	3 (1%)	11	39
32	DD	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
33	CE	199/201 (99%)	184 (92%)	14 (7%)	1 (0%)	29	61
33	DE	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
34	CF	175/178 (98%)	161 (92%)	14 (8%)	0	100	100
34	DF	175/178 (98%)	163 (93%)	12 (7%)	0	100	100
35	CG	174/176 (99%)	158 (91%)	12 (7%)	4 (2%)	6	30
35	DG	174/176 (99%)	160 (92%)	13 (8%)	1 (1%)	25	57
36	CH	147/149 (99%)	129 (88%)	12 (8%)	6 (4%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	DH	147/149 (99%)	131 (89%)	12 (8%)	4 (3%)	5	27
37	CJ	132/135 (98%)	120 (91%)	8 (6%)	4 (3%)	4	25
37	DJ	132/135 (98%)	120 (91%)	8 (6%)	4 (3%)	4	25
38	CK	140/142 (99%)	130 (93%)	7 (5%)	3 (2%)	7	32
38	DK	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	7	32
39	CL	120/123 (98%)	111 (92%)	7 (6%)	2 (2%)	9	36
39	DL	121/123 (98%)	114 (94%)	6 (5%)	1 (1%)	19	51
40	CM	142/144 (99%)	128 (90%)	8 (6%)	6 (4%)	3	18
40	DM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	7	32
41	CN	133/136 (98%)	121 (91%)	12 (9%)	0	100	100
41	DN	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
42	CO	118/127 (93%)	98 (83%)	16 (14%)	4 (3%)	3	23
42	DO	123/127 (97%)	106 (86%)	16 (13%)	1 (1%)	19	51
43	CP	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
43	DP	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
44	CQ	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	17	49
44	DQ	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	17	49
45	CR	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
45	DR	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
46	CS	101/103 (98%)	89 (88%)	10 (10%)	2 (2%)	7	33
46	DS	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	15	47
47	CT	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
47	DT	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	17	49
48	CU	91/100 (91%)	85 (93%)	5 (6%)	1 (1%)	14	45
48	DU	91/100 (91%)	86 (94%)	4 (4%)	1 (1%)	14	45
49	CV	100/103 (97%)	85 (85%)	12 (12%)	3 (3%)	4	25
49	DV	100/103 (97%)	87 (87%)	11 (11%)	2 (2%)	7	33
50	CW	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	14	45
50	DW	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	14	45
51	CX	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
51	DX	75/76 (99%)	71 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	CY	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
52	DY	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
53	CZ	60/62 (97%)	51 (85%)	8 (13%)	1 (2%)	9	36
53	DZ	60/62 (97%)	51 (85%)	8 (13%)	1 (2%)	9	36
54	DI	133/135 (98%)	112 (84%)	17 (13%)	4 (3%)	4	25
All	All	11407/11679 (98%)	10425 (91%)	815 (7%)	167 (2%)	10	38

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	95	ARG
2	AB	126	PHE
3	AC	156	ARG
13	AM	5	ALA
17	AQ	82	ALA
22	C1	25	VAL
22	C1	27	SER
23	C2	5	ILE
27	C0	4	THR
2	BB	95	ARG
2	BB	126	PHE
3	BC	156	ARG
6	BF	98	GLU
13	BM	7	ILE
17	BQ	82	ALA
20	BT	5	LYS
29	CC	108	LYS
29	CC	158	ALA
33	CE	83	VAL
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
48	CU	89	GLU
35	DG	46	ALA
36	DH	11	ASN

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Mol	Chain	Res	Type
37	DJ	19	ASN
49	DV	52	LEU
54	DI	91	ALA
3	AC	127	ARG
5	AE	162	GLU
8	AH	66	PHE
10	AJ	33	GLY
10	AJ	57	VAL
11	AK	89	PRO
14	AN	38	ASP
16	AP	31	ARG
19	AS	31	LEU
3	BC	61	ALA
3	BC	127	ARG
5	BE	110	ALA
6	BF	99	ALA
8	BH	66	PHE
10	BJ	38	GLY
10	BJ	57	VAL
11	BK	89	PRO
13	BM	5	ALA
14	BN	38	ASP
15	BO	88	ARG
16	BP	31	ARG
17	BQ	16	LYS
17	BQ	70	THR
29	CC	122	ALA
29	DC	122	ALA
29	DC	261	LYS
36	CH	11	ASN
38	CK	95	ARG
39	CL	35	VAL
40	CM	30	THR
40	CM	36	LYS
40	CM	69	ARG
44	CQ	105	GLY
49	CV	89	ASP
38	DK	95	ARG
40	DM	29	LYS
40	DM	36	LYS
44	DQ	105	GLY
46	DS	44	GLY

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Mol	Chain	Res	Type
48	DU	89	GLU
49	DV	89	ASP
54	DI	130	PRO
2	AB	127	ASP
7	AG	56	LYS
10	AJ	58	ASN
12	AL	48	ALA
12	AL	74	LEU
19	AS	8	GLY
22	C1	26	THR
2	BB	127	ASP
5	BE	103	THR
5	BE	109	GLY
7	BG	56	LYS
10	BJ	36	VAL
10	BJ	58	ASN
13	BM	114	LYS
19	BS	7	LYS
19	BS	31	LEU
29	CC	233	GLY
29	CC	253	LYS
30	CD	105	LYS
29	DC	233	GLY
36	CH	9	VAL
36	CH	122	LEU
37	CJ	23	PRO
37	CJ	32	GLY
39	CL	108	ARG
42	CO	119	SER
49	CV	7	ARG
49	CV	17	LYS
36	DH	122	LEU
37	DJ	23	PRO
37	DJ	32	GLY
39	DL	108	ARG
5	AE	109	GLY
6	AF	56	LYS
13	AM	7	ILE
17	AQ	16	LYS
17	AQ	68	SER
24	C3	45	SER
6	BF	56	LYS

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Mol	Chain	Res	Type
12	BL	74	LEU
13	BM	47	GLU
16	BP	44	SER
16	BP	80	LYS
30	CD	86	GLU
37	CJ	25	GLY
53	CZ	41	HIS
37	DJ	25	GLY
50	DW	23	ALA
53	DZ	41	HIS
54	DI	88	HIS
2	AB	125	THR
7	AG	17	LYS
13	AM	47	GLU
13	AM	105	ASN
16	AP	45	GLU
19	AS	7	LYS
2	BB	125	THR
5	BE	24	THR
7	BG	17	LYS
12	BL	44	LYS
13	BM	4	ILE
13	BM	105	ASN
17	BQ	17	MET
30	CD	149	ASN
29	DC	253	LYS
29	DC	262	ARG
36	CH	8	LYS
36	CH	34	GLY
40	CM	58	TYR
42	CO	32	GLU
42	CO	104	ALA
42	CO	118	ARG
46	CS	53	PHE
50	CW	23	ALA
38	DK	25	LEU
40	DM	58	TYR
42	DO	32	GLU
54	DI	108	VAL
8	AH	68	GLY
38	CK	25	LEU
40	CM	68	SER

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Mol	Chain	Res	Type
46	CS	48	LYS
36	DH	10	ALA
36	DH	34	GLY
47	DT	66	ILE
2	AB	71	GLY
2	BB	71	GLY
25	D4	7	VAL
27	C0	14	ILE
25	C4	7	VAL
5	BE	25	VAL
38	DK	83	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	168 (90%)	18 (10%)	8	30
2	BB	186/186 (100%)	168 (90%)	18 (10%)	8	30
3	AC	170/170 (100%)	158 (93%)	12 (7%)	14	44
3	BC	170/170 (100%)	155 (91%)	15 (9%)	10	34
4	AD	172/172 (100%)	163 (95%)	9 (5%)	23	55
4	BD	172/172 (100%)	162 (94%)	10 (6%)	20	51
5	AE	118/118 (100%)	102 (86%)	16 (14%)	3	16
5	BE	113/118 (96%)	97 (86%)	16 (14%)	3	15
6	AF	92/92 (100%)	83 (90%)	9 (10%)	8	29
6	BF	87/92 (95%)	77 (88%)	10 (12%)	5	22
7	AG	124/124 (100%)	108 (87%)	16 (13%)	4	18
7	BG	124/124 (100%)	107 (86%)	17 (14%)	3	16
8	AH	104/104 (100%)	92 (88%)	12 (12%)	5	22
8	BH	104/104 (100%)	93 (89%)	11 (11%)	6	25
9	AI	105/105 (100%)	97 (92%)	8 (8%)	13	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	BI	105/105 (100%)	97 (92%)	8 (8%)	13	40
10	AJ	87/87 (100%)	81 (93%)	6 (7%)	15	45
10	BJ	86/87 (99%)	77 (90%)	9 (10%)	7	26
11	AK	90/99 (91%)	86 (96%)	4 (4%)	28	60
11	BK	90/99 (91%)	81 (90%)	9 (10%)	7	28
12	AL	102/102 (100%)	96 (94%)	6 (6%)	19	50
12	BL	102/102 (100%)	95 (93%)	7 (7%)	15	45
13	AM	92/92 (100%)	81 (88%)	11 (12%)	5	21
13	BM	92/92 (100%)	81 (88%)	11 (12%)	5	21
14	AN	83/83 (100%)	81 (98%)	2 (2%)	49	74
14	BN	83/83 (100%)	81 (98%)	2 (2%)	49	74
15	AO	76/76 (100%)	71 (93%)	5 (7%)	16	47
15	BO	76/76 (100%)	68 (90%)	8 (10%)	7	26
16	AP	65/65 (100%)	60 (92%)	5 (8%)	13	40
16	BP	65/65 (100%)	61 (94%)	4 (6%)	18	49
17	AQ	74/74 (100%)	65 (88%)	9 (12%)	5	20
17	BQ	74/74 (100%)	64 (86%)	10 (14%)	4	17
18	AR	48/48 (100%)	47 (98%)	1 (2%)	53	76
18	BR	48/48 (100%)	48 (100%)	0	100	100
19	AS	70/70 (100%)	63 (90%)	7 (10%)	7	28
19	BS	70/70 (100%)	64 (91%)	6 (9%)	10	36
20	AT	65/65 (100%)	54 (83%)	11 (17%)	2	9
20	BT	65/65 (100%)	54 (83%)	11 (17%)	2	9
21	AU	48/48 (100%)	44 (92%)	4 (8%)	11	37
21	BU	48/48 (100%)	44 (92%)	4 (8%)	11	37
22	C1	47/47 (100%)	46 (98%)	1 (2%)	53	76
22	D1	47/47 (100%)	45 (96%)	2 (4%)	29	61
23	C2	45/46 (98%)	42 (93%)	3 (7%)	16	46
23	D2	45/46 (98%)	41 (91%)	4 (9%)	9	33
24	C3	38/38 (100%)	35 (92%)	3 (8%)	12	39
24	D3	38/38 (100%)	35 (92%)	3 (8%)	12	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	C4	51/51 (100%)	48 (94%)	3 (6%)	19	50
25	D4	51/51 (100%)	47 (92%)	4 (8%)	12	39
26	C5	34/34 (100%)	31 (91%)	3 (9%)	10	34
26	D5	34/34 (100%)	31 (91%)	3 (9%)	10	34
27	C0	48/48 (100%)	42 (88%)	6 (12%)	4	19
27	D0	49/48 (102%)	44 (90%)	5 (10%)	7	27
29	CC	216/217 (100%)	202 (94%)	14 (6%)	17	47
29	DC	216/217 (100%)	204 (94%)	12 (6%)	21	53
30	CD	164/164 (100%)	154 (94%)	10 (6%)	18	49
32	DD	163/163 (100%)	153 (94%)	10 (6%)	18	49
33	CE	165/165 (100%)	147 (89%)	18 (11%)	6	25
33	DE	165/165 (100%)	153 (93%)	12 (7%)	14	42
34	CF	148/149 (99%)	131 (88%)	17 (12%)	5	22
34	DF	148/149 (99%)	132 (89%)	16 (11%)	6	25
35	CG	137/137 (100%)	129 (94%)	8 (6%)	20	51
35	DG	137/137 (100%)	129 (94%)	8 (6%)	20	51
36	CH	114/114 (100%)	100 (88%)	14 (12%)	4	20
36	DH	114/114 (100%)	101 (89%)	13 (11%)	5	22
37	CJ	104/105 (99%)	95 (91%)	9 (9%)	10	35
37	DJ	104/105 (99%)	95 (91%)	9 (9%)	10	35
38	CK	116/116 (100%)	110 (95%)	6 (5%)	23	55
38	DK	116/116 (100%)	111 (96%)	5 (4%)	29	61
39	CL	103/104 (99%)	95 (92%)	8 (8%)	12	39
39	DL	104/104 (100%)	93 (89%)	11 (11%)	6	25
40	CM	103/103 (100%)	94 (91%)	9 (9%)	10	35
40	DM	103/103 (100%)	97 (94%)	6 (6%)	20	51
41	CN	108/108 (100%)	98 (91%)	10 (9%)	9	31
41	DN	109/108 (101%)	98 (90%)	11 (10%)	7	28
42	CO	100/103 (97%)	92 (92%)	8 (8%)	12	38
42	DO	102/103 (99%)	94 (92%)	8 (8%)	12	39
43	CP	86/87 (99%)	77 (90%)	9 (10%)	7	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	DP	87/87 (100%)	78 (90%)	9 (10%)	7	27
44	CQ	99/99 (100%)	91 (92%)	8 (8%)	11	37
44	DQ	99/99 (100%)	92 (93%)	7 (7%)	14	44
45	CR	89/89 (100%)	81 (91%)	8 (9%)	9	33
45	DR	89/89 (100%)	83 (93%)	6 (7%)	16	46
46	CS	84/84 (100%)	74 (88%)	10 (12%)	5	21
46	DS	84/84 (100%)	75 (89%)	9 (11%)	6	25
47	CT	93/93 (100%)	83 (89%)	10 (11%)	6	25
47	DT	93/93 (100%)	85 (91%)	8 (9%)	10	36
48	CU	80/84 (95%)	67 (84%)	13 (16%)	2	10
48	DU	80/84 (95%)	72 (90%)	8 (10%)	7	28
49	CV	83/84 (99%)	75 (90%)	8 (10%)	8	30
49	DV	83/84 (99%)	77 (93%)	6 (7%)	14	43
50	CW	78/78 (100%)	70 (90%)	8 (10%)	7	27
50	DW	78/78 (100%)	72 (92%)	6 (8%)	13	40
51	CX	56/58 (97%)	54 (96%)	2 (4%)	35	65
51	DX	58/58 (100%)	54 (93%)	4 (7%)	15	45
52	CY	67/67 (100%)	63 (94%)	4 (6%)	19	50
52	DY	67/67 (100%)	62 (92%)	5 (8%)	13	41
53	CZ	54/54 (100%)	50 (93%)	4 (7%)	13	41
53	DZ	54/54 (100%)	51 (94%)	3 (6%)	21	53
54	DI	103/103 (100%)	91 (88%)	12 (12%)	5	21
All	All	9461/9514 (99%)	8645 (91%)	816 (9%)	10	36

All (816) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	44	GLU
2	AB	57	LEU
2	AB	73	LYS
2	AB	93	ASN
2	AB	105	LYS
2	AB	108	ARG

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Mol	Chain	Res	Type
2	AB	116	ASP
2	AB	125	THR
2	AB	129	LEU
2	AB	130	THR
2	AB	135	LEU
2	AB	147	SER
2	AB	161	LEU
2	AB	168	HIS
2	AB	205	ASP
2	AB	207	ILE
2	AB	211	THR
3	AC	33	LEU
3	AC	36	ASP
3	AC	46	GLU
3	AC	55	ILE
3	AC	75	ILE
3	AC	107	ARG
3	AC	121	THR
3	AC	128	VAL
3	AC	178	LEU
3	AC	185	ASN
3	AC	186	THR
3	AC	207	ILE
4	AD	22	LYS
4	AD	26	ARG
4	AD	132	ILE
4	AD	142	VAL
4	AD	143	VAL
4	AD	192	SER
4	AD	194	ASP
4	AD	196	ASN
4	AD	198	HIS
5	AE	14	LYS
5	AE	46	VAL
5	AE	70	ASN
5	AE	78	ASN
5	AE	81	LEU
5	AE	82	GLN
5	AE	88	VAL
5	AE	94	VAL
5	AE	101	GLU
5	AE	120	VAL

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Mol	Chain	Res	Type
5	AE	123	VAL
5	AE	126	LYS
5	AE	134	ILE
5	AE	148	ASN
5	AE	159	LYS
5	AE	162	GLU
6	AF	14	GLN
6	AF	17	GLN
6	AF	39	LEU
6	AF	55	HIS
6	AF	69	GLU
6	AF	72	ASP
6	AF	79	ARG
6	AF	92	THR
6	AF	93	LYS
7	AG	4	ARG
7	AG	13	LEU
7	AG	18	PHE
7	AG	23	LEU
7	AG	30	LEU
7	AG	36	LYS
7	AG	63	GLU
7	AG	76	LYS
7	AG	83	SER
7	AG	89	VAL
7	AG	92	ARG
7	AG	95	ARG
7	AG	120	LEU
7	AG	131	LYS
7	AG	138	ARG
7	AG	142	HIS
8	AH	3	MET
8	AH	9	ASP
8	AH	13	ARG
8	AH	26	THR
8	AH	31	LYS
8	AH	47	GLU
8	AH	51	VAL
8	AH	52	GLU
8	AH	54	ASP
8	AH	55	THR
8	AH	60	GLU

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Mol	Chain	Res	Type
8	AH	63	LEU
9	AI	9	THR
9	AI	11	ARG
9	AI	36	GLU
9	AI	61	LEU
9	AI	63	LEU
9	AI	66	THR
9	AI	89	GLU
9	AI	111	VAL
10	AJ	6	ILE
10	AJ	62	ARG
10	AJ	65	TYR
10	AJ	69	THR
10	AJ	88	MET
10	AJ	89	ARG
11	AK	53	ARG
11	AK	85	MET
11	AK	97	ILE
11	AK	125	LYS
12	AL	24	LEU
12	AL	40	THR
12	AL	86	ARG
12	AL	110	ARG
12	AL	115	SER
12	AL	121	ARG
13	AM	3	ARG
13	AM	7	ILE
13	AM	8	ASN
13	AM	13	LYS
13	AM	27	LYS
13	AM	48	LEU
13	AM	58	ASP
13	AM	59	GLU
13	AM	64	VAL
13	AM	71	ARG
13	AM	101	ARG
14	AN	31	ILE
14	AN	77	PHE
15	AO	25	THR
15	AO	40	GLN
15	AO	58	ARG
15	AO	66	LEU

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Mol	Chain	Res	Type
15	AO	70	LEU
16	AP	1	MET
16	AP	2	VAL
16	AP	20	VAL
16	AP	33	ILE
16	AP	48	GLU
17	AQ	5	ILE
17	AQ	13	VAL
17	AQ	16	LYS
17	AQ	20	SER
17	AQ	29	VAL
17	AQ	38	ILE
17	AQ	65	ARG
17	AQ	75	LEU
17	AQ	83	VAL
18	AR	20	GLU
19	AS	5	LEU
19	AS	7	LYS
19	AS	13	LEU
19	AS	27	ASP
19	AS	37	ARG
19	AS	52	HIS
19	AS	63	THR
20	AT	12	ILE
20	AT	14	SER
20	AT	24	ARG
20	AT	26	SER
20	AT	43	ASP
20	AT	44	LYS
20	AT	54	MET
20	AT	64	LYS
20	AT	66	LEU
20	AT	85	LYS
20	AT	86	LEU
21	AU	13	ASP
21	AU	16	LEU
21	AU	20	LYS
21	AU	56	HIS
22	C1	40	ARG
23	C2	5	ILE
23	C2	28	ARG
23	C2	47	VAL

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Mol	Chain	Res	Type
24	C3	1	MET
24	C3	14	ARG
24	C3	41	ARG
25	C4	31	HIS
25	C4	52	LYS
25	C4	55	LEU
26	C5	2	LYS
26	C5	22	VAL
26	C5	26	ILE
27	C0	3	LYS
27	C0	4	THR
27	C0	5	ILE
27	C0	7	ILE
27	C0	36	VAL
27	C0	39	GLU
2	BB	23	TRP
2	BB	44	GLU
2	BB	57	LEU
2	BB	73	LYS
2	BB	93	ASN
2	BB	105	LYS
2	BB	108	ARG
2	BB	116	ASP
2	BB	125	THR
2	BB	129	LEU
2	BB	130	THR
2	BB	135	LEU
2	BB	147	SER
2	BB	161	LEU
2	BB	168	HIS
2	BB	205	ASP
2	BB	207	ILE
2	BB	211	THR
3	BC	3	GLN
3	BC	33	LEU
3	BC	36	ASP
3	BC	37	PHE
3	BC	46	GLU
3	BC	55	ILE
3	BC	75	ILE
3	BC	107	ARG
3	BC	121	THR

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Mol	Chain	Res	Type
3	BC	128	VAL
3	BC	152	GLU
3	BC	185	ASN
3	BC	186	THR
3	BC	193	TYR
3	BC	207	ILE
4	BD	22	LYS
4	BD	26	ARG
4	BD	130	VAL
4	BD	142	VAL
4	BD	143	VAL
4	BD	151	LYS
4	BD	194	ASP
4	BD	196	ASN
4	BD	198	HIS
4	BD	206	LYS
5	BE	14	LYS
5	BE	46	VAL
5	BE	65	GLU
5	BE	76	LEU
5	BE	81	LEU
5	BE	82	GLN
5	BE	88	VAL
5	BE	94	VAL
5	BE	105	ILE
5	BE	115	LEU
5	BE	120	VAL
5	BE	123	VAL
5	BE	126	LYS
5	BE	148	ASN
5	BE	157	ARG
5	BE	159	LYS
6	BF	9	MET
6	BF	14	GLN
6	BF	17	GLN
6	BF	39	LEU
6	BF	53	LYS
6	BF	55	HIS
6	BF	68	GLN
6	BF	69	GLU
6	BF	72	ASP
6	BF	93	LYS

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Mol	Chain	Res	Type
7	BG	5	ARG
7	BG	10	ARG
7	BG	23	LEU
7	BG	30	LEU
7	BG	36	LYS
7	BG	48	GLU
7	BG	50	LEU
7	BG	63	GLU
7	BG	72	THR
7	BG	76	LYS
7	BG	92	ARG
7	BG	95	ARG
7	BG	120	LEU
7	BG	131	LYS
7	BG	138	ARG
7	BG	142	HIS
7	BG	144	MET
8	BH	3	MET
8	BH	9	ASP
8	BH	13	ARG
8	BH	26	THR
8	BH	47	GLU
8	BH	52	GLU
8	BH	60	GLU
8	BH	76	GLN
8	BH	77	ARG
8	BH	80	ARG
8	BH	83	LEU
9	BI	9	THR
9	BI	11	ARG
9	BI	36	GLU
9	BI	61	LEU
9	BI	63	LEU
9	BI	66	THR
9	BI	89	GLU
9	BI	111	VAL
10	BJ	5	ARG
10	BJ	6	ILE
10	BJ	62	ARG
10	BJ	65	TYR
10	BJ	69	THR
10	BJ	78	GLU

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Mol	Chain	Res	Type
10	BJ	88	MET
10	BJ	89	ARG
10	BJ	90	LEU
11	BK	18	ASP
11	BK	22	HIS
11	BK	31	ILE
11	BK	38	GLN
11	BK	53	ARG
11	BK	85	MET
11	BK	97	ILE
11	BK	118	HIS
11	BK	125	LYS
12	BL	24	LEU
12	BL	55	VAL
12	BL	58	THR
12	BL	86	ARG
12	BL	110	ARG
12	BL	115	SER
12	BL	121	ARG
13	BM	7	ILE
13	BM	8	ASN
13	BM	11	ASP
13	BM	16	VAL
13	BM	27	LYS
13	BM	29	ARG
13	BM	41	GLU
13	BM	48	LEU
13	BM	59	GLU
13	BM	64	VAL
13	BM	101	ARG
14	BN	26	GLU
14	BN	77	PHE
15	BO	25	THR
15	BO	40	GLN
15	BO	58	ARG
15	BO	64	ARG
15	BO	66	LEU
15	BO	70	LEU
15	BO	87	LEU
15	BO	88	ARG
16	BP	1	MET
16	BP	2	VAL

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Mol	Chain	Res	Type
16	BP	33	ILE
16	BP	46	LYS
17	BQ	13	VAL
17	BQ	17	MET
17	BQ	20	SER
17	BQ	21	ILE
17	BQ	26	GLU
17	BQ	28	PHE
17	BQ	38	ILE
17	BQ	40	ARG
17	BQ	65	ARG
17	BQ	75	LEU
19	BS	6	LYS
19	BS	7	LYS
19	BS	13	LEU
19	BS	37	ARG
19	BS	52	HIS
19	BS	63	THR
20	BT	12	ILE
20	BT	14	SER
20	BT	26	SER
20	BT	36	TYR
20	BT	43	ASP
20	BT	54	MET
20	BT	58	VAL
20	BT	64	LYS
20	BT	66	LEU
20	BT	69	LYS
20	BT	84	ASN
21	BU	13	ASP
21	BU	16	LEU
21	BU	20	LYS
21	BU	56	HIS
22	D1	27	SER
22	D1	40	ARG
23	D2	5	ILE
23	D2	12	VAL
23	D2	47	VAL
23	D2	48	ILE
24	D3	1	MET
24	D3	14	ARG
24	D3	41	ARG

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Mol	Chain	Res	Type
25	D4	15	LYS
25	D4	31	HIS
25	D4	52	LYS
25	D4	55	LEU
26	D5	2	LYS
26	D5	22	VAL
26	D5	26	ILE
27	D0	7	ILE
27	D0	36	VAL
27	D0	39	GLU
27	D0	55	VAL
27	D0	58	GLU
29	CC	28	LYS
29	CC	116	ILE
29	CC	118	SER
29	CC	120	VAL
29	CC	130	LEU
29	CC	157	SER
29	CC	168	ASP
29	CC	185	GLU
29	CC	195	VAL
29	CC	204	VAL
29	CC	236	GLU
29	CC	245	VAL
29	CC	266	PHE
29	CC	271	ARG
30	CD	4	LEU
30	CD	13	ARG
30	CD	18	ASP
30	CD	32	ASN
30	CD	79	LEU
30	CD	95	SER
30	CD	126	ASN
30	CD	131	ASP
30	CD	138	LEU
30	CD	150	GLN
29	DC	28	LYS
29	DC	70	ASN
29	DC	116	ILE
29	DC	118	SER
29	DC	120	VAL
29	DC	130	LEU

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Mol	Chain	Res	Type
29	DC	185	GLU
29	DC	205	LEU
29	DC	236	GLU
29	DC	245	VAL
29	DC	265	LYS
29	DC	271	ARG
32	DD	13	ARG
32	DD	18	ASP
32	DD	32	ASN
32	DD	79	LEU
32	DD	86	GLU
32	DD	95	SER
32	DD	126	ASN
32	DD	129	THR
32	DD	131	ASP
32	DD	138	LEU
33	CE	7	ASP
33	CE	12	LEU
33	CE	25	GLU
33	CE	32	VAL
33	CE	44	ARG
33	CE	69	ARG
33	CE	72	SER
33	CE	78	TRP
33	CE	83	VAL
33	CE	107	SER
33	CE	120	VAL
33	CE	122	GLU
33	CE	127	GLU
33	CE	149	ILE
33	CE	152	GLU
33	CE	173	THR
33	CE	176	ASP
33	CE	189	THR
34	CF	35	THR
34	CF	36	LEU
34	CF	37	ASN
34	CF	50	LEU
34	CF	57	LEU
34	CF	72	LYS
34	CF	80	ARG
34	CF	94	GLU

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Mol	Chain	Res	Type
34	CF	98	GLU
34	CF	115	ARG
34	CF	117	LEU
34	CF	123	ASP
34	CF	134	GLU
34	CF	136	ILE
34	CF	150	ARG
34	CF	152	LEU
34	CF	174	ASP
35	CG	49	THR
35	CG	50	LEU
35	CG	56	ASP
35	CG	72	LEU
35	CG	127	THR
35	CG	155	GLU
35	CG	167	GLU
35	CG	171	THR
36	CH	3	VAL
36	CH	6	LEU
36	CH	15	LEU
36	CH	21	VAL
36	CH	48	GLU
36	CH	50	ARG
36	CH	51	ARG
36	CH	53	GLU
36	CH	55	GLU
36	CH	62	LEU
36	CH	89	LYS
36	CH	108	VAL
36	CH	110	VAL
36	CH	145	ASN
37	CJ	9	VAL
37	CJ	11	LEU
37	CJ	13	VAL
37	CJ	28	LEU
37	CJ	55	ILE
37	CJ	61	VAL
37	CJ	80	LEU
37	CJ	98	VAL
37	CJ	113	LYS
38	CK	5	THR
38	CK	7	LYS

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Mol	Chain	Res	Type
38	CK	9	GLU
38	CK	76	HIS
38	CK	124	VAL
38	CK	142	ILE
39	CL	18	ARG
39	CL	49	ARG
39	CL	58	LEU
39	CL	66	LYS
39	CL	80	ASP
39	CL	89	ASN
39	CL	91	SER
39	CL	98	ARG
40	CM	33	ARG
40	CM	40	SER
40	CM	68	SER
40	CM	92	LEU
40	CM	93	ASN
40	CM	100	ILE
40	CM	107	PHE
40	CM	115	GLU
40	CM	120	VAL
41	CN	6	ARG
41	CN	13	HIS
41	CN	20	LEU
41	CN	55	ARG
41	CN	59	ARG
41	CN	128	THR
41	CN	131	VAL
41	CN	132	THR
41	CN	134	THR
41	CN	135	VAL
42	CO	1	MET
42	CO	2	ARG
42	CO	6	SER
42	CO	14	SER
42	CO	53	THR
42	CO	59	SER
42	CO	69	ARG
42	CO	95	THR
43	CP	24	THR
43	CP	31	THR
43	CP	35	ILE

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Mol	Chain	Res	Type
43	CP	38	GLN
43	CP	45	SER
43	CP	47	VAL
43	CP	48	LEU
43	CP	78	VAL
43	CP	106	LEU
44	CQ	10	GLN
44	CQ	39	ARG
44	CQ	63	LYS
44	CQ	65	SER
44	CQ	85	SER
44	CQ	102	GLU
44	CQ	114	LEU
44	CQ	115	ASN
45	CR	5	LYS
45	CR	6	ARG
45	CR	9	ILE
45	CR	16	LYS
45	CR	51	ARG
45	CR	64	ARG
45	CR	109	LEU
45	CR	117	LEU
46	CS	1	MET
46	CS	12	HIS
46	CS	13	ARG
46	CS	15	SER
46	CS	26	ASP
46	CS	45	GLU
46	CS	46	GLU
46	CS	48	LYS
46	CS	51	VAL
46	CS	66	HIS
47	CT	29	VAL
47	CT	50	VAL
47	CT	53	SER
47	CT	59	GLU
47	CT	74	ILE
47	CT	83	LYS
47	CT	86	MET
47	CT	97	LEU
47	CT	109	ASP
47	CT	110	ARG

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Mol	Chain	Res	Type
48	CU	1	MET
48	CU	2	ILE
48	CU	3	ARG
48	CU	18	GLU
48	CU	30	ILE
48	CU	36	LYS
48	CU	49	LYS
48	CU	53	VAL
48	CU	69	ARG
48	CU	73	ARG
48	CU	79	ASP
48	CU	86	THR
48	CU	93	LEU
49	CV	9	ASP
49	CV	28	VAL
49	CV	29	LEU
49	CV	44	LYS
49	CV	52	LEU
49	CV	61	LYS
49	CV	81	ASP
49	CV	98	SER
50	CW	7	GLU
50	CW	10	LYS
50	CW	20	LEU
50	CW	53	LYS
50	CW	61	LEU
50	CW	62	THR
50	CW	68	LYS
50	CW	93	ARG
51	CX	41	ARG
51	CX	78	LYS
52	CY	4	VAL
52	CY	25	THR
52	CY	28	ARG
52	CY	71	LEU
53	CZ	18	LEU
53	CZ	19	LEU
53	CZ	22	LEU
53	CZ	58	ASN
33	DE	12	LEU
33	DE	32	VAL
33	DE	69	ARG

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Mol	Chain	Res	Type
33	DE	88	ARG
33	DE	107	SER
33	DE	120	VAL
33	DE	122	GLU
33	DE	127	GLU
33	DE	153	LEU
33	DE	173	THR
33	DE	176	ASP
33	DE	189	THR
34	DF	10	ASP
34	DF	35	THR
34	DF	37	ASN
34	DF	57	LEU
34	DF	72	LYS
34	DF	94	GLU
34	DF	98	GLU
34	DF	117	LEU
34	DF	134	GLU
34	DF	136	ILE
34	DF	148	ARG
34	DF	150	ARG
34	DF	152	LEU
34	DF	158	THR
34	DF	174	ASP
34	DF	178	ARG
35	DG	18	LYS
35	DG	50	LEU
35	DG	56	ASP
35	DG	72	LEU
35	DG	127	THR
35	DG	155	GLU
35	DG	167	GLU
35	DG	171	THR
36	DH	3	VAL
36	DH	6	LEU
36	DH	15	LEU
36	DH	21	VAL
36	DH	48	GLU
36	DH	50	ARG
36	DH	53	GLU
36	DH	58	LEU
36	DH	62	LEU

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Mol	Chain	Res	Type
36	DH	89	LYS
36	DH	108	VAL
36	DH	110	VAL
36	DH	145	ASN
37	DJ	9	VAL
37	DJ	11	LEU
37	DJ	13	VAL
37	DJ	28	LEU
37	DJ	55	ILE
37	DJ	61	VAL
37	DJ	80	LEU
37	DJ	98	VAL
37	DJ	113	LYS
38	DK	7	LYS
38	DK	30	THR
38	DK	76	HIS
38	DK	124	VAL
38	DK	142	ILE
39	DL	18	ARG
39	DL	49	ARG
39	DL	58	LEU
39	DL	66	LYS
39	DL	75	SER
39	DL	80	ASP
39	DL	89	ASN
39	DL	91	SER
39	DL	109	SER
39	DL	110	GLU
39	DL	113	MET
40	DM	40	SER
40	DM	86	GLU
40	DM	92	LEU
40	DM	107	PHE
40	DM	115	GLU
40	DM	120	VAL
41	DN	6	ARG
41	DN	10	ARG
41	DN	55	ARG
41	DN	58	LYS
41	DN	100	LYS
41	DN	126	ILE
41	DN	128	THR

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Mol	Chain	Res	Type
41	DN	131	VAL
41	DN	132	THR
41	DN	134	THR
41	DN	135	VAL
42	DO	1	MET
42	DO	2	ARG
42	DO	6	SER
42	DO	14	SER
42	DO	46	ARG
42	DO	53	THR
42	DO	59	SER
42	DO	69	ARG
43	DP	1	MET
43	DP	24	THR
43	DP	31	THR
43	DP	35	ILE
43	DP	45	SER
43	DP	47	VAL
43	DP	48	LEU
43	DP	78	VAL
43	DP	106	LEU
44	DQ	10	GLN
44	DQ	40	LEU
44	DQ	63	LYS
44	DQ	65	SER
44	DQ	85	SER
44	DQ	102	GLU
44	DQ	115	ASN
45	DR	5	LYS
45	DR	6	ARG
45	DR	51	ARG
45	DR	64	ARG
45	DR	109	LEU
45	DR	117	LEU
46	DS	1	MET
46	DS	7	SER
46	DS	13	ARG
46	DS	15	SER
46	DS	20	VAL
46	DS	26	ASP
46	DS	38	VAL
46	DS	58	VAL

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Mol	Chain	Res	Type
46	DS	66	HIS
47	DT	29	VAL
47	DT	50	VAL
47	DT	53	SER
47	DT	59	GLU
47	DT	74	ILE
47	DT	86	MET
47	DT	109	ASP
47	DT	110	ARG
48	DU	2	ILE
48	DU	3	ARG
48	DU	25	GLU
48	DU	53	VAL
48	DU	69	ARG
48	DU	74	ILE
48	DU	79	ASP
48	DU	86	THR
49	DV	26	LYS
49	DV	28	VAL
49	DV	29	LEU
49	DV	44	LYS
49	DV	61	LYS
49	DV	81	ASP
50	DW	7	GLU
50	DW	20	LEU
50	DW	53	LYS
50	DW	61	LEU
50	DW	62	THR
50	DW	93	ARG
51	DX	11	ARG
51	DX	41[A]	ARG
51	DX	41[B]	ARG
51	DX	78	LYS
52	DY	4	VAL
52	DY	25	THR
52	DY	28	ARG
52	DY	48	THR
52	DY	51	VAL
53	DZ	6	LEU
53	DZ	19	LEU
53	DZ	22	LEU
54	DI	7	ASP

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Mol	Chain	Res	Type
54	DI	23	LEU
54	DI	31	ARG
54	DI	53	ARG
54	DI	58	THR
54	DI	61	ARG
54	DI	64	VAL
54	DI	67	THR
54	DI	74	ASP
54	DI	82	ILE
54	DI	95	LEU
54	DI	117	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	39	HIS
2	AB	93	ASN
2	AB	120	GLN
2	AB	177	ASN
3	AC	139	GLN
4	AD	136	GLN
4	AD	196	ASN
5	AE	82	GLN
5	AE	89	HIS
5	AE	97	GLN
6	AF	14	GLN
6	AF	63	ASN
7	AG	97	ASN
9	AI	31	ASN
10	AJ	58	ASN
11	AK	24	HIS
11	AK	101	ASN
16	AP	63	GLN
19	AS	52	HIS
19	AS	53	ASN
19	AS	56	GLN
19	AS	57	HIS
20	AT	48	GLN
22	C1	6	ASN
22	C1	42	HIS
2	BB	39	HIS
2	BB	93	ASN

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Mol	Chain	Res	Type
2	BB	120	GLN
2	BB	177	ASN
3	BC	139	GLN
5	BE	82	GLN
5	BE	89	HIS
5	BE	97	GLN
6	BF	14	GLN
7	BG	97	ASN
7	BG	142	HIS
9	BI	31	ASN
11	BK	101	ASN
16	BP	63	GLN
19	BS	53	ASN
19	BS	57	HIS
20	BT	13	GLN
20	BT	20	HIS
29	CC	45	ASN
29	CC	70	ASN
30	CD	130	GLN
30	CD	150	GLN
30	CD	164	GLN
29	DC	45	ASN
29	DC	70	ASN
34	CF	27	GLN
35	CG	38	ASN
37	CJ	43	ASN
38	CK	47	HIS
40	CM	38	GLN
43	CP	100	HIS
49	CV	74	ASN
52	CY	16	ASN
35	DG	22	GLN
37	DJ	30	GLN
37	DJ	43	ASN
38	DK	47	HIS
41	DN	60	GLN
42	DO	13	ASN
43	DP	38	GLN
44	DQ	115	ASN
45	DR	56	GLN
49	DV	54	GLN
50	DW	24	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	296 (19%)	48 (3%)
1	BA	1529/1534 (99%)	300 (19%)	52 (3%)
28	CB	117/120 (97%)	13 (11%)	2 (1%)
28	DB	119/120 (99%)	13 (10%)	1 (0%)
31	CA	2892/2904 (99%)	572 (19%)	110 (3%)
55	DA	2880/2904 (99%)	490 (17%)	73 (2%)
All	All	9067/9116 (99%)	1684 (18%)	286 (3%)

All (1684) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	8	A
1	AA	9	G
1	AA	22	G
1	AA	28	A
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	49	U
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	54	C
1	AA	69	G
1	AA	70	U
1	AA	71	A
1	AA	72	A
1	AA	74	A
1	AA	79	G
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	88	U

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Mol	Chain	Res	Type
1	AA	89	U
1	AA	90	C
1	AA	92	U
1	AA	94	G
1	AA	95	C
1	AA	108	G
1	AA	119	A
1	AA	120	A
1	AA	127	G
1	AA	128	G
1	AA	130	A
1	AA	131	A
1	AA	141	G
1	AA	142	G
1	AA	143	A
1	AA	144	G
1	AA	146	G
1	AA	149	A
1	AA	159	G
1	AA	163	C
1	AA	168	G
1	AA	189	A
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	251	G
1	AA	262	A
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	306	A
1	AA	308	C
1	AA	321	A
1	AA	328	C
1	AA	329	A

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Mol	Chain	Res	Type
1	AA	332	G
1	AA	346	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	368	U
1	AA	372	C
1	AA	373	A
1	AA	376	G
1	AA	384	G
1	AA	396	C
1	AA	397	A
1	AA	398	U
1	AA	406	G
1	AA	411	A
1	AA	413	G
1	AA	414	A
1	AA	421	U
1	AA	422	C
1	AA	424	G
1	AA	429	U
1	AA	436	C
1	AA	451	A
1	AA	457	G
1	AA	458	U
1	AA	463	U
1	AA	467	U
1	AA	468	A
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	505	G
1	AA	509	A
1	AA	511	C
1	AA	521	G
1	AA	524	G
1	AA	527	7MG
1	AA	530	G
1	AA	531	U
1	AA	533	A
1	AA	547	A

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Mol	Chain	Res	Type
1	AA	559	A
1	AA	564	C
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	596	A
1	AA	615	G
1	AA	633	G
1	AA	639	G
1	AA	642	A
1	AA	650	G
1	AA	653	U
1	AA	656	G
1	AA	665	A
1	AA	671	G
1	AA	675	A
1	AA	677	U
1	AA	702	A
1	AA	703	G
1	AA	721	G
1	AA	723	U
1	AA	724	G
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	758	C
1	AA	774	G
1	AA	777	A
1	AA	782	A
1	AA	793	U
1	AA	794	A
1	AA	809	G
1	AA	815	A
1	AA	817	C
1	AA	821	G
1	AA	828	U
1	AA	832	G
1	AA	836	G
1	AA	839	C
1	AA	841	C
1	AA	842	U

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Mol	Chain	Res	Type
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	884	U
1	AA	902	G
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	942	G
1	AA	955	U
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	971	G
1	AA	972	C
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	985	C
1	AA	987	G
1	AA	992	U
1	AA	993	G
1	AA	1004	A
1	AA	1008	U
1	AA	1015	G
1	AA	1019	A
1	AA	1024	G
1	AA	1026	G
1	AA	1027	C
1	AA	1029	U
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1036	A
1	AA	1037	C
1	AA	1043	G
1	AA	1044	A
1	AA	1053	G
1	AA	1054	C

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Mol	Chain	Res	Type
1	AA	1055	A
1	AA	1064	G
1	AA	1065	U
1	AA	1070	U
1	AA	1086	U
1	AA	1089	G
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1104	G
1	AA	1124	G
1	AA	1125	U
1	AA	1132	C
1	AA	1133	G
1	AA	1136	C
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1142	G
1	AA	1145	A
1	AA	1152	A
1	AA	1159	U
1	AA	1160	G
1	AA	1168	U
1	AA	1182	G
1	AA	1183	U
1	AA	1184	G
1	AA	1186	G
1	AA	1196	A
1	AA	1197	A
1	AA	1198	G
1	AA	1201	A
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1221	G
1	AA	1224	U
1	AA	1225	A

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Mol	Chain	Res	Type
1	AA	1226	C
1	AA	1227	A
1	AA	1233	G
1	AA	1236	A
1	AA	1238	A
1	AA	1239	A
1	AA	1256	A
1	AA	1257	A
1	AA	1258	G
1	AA	1260	G
1	AA	1274	A
1	AA	1280	A
1	AA	1281	C
1	AA	1286	U
1	AA	1287	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1312	G
1	AA	1317	C
1	AA	1318	A
1	AA	1319	A
1	AA	1320	C
1	AA	1323	G
1	AA	1338	G
1	AA	1351	U
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1379	G
1	AA	1381	U
1	AA	1398	A
1	AA	1419	G
1	AA	1422	G
1	AA	1441	A
1	AA	1446	A
1	AA	1448	C
1	AA	1451	U
1	AA	1452	C
1	AA	1453	G
1	AA	1475	G
1	AA	1483	A

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Mol	Chain	Res	Type
1	AA	1484	C
1	AA	1487	G
1	AA	1492	A
1	AA	1493	A
1	AA	1497	G
1	AA	1503	A
1	AA	1505	G
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1533	C
1	AA	1534	A
1	BA	5	U
1	BA	6	G
1	BA	7	A
1	BA	8	A
1	BA	9	G
1	BA	22	G
1	BA	28	A
1	BA	31	G
1	BA	32	A
1	BA	39	G
1	BA	47	C
1	BA	48	C
1	BA	49	U
1	BA	50	A
1	BA	51	A
1	BA	52	C
1	BA	54	C
1	BA	69	G
1	BA	70	U
1	BA	71	A
1	BA	72	A
1	BA	74	A
1	BA	79	G
1	BA	82	G
1	BA	83	C
1	BA	84	U
1	BA	85	U
1	BA	86	G

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Mol	Chain	Res	Type
1	BA	87	C
1	BA	89	U
1	BA	90	C
1	BA	92	U
1	BA	94	G
1	BA	95	C
1	BA	108	G
1	BA	119	A
1	BA	120	A
1	BA	127	G
1	BA	128	G
1	BA	130	A
1	BA	131	A
1	BA	141	G
1	BA	142	G
1	BA	143	A
1	BA	144	G
1	BA	146	G
1	BA	149	A
1	BA	159	G
1	BA	163	C
1	BA	168	G
1	BA	189	A
1	BA	197	A
1	BA	200	G
1	BA	205	A
1	BA	210	C
1	BA	211	G
1	BA	212	G
1	BA	226	G
1	BA	240	G
1	BA	245	U
1	BA	247	G
1	BA	251	G
1	BA	262	A
1	BA	266	G
1	BA	267	C
1	BA	289	G
1	BA	306	A
1	BA	308	C
1	BA	321	A
1	BA	328	C

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Mol	Chain	Res	Type
1	BA	329	A
1	BA	332	G
1	BA	346	G
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	368	U
1	BA	372	C
1	BA	373	A
1	BA	376	G
1	BA	384	G
1	BA	396	C
1	BA	397	A
1	BA	398	U
1	BA	406	G
1	BA	411	A
1	BA	412	A
1	BA	413	G
1	BA	414	A
1	BA	421	U
1	BA	422	C
1	BA	424	G
1	BA	429	U
1	BA	436	C
1	BA	451	A
1	BA	457	G
1	BA	458	U
1	BA	463	U
1	BA	467	U
1	BA	468	A
1	BA	481	G
1	BA	484	G
1	BA	486	U
1	BA	495	A
1	BA	505	G
1	BA	509	A
1	BA	511	C
1	BA	521	G
1	BA	524	G
1	BA	525	C
1	BA	527	7MG
1	BA	530	G

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Mol	Chain	Res	Type
1	BA	531	U
1	BA	532	A
1	BA	533	A
1	BA	547	A
1	BA	559	A
1	BA	560	A
1	BA	564	C
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
1	BA	596	A
1	BA	615	G
1	BA	633	G
1	BA	639	G
1	BA	642	A
1	BA	650	G
1	BA	653	U
1	BA	656	G
1	BA	665	A
1	BA	671	G
1	BA	675	A
1	BA	677	U
1	BA	702	A
1	BA	703	G
1	BA	721	G
1	BA	723	U
1	BA	724	G
1	BA	734	G
1	BA	748	G
1	BA	755	G
1	BA	758	C
1	BA	774	G
1	BA	777	A
1	BA	782	A
1	BA	793	U
1	BA	794	A
1	BA	809	G
1	BA	815	A
1	BA	817	C
1	BA	821	G
1	BA	828	U

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Mol	Chain	Res	Type
1	BA	832	G
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	845	A
1	BA	846	G
1	BA	902	G
1	BA	914	A
1	BA	926	G
1	BA	927	G
1	BA	934	C
1	BA	935	A
1	BA	942	G
1	BA	955	U
1	BA	960	U
1	BA	966	2MG
1	BA	969	A
1	BA	971	G
1	BA	972	C
1	BA	975	A
1	BA	976	G
1	BA	977	A
1	BA	985	C
1	BA	987	G
1	BA	992	U
1	BA	993	G
1	BA	1004	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	1024	G
1	BA	1026	G
1	BA	1027	C
1	BA	1029	U
1	BA	1030	U
1	BA	1031	C
1	BA	1032	G
1	BA	1033	G

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Mol	Chain	Res	Type
1	BA	1036	A
1	BA	1037	C
1	BA	1043	G
1	BA	1044	A
1	BA	1053	G
1	BA	1054	C
1	BA	1055	A
1	BA	1064	G
1	BA	1065	U
1	BA	1066	C
1	BA	1086	U
1	BA	1089	G
1	BA	1094	G
1	BA	1095	U
1	BA	1101	A
1	BA	1104	G
1	BA	1124	G
1	BA	1125	U
1	BA	1132	C
1	BA	1133	G
1	BA	1136	C
1	BA	1137	C
1	BA	1138	G
1	BA	1139	G
1	BA	1140	C
1	BA	1141	C
1	BA	1142	G
1	BA	1145	A
1	BA	1152	A
1	BA	1159	U
1	BA	1160	G
1	BA	1168	U
1	BA	1182	G
1	BA	1183	U
1	BA	1186	G
1	BA	1196	A
1	BA	1197	A
1	BA	1198	G
1	BA	1201	A
1	BA	1202	U
1	BA	1212	U
1	BA	1213	A

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Mol	Chain	Res	Type
1	BA	1214	C
1	BA	1215	G
1	BA	1221	G
1	BA	1224	U
1	BA	1225	A
1	BA	1226	C
1	BA	1227	A
1	BA	1233	G
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	1274	A
1	BA	1280	A
1	BA	1281	C
1	BA	1286	U
1	BA	1287	A
1	BA	1300	G
1	BA	1302	C
1	BA	1305	G
1	BA	1312	G
1	BA	1317	C
1	BA	1318	A
1	BA	1319	A
1	BA	1320	C
1	BA	1323	G
1	BA	1337	G
1	BA	1338	G
1	BA	1351	U
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	1419	G
1	BA	1422	G
1	BA	1441	A

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Mol	Chain	Res	Type
1	BA	1446	A
1	BA	1448	C
1	BA	1451	U
1	BA	1452	C
1	BA	1453	G
1	BA	1475	G
1	BA	1483	A
1	BA	1484	C
1	BA	1487	G
1	BA	1493	A
1	BA	1497	G
1	BA	1499	A
1	BA	1505	G
1	BA	1506	U
1	BA	1507	A
1	BA	1517	G
1	BA	1529	G
1	BA	1530	G
1	BA	1533	C
1	BA	1534	A
28	CB	25	U
28	CB	35	C
28	CB	44	G
28	CB	45	A
28	CB	51	G
28	CB	56	G
28	CB	57	A
28	CB	87	U
28	CB	88	C
28	CB	89	U
28	CB	90	C
28	CB	99	A
28	CB	109	A
31	CA	10	A
31	CA	13	A
31	CA	34	U
31	CA	36	G
31	CA	39	G
31	CA	42	A
31	CA	46	G
31	CA	49	A
31	CA	71	A

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Mol	Chain	Res	Type
31	CA	73	A
31	CA	74	A
31	CA	75	G
31	CA	80	G
31	CA	83	A
31	CA	84	A
31	CA	86	G
31	CA	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	177	G
31	CA	178	G
31	CA	186	G
31	CA	188	G
31	CA	196	A
31	CA	197	A
31	CA	199	A
31	CA	201	C
31	CA	204	A
31	CA	215	G
31	CA	216	A
31	CA	222	A
31	CA	245	G
31	CA	248	G
31	CA	250	G
31	CA	265	A
31	CA	266	G
31	CA	267	C
31	CA	272	A
31	CA	276	U
31	CA	277	G
31	CA	278	A
31	CA	285	G
31	CA	310	A
31	CA	311	A

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Mol	Chain	Res	Type
31	CA	317	G
31	CA	324	A
31	CA	329	G
31	CA	330	A
31	CA	331	C
31	CA	343	C
31	CA	346	A
31	CA	352	A
31	CA	353	C
31	CA	361	G
31	CA	362	A
31	CA	371	A
31	CA	372	G
31	CA	383	C
31	CA	385	C
31	CA	386	G
31	CA	391	A
31	CA	396	G
31	CA	399	U
31	CA	403	U
31	CA	405	U
31	CA	411	G
31	CA	412	A
31	CA	420	C
31	CA	424	G
31	CA	435	C
31	CA	451	U
31	CA	455	C
31	CA	456	C
31	CA	457	A
31	CA	475	C
31	CA	479	A
31	CA	480	A
31	CA	481	G
31	CA	482	A
31	CA	491	G
31	CA	496	G
31	CA	501	A
31	CA	504	A
31	CA	505	A
31	CA	507	A
31	CA	508	A

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Mol	Chain	Res	Type
31	CA	527	C
31	CA	528	A
31	CA	529	A
31	CA	531	C
31	CA	532	A
31	CA	533	G
31	CA	543	G
31	CA	544	C
31	CA	546	U
31	CA	547	A
31	CA	548	G
31	CA	549	G
31	CA	550	C
31	CA	563	A
31	CA	569	U
31	CA	572	A
31	CA	573	U
31	CA	574	A
31	CA	575	A
31	CA	586	A
31	CA	592	A
31	CA	603	A
31	CA	614	A
31	CA	615	U
31	CA	620	G
31	CA	621	A
31	CA	622	G
31	CA	627	A
31	CA	628	G
31	CA	632	A
31	CA	634	C
31	CA	637	A
31	CA	645	C
31	CA	647	G
31	CA	651	G
31	CA	653	U
31	CA	654	A
31	CA	655	A
31	CA	659	G
31	CA	669	G
31	CA	670	A
31	CA	684	G

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Mol	Chain	Res	Type
31	CA	685	A
31	CA	686	U
31	CA	694	U
31	CA	695	G
31	CA	696	G
31	CA	701	G
31	CA	702	U
31	CA	717	C
31	CA	730	A
31	CA	740	C
31	CA	747	5MU
31	CA	763	G
31	CA	764	A
31	CA	765	C
31	CA	774	G
31	CA	775	G
31	CA	776	G
31	CA	781	A
31	CA	782	A
31	CA	784	G
31	CA	785	G
31	CA	792	A
31	CA	798	G
31	CA	800	A
31	CA	805	G
31	CA	812	C
31	CA	819	A
31	CA	827	U
31	CA	828	U
31	CA	831	G
31	CA	845	A
31	CA	846	U
31	CA	847	U
31	CA	858	G
31	CA	859	G
31	CA	866	A
31	CA	869	G
31	CA	878	A
31	CA	882	G
31	CA	896	A
31	CA	897	C
31	CA	907	G

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Mol	Chain	Res	Type
31	CA	910	A
31	CA	914	G
31	CA	931	U
31	CA	932	U
31	CA	941	A
31	CA	946	C
31	CA	953	G
31	CA	957	C
31	CA	961	C
31	CA	973	A
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	999	U
31	CA	1009	A
31	CA	1012	U
31	CA	1013	C
31	CA	1017	G
31	CA	1020	A
31	CA	1021	A
31	CA	1022	G
31	CA	1024	G
31	CA	1026	G
31	CA	1033	U
31	CA	1040	A
31	CA	1045	C
31	CA	1046	A
31	CA	1047	G
31	CA	1051	G
31	CA	1061	U
31	CA	1062	G
31	CA	1068	G
31	CA	1069	A
31	CA	1070	A
31	CA	1073	A
31	CA	1083	U
31	CA	1088	A
31	CA	1090	A
31	CA	1097	U

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Mol	Chain	Res	Type
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	1135	C
31	CA	1136	G
31	CA	1141	U
31	CA	1142	A
31	CA	1143	A
31	CA	1151	A
31	CA	1168	G
31	CA	1169	A
31	CA	1172	C
31	CA	1175	A
31	CA	1176	U
31	CA	1177	G
31	CA	1179	G
31	CA	1180	U
31	CA	1186	G
31	CA	1212	G
31	CA	1236	G
31	CA	1238	G
31	CA	1244	A
31	CA	1247	A
31	CA	1248	G
31	CA	1250	G
31	CA	1253	A
31	CA	1256	G
31	CA	1262	A
31	CA	1266	G
31	CA	1271	G
31	CA	1272	A
31	CA	1288	G
31	CA	1289	C
31	CA	1294	U
31	CA	1300	G
31	CA	1301	A
31	CA	1306	C

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Mol	Chain	Res	Type
31	CA	1312	U
31	CA	1313	U
31	CA	1321	A
31	CA	1328	A
31	CA	1329	U
31	CA	1330	C
31	CA	1332	G
31	CA	1344	U
31	CA	1352	U
31	CA	1355	G
31	CA	1359	A
31	CA	1365	A
31	CA	1370	C
31	CA	1376	C
31	CA	1379	U
31	CA	1380	G
31	CA	1383	A
31	CA	1386	C
31	CA	1395	A
31	CA	1398	C
31	CA	1403	A
31	CA	1416	G
31	CA	1417	C
31	CA	1420	A
31	CA	1424	G
31	CA	1427	A
31	CA	1428	C
31	CA	1434	A
31	CA	1437	C
31	CA	1452	G
31	CA	1458	U
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

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Mol	Chain	Res	Type
31	CA	1515	A
31	CA	1522	A
31	CA	1523	U
31	CA	1529	G
31	CA	1532	A
31	CA	1534	U
31	CA	1535	A
31	CA	1536	C
31	CA	1537	G
31	CA	1544	A
31	CA	1555	G
31	CA	1565	C
31	CA	1566	A
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	1611	C
31	CA	1613	G
31	CA	1617	C
31	CA	1634	A
31	CA	1647	U
31	CA	1648	U
31	CA	1649	G
31	CA	1663	G
31	CA	1664	A
31	CA	1674	G
31	CA	1677	A
31	CA	1694	C
31	CA	1697	G
31	CA	1698	A
31	CA	1699	G
31	CA	1703	G
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

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Mol	Chain	Res	Type
31	CA	1758	U
31	CA	1764	C
31	CA	1773	A
31	CA	1781	U
31	CA	1782	U
31	CA	1784	A
31	CA	1786	A
31	CA	1787	A
31	CA	1800	C
31	CA	1801	A
31	CA	1808	A
31	CA	1812	U
31	CA	1815	A
31	CA	1816	C
31	CA	1821	A
31	CA	1822	C
31	CA	1823	G
31	CA	1828	G
31	CA	1829	A
31	CA	1833	C
31	CA	1834	U
31	CA	1839	G
31	CA	1869	G
31	CA	1870	C
31	CA	1871	A
31	CA	1872	A
31	CA	1873	G
31	CA	1882	U
31	CA	1900	A
31	CA	1902	C
31	CA	1903	G
31	CA	1906	G
31	CA	1907	G
31	CA	1914	C
31	CA	1928	A
31	CA	1929	G
31	CA	1930	G
31	CA	1931	U
31	CA	1934	C
31	CA	1938	A
31	CA	1940	U
31	CA	1955	U

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Mol	Chain	Res	Type
31	CA	1965	C
31	CA	1966	A
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	2020	A
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	2051	A
31	CA	2055	C
31	CA	2056	G
31	CA	2060	A
31	CA	2061	G
31	CA	2062	A
31	CA	2069	7MG
31	CA	2072	C
31	CA	2092	U
31	CA	2093	G
31	CA	2095	A
31	CA	2100	G
31	CA	2101	A
31	CA	2108	A
31	CA	2110	G
31	CA	2111	U
31	CA	2112	G
31	CA	2113	U
31	CA	2114	A
31	CA	2115	G
31	CA	2117	A
31	CA	2118	U
31	CA	2119	A

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Mol	Chain	Res	Type
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	2145	C
31	CA	2146	C
31	CA	2147	A
31	CA	2157	G
31	CA	2158	A
31	CA	2159	G
31	CA	2161	C
31	CA	2162	G
31	CA	2163	A
31	CA	2164	C
31	CA	2165	C
31	CA	2171	A
31	CA	2172	U
31	CA	2173	A
31	CA	2174	C
31	CA	2178	C
31	CA	2190	G
31	CA	2198	A
31	CA	2203	U
31	CA	2204	G
31	CA	2211	A
31	CA	2225	A
31	CA	2226	C
31	CA	2238	G
31	CA	2239	G
31	CA	2243	U
31	CA	2259	U
31	CA	2268	A
31	CA	2278	A
31	CA	2282	G
31	CA	2283	C
31	CA	2287	A

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Mol	Chain	Res	Type
31	CA	2288	A
31	CA	2305	U
31	CA	2311	A
31	CA	2325	G
31	CA	2326	C
31	CA	2327	A
31	CA	2331	G
31	CA	2333	A
31	CA	2335	A
31	CA	2345	G
31	CA	2347	C
31	CA	2350	C
31	CA	2354	C
31	CA	2357	G
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	2423	U
31	CA	2424	C
31	CA	2425	A
31	CA	2426	A
31	CA	2429	G
31	CA	2430	A
31	CA	2435	A
31	CA	2436	G
31	CA	2441	U
31	CA	2446	G
31	CA	2448	A
31	CA	2449	U
31	CA	2469	A
31	CA	2474	U
31	CA	2476	A
31	CA	2491	U
31	CA	2498	OMC
31	CA	2502	G
31	CA	2505	G
31	CA	2512	C
31	CA	2513	A
31	CA	2518	A

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Mol	Chain	Res	Type
31	CA	2520	C
31	CA	2529	G
31	CA	2535	G
31	CA	2543	G
31	CA	2544	G
31	CA	2547	A
31	CA	2554	U
31	CA	2564	A
31	CA	2566	A
31	CA	2567	G
31	CA	2573	C
31	CA	2582	G
31	CA	2585	U
31	CA	2600	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	2673	G
31	CA	2681	C
31	CA	2682	A
31	CA	2689	U
31	CA	2690	U
31	CA	2714	G
31	CA	2718	G
31	CA	2726	A
31	CA	2733	A
31	CA	2744	G
31	CA	2748	A
31	CA	2762	C
31	CA	2765	A
31	CA	2776	A
31	CA	2777	G
31	CA	2778	A
31	CA	2779	U
31	CA	2791	G
31	CA	2794	C
31	CA	2798	U

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Mol	Chain	Res	Type
31	CA	2799	A
31	CA	2818	U
31	CA	2820	A
31	CA	2821	A
31	CA	2835	A
31	CA	2836	U
31	CA	2849	U
31	CA	2850	A
31	CA	2861	U
31	CA	2867	G
31	CA	2870	C
31	CA	2872	A
31	CA	2879	A
31	CA	2883	A
31	CA	2886	A
31	CA	2893	A
31	CA	2894	G
28	DB	25	U
28	DB	35	C
28	DB	37	C
28	DB	44	G
28	DB	45	A
28	DB	51	G
28	DB	56	G
28	DB	57	A
28	DB	87	U
28	DB	88	C
28	DB	89	U
28	DB	90	C
28	DB	109	A
55	DA	10	A
55	DA	12	U
55	DA	13	A
55	DA	14	A
55	DA	15	G
55	DA	34	U
55	DA	46	G
55	DA	58	G
55	DA	71	A
55	DA	74	A
55	DA	75	G
55	DA	80	G

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Mol	Chain	Res	Type
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	137	U
55	DA	138	U
55	DA	139	U
55	DA	140	C
55	DA	141	G
55	DA	142	A
55	DA	186	G
55	DA	188	G
55	DA	193	U
55	DA	196	A
55	DA	197	A
55	DA	198	C
55	DA	199	A
55	DA	200	U
55	DA	215	G
55	DA	216	A
55	DA	221	A
55	DA	222	A
55	DA	230	G
55	DA	248	G
55	DA	265	A
55	DA	266	G
55	DA	267	C
55	DA	272	A
55	DA	276	U
55	DA	277	G
55	DA	278	A
55	DA	285	G
55	DA	302	C
55	DA	311	A
55	DA	317	G
55	DA	324	A
55	DA	329	G
55	DA	330	A

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Mol	Chain	Res	Type
55	DA	331	C
55	DA	343	C
55	DA	346	A
55	DA	352	A
55	DA	353	C
55	DA	361	G
55	DA	362	A
55	DA	372	G
55	DA	383	C
55	DA	386	G
55	DA	396	G
55	DA	399	U
55	DA	403	U
55	DA	406	G
55	DA	411	G
55	DA	412	A
55	DA	420	C
55	DA	424	G
55	DA	435	C
55	DA	451	U
55	DA	455	C
55	DA	456	C
55	DA	459	U
55	DA	475	C
55	DA	479	A
55	DA	480	A
55	DA	481	G
55	DA	482	A
55	DA	491	G
55	DA	496	G
55	DA	504	A
55	DA	505	A
55	DA	508	A
55	DA	510	C
55	DA	513	A
55	DA	531	C
55	DA	532	A
55	DA	533	G
55	DA	543	G
55	DA	544	C
55	DA	546	U
55	DA	547	A

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Mol	Chain	Res	Type
55	DA	548	G
55	DA	549	G
55	DA	550	C
55	DA	563	A
55	DA	573	U
55	DA	575	A
55	DA	586	A
55	DA	603	A
55	DA	613	A
55	DA	614	A
55	DA	615	U
55	DA	620	G
55	DA	622	G
55	DA	627	A
55	DA	637	A
55	DA	645	C
55	DA	647	G
55	DA	651	G
55	DA	653	U
55	DA	654	A
55	DA	655	A
55	DA	659	G
55	DA	684	G
55	DA	685	A
55	DA	686	U
55	DA	717	C
55	DA	730	A
55	DA	738	G
55	DA	747	5MU
55	DA	764	A
55	DA	765	C
55	DA	772	C
55	DA	775	G
55	DA	776	G
55	DA	782	A
55	DA	783	A
55	DA	784	G
55	DA	785	G
55	DA	790	U
55	DA	801	G
55	DA	802	A
55	DA	805	G

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Mol	Chain	Res	Type
55	DA	806	C
55	DA	812	C
55	DA	827	U
55	DA	828	U
55	DA	858	G
55	DA	859	G
55	DA	866	A
55	DA	878	A
55	DA	882	G
55	DA	885	C
55	DA	896	A
55	DA	897	C
55	DA	907	G
55	DA	910	A
55	DA	914	G
55	DA	915	C
55	DA	931	U
55	DA	932	U
55	DA	946	C
55	DA	947	A
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	1010	A
55	DA	1012	U
55	DA	1013	C
55	DA	1022	G
55	DA	1023	U
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	1069	A
55	DA	1070	A
55	DA	1073	A

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Mol	Chain	Res	Type
55	DA	1083	U
55	DA	1088	A
55	DA	1090	A
55	DA	1096	A
55	DA	1097	U
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	1135	C
55	DA	1136	G
55	DA	1141	U
55	DA	1142	A
55	DA	1151	A
55	DA	1168	G
55	DA	1172	C
55	DA	1174	U
55	DA	1176	U
55	DA	1177	G
55	DA	1180	U
55	DA	1212	G
55	DA	1238	G
55	DA	1244	A
55	DA	1250	G
55	DA	1253	A
55	DA	1256	G
55	DA	1262	A
55	DA	1269	A
55	DA	1271	G
55	DA	1272	A
55	DA	1273	U
55	DA	1294	U
55	DA	1297	C
55	DA	1300	G
55	DA	1301	A
55	DA	1306	C
55	DA	1321	A
55	DA	1328	A
55	DA	1332	G
55	DA	1352	U

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Mol	Chain	Res	Type
55	DA	1355	G
55	DA	1359	A
55	DA	1365	A
55	DA	1379	U
55	DA	1383	A
55	DA	1386	C
55	DA	1398	C
55	DA	1403	A
55	DA	1416	G
55	DA	1417	C
55	DA	1420	A
55	DA	1427	A
55	DA	1428	C
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
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	1534	U
55	DA	1535	A
55	DA	1537	G
55	DA	1544	A
55	DA	1554	U
55	DA	1566	A
55	DA	1569	A
55	DA	1578	U
55	DA	1583	A
55	DA	1585	C
55	DA	1607	C

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Mol	Chain	Res	Type
55	DA	1608	A
55	DA	1613	G
55	DA	1647	U
55	DA	1648	U
55	DA	1649	G
55	DA	1663	G
55	DA	1674	G
55	DA	1694	C
55	DA	1699	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	1758	U
55	DA	1764	C
55	DA	1773	A
55	DA	1781	U
55	DA	1782	U
55	DA	1786	A
55	DA	1800	C
55	DA	1801	A
55	DA	1808	A
55	DA	1812	U
55	DA	1816	C
55	DA	1826	G
55	DA	1829	A
55	DA	1869	G
55	DA	1870	C
55	DA	1871	A
55	DA	1872	A
55	DA	1873	G
55	DA	1900	A
55	DA	1906	G
55	DA	1907	G
55	DA	1913	A
55	DA	1914	C
55	DA	1927	A
55	DA	1929	G
55	DA	1930	G
55	DA	1931	U

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Mol	Chain	Res	Type
55	DA	1932	A
55	DA	1938	A
55	DA	1941	C
55	DA	1955	U
55	DA	1965	C
55	DA	1967	C
55	DA	1970	A
55	DA	1972	G
55	DA	1974	C
55	DA	1991	U
55	DA	1992	G
55	DA	1993	U
55	DA	1997	C
55	DA	2020	A
55	DA	2023	C
55	DA	2031	A
55	DA	2033	A
55	DA	2043	C
55	DA	2049	G
55	DA	2055	C
55	DA	2056	G
55	DA	2060	A
55	DA	2061	G
55	DA	2062	A
55	DA	2069	7MG
55	DA	2093	G
55	DA	2095	A
55	DA	2097	A
55	DA	2100	G
55	DA	2101	A
55	DA	2105	U
55	DA	2108	A
55	DA	2111	U
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	2121	G
55	DA	2123	G

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Mol	Chain	Res	Type
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	2147	A
55	DA	2148	G
55	DA	2157	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	2185	U
55	DA	2186	G
55	DA	2198	A
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

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Mol	Chain	Res	Type
55	DA	2280	G
55	DA	2283	C
55	DA	2286	G
55	DA	2287	A
55	DA	2288	A
55	DA	2292	U
55	DA	2305	U
55	DA	2308	G
55	DA	2311	A
55	DA	2312	U
55	DA	2320	U
55	DA	2325	G
55	DA	2327	A
55	DA	2328	A
55	DA	2331	G
55	DA	2333	A
55	DA	2335	A
55	DA	2347	C
55	DA	2350	C
55	DA	2357	G
55	DA	2383	G
55	DA	2385	C
55	DA	2402	U
55	DA	2403	C
55	DA	2406	A
55	DA	2410	G
55	DA	2423	U
55	DA	2424	C
55	DA	2425	A
55	DA	2426	A
55	DA	2427	C
55	DA	2434	A
55	DA	2435	A
55	DA	2441	U
55	DA	2448	A
55	DA	2464	G
55	DA	2465	C
55	DA	2469	A
55	DA	2474	U
55	DA	2476	A
55	DA	2478	A
55	DA	2480	C

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Mol	Chain	Res	Type
55	DA	2491	U
55	DA	2502	G
55	DA	2505	G
55	DA	2518	A
55	DA	2520	C
55	DA	2529	G
55	DA	2535	G
55	DA	2547	A
55	DA	2564	A
55	DA	2566	A
55	DA	2567	G
55	DA	2573	C
55	DA	2578	G
55	DA	2582	G
55	DA	2585	U
55	DA	2586	U
55	DA	2596	U
55	DA	2603	G
55	DA	2609	U
55	DA	2613	U
55	DA	2621	G
55	DA	2629	U
55	DA	2630	G
55	DA	2661	G
55	DA	2663	G
55	DA	2673	G
55	DA	2689	U
55	DA	2690	U
55	DA	2706	A
55	DA	2714	G
55	DA	2719	G
55	DA	2720	U
55	DA	2721	A
55	DA	2726	A
55	DA	2729	G
55	DA	2733	A
55	DA	2744	G
55	DA	2748	A
55	DA	2762	C
55	DA	2765	A
55	DA	2769	U
55	DA	2778	A

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Mol	Chain	Res	Type
55	DA	2791	G
55	DA	2798	U
55	DA	2799	A
55	DA	2811	G
55	DA	2815	C
55	DA	2818	U
55	DA	2820	A
55	DA	2821	A
55	DA	2825	G
55	DA	2835	A
55	DA	2836	U
55	DA	2861	U
55	DA	2867	G
55	DA	2872	A
55	DA	2879	A
55	DA	2883	A

All (286) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	A
1	AA	30	U
1	AA	49	U
1	AA	70	U
1	AA	89	U
1	AA	142	G
1	AA	209	U
1	AA	250	A
1	AA	305	G
1	AA	327	A
1	AA	367	U
1	AA	413	G
1	AA	422	C
1	AA	438	U
1	AA	518	C
1	AA	559	A
1	AA	576	C
1	AA	641	U
1	AA	702	A
1	AA	733	G
1	AA	793	U

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Mol	Chain	Res	Type
1	AA	841	C
1	AA	870	U
1	AA	884	U
1	AA	965	U
1	AA	971	G
1	AA	974	A
1	AA	991	U
1	AA	992	U
1	AA	1053	G
1	AA	1129	C
1	AA	1136	C
1	AA	1137	C
1	AA	1140	C
1	AA	1141	C
1	AA	1195	C
1	AA	1197	A
1	AA	1224	U
1	AA	1225	A
1	AA	1278	G
1	AA	1281	C
1	AA	1319	A
1	AA	1345	U
1	AA	1380	U
1	AA	1397	C
1	AA	1432	G
1	AA	1452	C
1	BA	5	U
1	BA	7	A
1	BA	30	U
1	BA	49	U
1	BA	70	U
1	BA	83	C
1	BA	86	G
1	BA	89	U
1	BA	142	G
1	BA	209	U
1	BA	246	A
1	BA	250	A
1	BA	305	G
1	BA	327	A
1	BA	367	U
1	BA	422	C

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Mol	Chain	Res	Type
1	BA	438	U
1	BA	518	C
1	BA	559	A
1	BA	561	U
1	BA	576	C
1	BA	641	U
1	BA	702	A
1	BA	733	G
1	BA	793	U
1	BA	842	U
1	BA	870	U
1	BA	884	U
1	BA	965	U
1	BA	971	G
1	BA	974	A
1	BA	991	U
1	BA	992	U
1	BA	1008	U
1	BA	1053	G
1	BA	1129	C
1	BA	1136	C
1	BA	1137	C
1	BA	1140	C
1	BA	1141	C
1	BA	1196	A
1	BA	1224	U
1	BA	1225	A
1	BA	1278	G
1	BA	1281	C
1	BA	1319	A
1	BA	1345	U
1	BA	1362	A
1	BA	1363	A
1	BA	1380	U
1	BA	1397	C
1	BA	1452	C
28	CB	51	G
28	CB	89	U
31	CA	83	A
31	CA	137	U
31	CA	138	U
31	CA	139	U

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Mol	Chain	Res	Type
31	CA	141	G
31	CA	177	G
31	CA	196	A
31	CA	199	A
31	CA	215	G
31	CA	271	G
31	CA	278	A
31	CA	310	A
31	CA	345	A
31	CA	361	G
31	CA	386	G
31	CA	390	U
31	CA	403	U
31	CA	404	A
31	CA	411	G
31	CA	455	C
31	CA	503	A
31	CA	506	G
31	CA	527	C
31	CA	531	C
31	CA	571	U
31	CA	572	A
31	CA	573	U
31	CA	603	A
31	CA	620	G
31	CA	637	A
31	CA	669	G
31	CA	684	G
31	CA	685	A
31	CA	752	A
31	CA	764	A
31	CA	774	G
31	CA	781	A
31	CA	784	G
31	CA	827	U
31	CA	846	U
31	CA	913	U
31	CA	945	A
31	CA	957	C
31	CA	973	A
31	CA	984	A
31	CA	1021	A

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Mol	Chain	Res	Type
31	CA	1045	C
31	CA	1061	U
31	CA	1069	A
31	CA	1070	A
31	CA	1087	G
31	CA	1089	A
31	CA	1128	G
31	CA	1133	A
31	CA	1141	U
31	CA	1212	G
31	CA	1247	A
31	CA	1288	G
31	CA	1300	G
31	CA	1329	U
31	CA	1379	U
31	CA	1397	U
31	CA	1452	G
31	CA	1490	A
31	CA	1497	U
31	CA	1509	A
31	CA	1535	A
31	CA	1536	C
31	CA	1607	C
31	CA	1647	U
31	CA	1776	G
31	CA	1786	A
31	CA	1800	C
31	CA	1818	U
31	CA	1838	C
31	CA	1870	C
31	CA	1871	A
31	CA	1900	A
31	CA	1937	A
31	CA	1970	A
31	CA	2035	G
31	CA	2043	C
31	CA	2095	A
31	CA	2119	A
31	CA	2126	A
31	CA	2145	C
31	CA	2146	C
31	CA	2157	G

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Mol	Chain	Res	Type
31	CA	2164	C
31	CA	2225	A
31	CA	2238	G
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	2426	A
31	CA	2448	A
31	CA	2468	A
31	CA	2542	A
31	CA	2572	A
31	CA	2645	G
31	CA	2680	U
31	CA	2776	A
31	CA	2778	A
31	CA	2779	U
31	CA	2849	U
31	CA	2873	A
31	CA	2893	A
28	DB	51	G
55	DA	119	A
55	DA	125	A
55	DA	137	U
55	DA	138	U
55	DA	141	G
55	DA	177	G
55	DA	196	A
55	DA	199	A
55	DA	215	G
55	DA	271	G
55	DA	278	A
55	DA	345	A
55	DA	361	G
55	DA	403	U
55	DA	411	G
55	DA	455	C
55	DA	503	A
55	DA	512	G
55	DA	603	A

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Mol	Chain	Res	Type
55	DA	614	A
55	DA	620	G
55	DA	764	A
55	DA	784	G
55	DA	858	G
55	DA	945	A
55	DA	984	A
55	DA	1061	U
55	DA	1069	A
55	DA	1070	A
55	DA	1087	G
55	DA	1089	A
55	DA	1128	G
55	DA	1133	A
55	DA	1171	G
55	DA	1300	G
55	DA	1329	U
55	DA	1396	U
55	DA	1397	U
55	DA	1420	A
55	DA	1427	A
55	DA	1490	A
55	DA	1509	A
55	DA	1535	A
55	DA	1558	C
55	DA	1607	C
55	DA	1647	U
55	DA	1786	A
55	DA	1800	C
55	DA	1870	C
55	DA	1871	A
55	DA	1900	A
55	DA	1939	5MU
55	DA	2035	G
55	DA	2051	A
55	DA	2097	A
55	DA	2119	A
55	DA	2126	A
55	DA	2127	G
55	DA	2146	C
55	DA	2157	G
55	DA	2158	A

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Mol	Chain	Res	Type
55	DA	2164	C
55	DA	2238	G
55	DA	2282	G
55	DA	2286	G
55	DA	2311	A
55	DA	2406	A
55	DA	2423	U
55	DA	2572	A
55	DA	2581	G
55	DA	2585	U
55	DA	2866	U
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
55	2MA	DA	2503	55,56	17,25,26	0.95	0	19,37,40	1.93	4 (21%)
55	PSU	DA	2457	55	17,21,22	1.39	3 (17%)	20,30,33	5.27	4 (20%)
31	OMC	CA	2498	31,56	15,22,23	0.94	1 (6%)	17,31,34	1.11	1 (5%)
1	2MG	BA	966	1	19,26,27	1.31	2 (10%)	21,38,41	2.43	4 (19%)
55	PSU	DA	2504	55	17,21,22	1.24	3 (17%)	20,30,33	5.30	4 (20%)
55	7MG	DA	2069	55	22,26,27	1.71	3 (13%)	28,39,42	2.37	6 (21%)
1	2MG	BA	1207	1	19,26,27	1.22	2 (10%)	21,38,41	2.40	4 (19%)
31	PSU	CA	955	31	17,21,22	1.17	2 (11%)	20,30,33	5.31	5 (25%)
1	2MG	AA	1516	1	19,26,27	1.15	2 (10%)	21,38,41	2.40	4 (19%)
1	MA6	AA	1518	1	19,26,27	0.86	0	18,38,41	1.25	1 (5%)
31	PSU	CA	2504	31	17,21,22	1.22	3 (17%)	20,30,33	5.32	4 (20%)
41	4D4	DN	81[B]	-	9,11,12	1.73	2 (22%)	8,13,15	2.07	2 (25%)
41	4D4	DN	81[A]	-	9,11,12	1.60	1 (11%)	8,13,15	2.99	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	2MG	CA	1835	31	19,26,27	1.14	2 (10%)	21,38,41	2.38	4 (19%)
1	4OC	BA	1402	1	16,23,24	0.79	1 (6%)	17,32,35	0.84	1 (5%)
55	6MZ	DA	2030	55	18,25,26	0.78	0	16,36,39	0.98	1 (6%)
1	UR3	BA	1498	1	14,22,23	1.01	1 (7%)	15,32,35	0.56	0
31	2MA	CA	2503	31	17,25,26	0.98	0	19,37,40	2.01	4 (21%)
1	MA6	BA	1519	1	19,26,27	0.90	0	18,38,41	0.87	0
1	2MG	AA	966	1	19,26,27	1.38	2 (10%)	21,38,41	2.34	3 (14%)
55	PSU	DA	2604	55	17,21,22	1.51	4 (23%)	20,30,33	5.31	4 (20%)
55	PSU	DA	2580	55	17,21,22	1.31	2 (11%)	20,30,33	5.35	4 (20%)
31	PSU	CA	2580	31	17,21,22	1.39	3 (17%)	20,30,33	5.32	5 (25%)
1	PSU	BA	516	1	17,21,22	1.39	3 (17%)	20,30,33	5.29	4 (20%)
32	MEQ	DD	150[B]	32	8,9,10	1.65	1 (12%)	5,10,12	1.46	1 (20%)
55	PSU	DA	1911	55	17,21,22	1.28	2 (11%)	20,30,33	5.26	4 (20%)
55	OMC	DA	2498	55,56	15,22,23	1.25	2 (13%)	17,31,34	1.10	1 (5%)
12	D2T	BL	89	12	4,9,10	0.66	0	3,11,13	0.88	0
1	2MG	BA	1516	1	19,26,27	1.20	2 (10%)	21,38,41	2.42	4 (19%)
1	5MC	AA	1407	1	15,22,23	0.80	1 (6%)	19,32,35	1.21	2 (10%)
31	PSU	CA	1911	31	17,21,22	1.26	2 (11%)	20,30,33	5.30	4 (20%)
32	MEQ	DD	150[A]	32	8,9,10	0.39	0	5,10,12	0.54	0
55	OMG	DA	2251	55	18,26,27	1.01	1 (5%)	20,38,41	2.50	5 (25%)
1	MA6	BA	1518	1	19,26,27	0.86	0	18,38,41	1.36	1 (5%)
55	PSU	DA	2605	55	17,21,22	1.26	2 (11%)	20,30,33	5.27	4 (20%)
55	5MU	DA	747	55	15,22,23	1.22	2 (13%)	16,32,35	3.70	1 (6%)
1	5MC	AA	967	1	15,22,23	0.87	1 (6%)	19,32,35	1.16	2 (10%)
1	7MG	BA	527	1	22,26,27	1.73	3 (13%)	28,39,42	2.47	8 (28%)
55	2MG	DA	1835	55	19,26,27	1.25	2 (10%)	21,38,41	2.43	4 (19%)
1	7MG	AA	527	1	22,26,27	1.61	3 (13%)	28,39,42	2.50	7 (25%)
31	PSU	CA	746	31,56	17,21,22	1.44	3 (17%)	20,30,33	5.32	4 (20%)
31	PSU	CA	2457	31	17,21,22	1.59	4 (23%)	20,30,33	5.30	4 (20%)
55	5MC	DA	1962	55	15,22,23	1.10	2 (13%)	19,32,35	1.19	2 (10%)
55	PSU	DA	955	55	17,21,22	1.43	3 (17%)	20,30,33	5.32	5 (25%)
31	3TD	CA	1915	31	17,22,23	1.29	4 (23%)	19,32,35	1.51	2 (10%)
31	5MU	CA	1939	31	15,22,23	1.20	2 (13%)	16,32,35	3.65	1 (6%)
31	PSU	CA	1917	31	17,21,22	1.28	2 (11%)	20,30,33	5.32	4 (20%)
31	5MC	CA	1962	31	15,22,23	0.74	0	19,32,35	1.20	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	BA	1407	1	15,22,23	0.90	0	19,32,35	1.17	2 (10%)
55	PSU	DA	746	55,56	17,21,22	1.75	4 (23%)	20,30,33	5.31	5 (25%)
12	D2T	AL	89	12	4,9,10	0.59	0	3,11,13	0.94	0
55	PSU	DA	1917	55	17,21,22	1.44	3 (17%)	20,30,33	5.29	4 (20%)
31	PSU	CA	2605	31	17,21,22	1.21	2 (11%)	20,30,33	5.34	4 (20%)
31	6MZ	CA	1618	31	18,25,26	0.90	1 (5%)	16,36,39	1.04	1 (6%)
1	2MG	AA	1207	1	19,26,27	1.18	2 (10%)	21,38,41	2.39	4 (19%)
41	4D4	CN	81	41	9,11,12	2.26	2 (22%)	8,13,15	2.20	2 (25%)
31	6MZ	CA	2030	31	18,25,26	0.71	0	16,36,39	0.85	1 (6%)
55	2MG	DA	2445	55	19,26,27	1.14	1 (5%)	21,38,41	2.40	4 (19%)
1	PSU	AA	516	1,56	17,21,22	1.40	3 (17%)	20,30,33	5.32	4 (20%)
55	6MZ	DA	1618	55	18,25,26	1.09	0	16,36,39	2.01	2 (12%)
55	1MG	DA	745	55	18,26,27	1.15	2 (11%)	19,39,42	1.20	2 (10%)
1	MA6	AA	1519	1	19,26,27	0.93	1 (5%)	18,38,41	0.90	1 (5%)
31	7MG	CA	2069	31	22,26,27	1.70	4 (18%)	28,39,42	2.37	7 (25%)
31	OMG	CA	2251	31	18,26,27	1.27	2 (11%)	20,38,41	2.51	4 (20%)
31	1MG	CA	745	31	18,26,27	1.20	2 (11%)	19,39,42	1.29	2 (10%)
1	UR3	AA	1498	1	14,22,23	1.05	1 (7%)	15,32,35	0.53	0
1	4OC	AA	1402	1	16,23,24	0.79	1 (6%)	17,32,35	0.79	1 (5%)
55	3TD	DA	1915	55	17,22,23	1.28	2 (11%)	19,32,35	1.50	2 (10%)
31	OMU	CA	2552	31	14,22,23	1.27	2 (14%)	14,31,34	1.16	1 (7%)
31	5MU	CA	747	31	15,22,23	1.13	1 (6%)	16,32,35	3.68	2 (12%)
55	5MU	DA	1939	55	15,22,23	1.58	2 (13%)	16,32,35	3.68	2 (12%)
55	OMU	DA	2552	55	14,22,23	1.28	2 (14%)	14,31,34	1.10	1 (7%)
1	5MC	BA	967	1	15,22,23	0.87	0	19,32,35	1.16	2 (10%)
31	2MG	CA	2445	31	19,26,27	1.22	1 (5%)	21,38,41	2.31	3 (14%)
55	H2U	DA	2449	55	18,21,22	0.84	0	21,30,33	0.45	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
55	2MA	DA	2503	55,56	-	2/3/25/26	0/3/3/3
55	PSU	DA	2457	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	OMC	CA	2498	31,56	-	2/7/27/28	0/2/2/2
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
55	PSU	DA	2504	55	-	2/7/25/26	0/2/2/2
55	7MG	DA	2069	55	-	2/7/37/38	0/3/3/3
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
31	PSU	CA	955	31	-	0/7/25/26	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
31	PSU	CA	2504	31	-	2/7/25/26	0/2/2/2
41	4D4	DN	81[B]	-	-	4/11/12/14	-
41	4D4	DN	81[A]	-	-	1/11/12/14	-
31	2MG	CA	1835	31	-	0/5/27/28	0/3/3/3
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2
55	6MZ	DA	2030	55	-	2/5/27/28	0/3/3/3
1	UR3	BA	1498	1	-	0/5/25/26	0/2/2/2
31	2MA	CA	2503	31	-	2/3/25/26	0/3/3/3
1	MA6	BA	1519	1	-	3/7/29/30	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
55	PSU	DA	2604	55	-	1/7/25/26	0/2/2/2
55	PSU	DA	2580	55	-	2/7/25/26	0/2/2/2
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[B]	32	-	3/8/9/11	-
55	PSU	DA	1911	55	-	0/7/25/26	0/2/2/2
55	OMC	DA	2498	55,56	-	0/7/27/28	0/2/2/2
12	D2T	BL	89	12	-	3/3/12/14	-
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/5/25/26	0/2/2/2
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[A]	32	-	4/8/9/11	-
55	OMG	DA	2251	55	-	0/5/27/28	0/3/3/3
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
55	PSU	DA	2605	55	-	0/7/25/26	0/2/2/2
55	5MU	DA	747	55	-	0/5/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/5/25/26	0/2/2/2
1	7MG	BA	527	1	-	2/7/37/38	0/3/3/3
55	2MG	DA	1835	55	-	0/5/27/28	0/3/3/3
1	7MG	AA	527	1	-	2/7/37/38	0/3/3/3
31	PSU	CA	746	31,56	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
55	5MC	DA	1962	55	-	2/5/25/26	0/2/2/2
55	PSU	DA	955	55	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	2/5/25/26	0/2/2/2
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/5/25/26	0/2/2/2
1	5MC	BA	1407	1	-	0/5/25/26	0/2/2/2
55	PSU	DA	746	55,56	-	3/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	3/3/12/14	-
55	PSU	DA	1917	55	-	0/7/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	1/5/27/28	0/3/3/3
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
41	4D4	CN	81	41	-	1/11/12/14	-
31	6MZ	CA	2030	31	-	2/5/27/28	0/3/3/3
55	2MG	DA	2445	55	-	2/5/27/28	0/3/3/3
1	PSU	AA	516	1,56	-	0/7/25/26	0/2/2/2
55	6MZ	DA	1618	55	-	0/5/27/28	0/3/3/3
55	1MG	DA	745	55	-	0/3/25/26	0/3/3/3
1	MA6	AA	1519	1	-	3/7/29/30	0/3/3/3
31	7MG	CA	2069	31	-	1/7/37/38	0/3/3/3
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
1	UR3	AA	1498	1	-	0/5/25/26	0/2/2/2
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
55	3TD	DA	1915	55	-	0/7/25/26	0/2/2/2
31	OMU	CA	2552	31	-	0/7/27/28	0/2/2/2
31	5MU	CA	747	31	-	0/5/25/26	0/2/2/2
55	5MU	DA	1939	55	-	0/5/25/26	0/2/2/2
55	OMU	DA	2552	55	-	0/7/27/28	0/2/2/2
1	5MC	BA	967	1	-	0/5/25/26	0/2/2/2
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
55	H2U	DA	2449	55	-	1/7/38/39	0/2/2/2

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	CN	81	4D4	CZ-NE	6.18	1.45	1.33
55	DA	2069	7MG	C8-N9	-5.42	1.33	1.45
1	BA	527	7MG	C8-N9	-5.38	1.33	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2069	7MG	C8-N9	-5.23	1.33	1.45
1	AA	527	7MG	C8-N9	-5.21	1.33	1.45
41	DN	81[B]	4D4	CZ-NE	4.54	1.42	1.33
32	DD	150[B]	MEQ	CB-CA	4.46	1.59	1.53
41	DN	81[A]	4D4	CZ-NE	4.33	1.41	1.33
55	DA	746	PSU	O4'-C1'	-4.14	1.38	1.44
1	AA	966	2MG	C6-N1	3.69	1.39	1.33
1	AA	966	2MG	C6-C5	3.67	1.47	1.41
1	AA	527	7MG	C6-N1	3.66	1.39	1.33
1	BA	966	2MG	C6-N1	3.61	1.39	1.33
1	BA	1516	2MG	C6-N1	3.60	1.39	1.33
31	CA	746	PSU	C4-N3	3.58	1.39	1.33
31	CA	2504	PSU	C4-N3	3.55	1.39	1.33
55	DA	2069	7MG	C6-C5	3.52	1.46	1.41
31	CA	2580	PSU	C4-N3	3.51	1.39	1.33
1	BA	1207	2MG	C6-N1	3.50	1.39	1.33
55	DA	2605	PSU	C4-N3	3.50	1.39	1.33
55	DA	2504	PSU	C4-N3	3.50	1.39	1.33
31	CA	745	1MG	C6-C5	3.49	1.46	1.41
31	CA	2552	OMU	C4-N3	3.48	1.39	1.33
1	AA	516	PSU	C4-N3	3.48	1.39	1.33
55	DA	1917	PSU	C4-N3	3.48	1.39	1.33
1	BA	516	PSU	C4-N3	3.46	1.39	1.33
1	AA	1207	2MG	C6-N1	3.44	1.39	1.33
55	DA	1911	PSU	C4-N3	3.43	1.39	1.33
31	CA	1911	PSU	C4-N3	3.40	1.39	1.33
31	CA	955	PSU	C4-N3	3.39	1.38	1.33
55	DA	1939	5MU	C2'-C1'	-3.39	1.48	1.53
31	CA	2069	7MG	C6-N1	3.38	1.38	1.33
55	DA	1939	5MU	C4-N3	3.38	1.38	1.33
31	CA	2457	PSU	C4-N3	3.37	1.38	1.33
1	AA	1516	2MG	C6-N1	3.34	1.38	1.33
31	CA	2605	PSU	C4-N3	3.34	1.38	1.33
55	DA	746	PSU	C4-N3	3.33	1.38	1.33
31	CA	2445	2MG	C6-N1	3.32	1.38	1.33
31	CA	1917	PSU	C4-N3	3.32	1.38	1.33
31	CA	1835	2MG	C6-N1	3.30	1.38	1.33
55	DA	1915	3TD	C4-C5	3.27	1.48	1.41
1	BA	527	7MG	C6-C5	3.25	1.45	1.41
31	CA	2251	OMG	C6-N1	3.25	1.38	1.33
31	CA	747	5MU	C4-N3	3.24	1.38	1.33
55	DA	2251	OMG	C6-N1	3.24	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2069	7MG	C1'-N9	-3.23	1.40	1.46
55	DA	2457	PSU	C4-N3	3.17	1.38	1.33
55	DA	2069	7MG	C6-N1	3.15	1.38	1.33
55	DA	2580	PSU	C4-N3	3.13	1.38	1.33
55	DA	955	PSU	C4-N3	3.12	1.38	1.33
1	BA	966	2MG	C6-C5	3.11	1.46	1.41
31	CA	1939	5MU	C4-N3	3.11	1.38	1.33
1	BA	527	7MG	C6-N1	3.10	1.38	1.33
55	DA	1835	2MG	C6-C5	3.05	1.46	1.41
55	DA	746	PSU	C2'-C1'	-3.03	1.50	1.54
55	DA	747	5MU	C4-N3	3.01	1.38	1.33
1	AA	1498	UR3	C6-N1	2.89	1.39	1.35
55	DA	2552	OMU	C4-N3	2.88	1.38	1.33
55	DA	2498	OMC	O5'-C5'	-2.88	1.37	1.44
31	CA	1915	3TD	C4-C5	2.87	1.47	1.41
55	DA	1835	2MG	C6-N1	2.87	1.38	1.33
55	DA	2604	PSU	C5-C1'	-2.85	1.49	1.52
1	BA	1207	2MG	C6-C5	2.82	1.46	1.41
55	DA	2445	2MG	C6-N1	2.80	1.37	1.33
55	DA	2604	PSU	C4-N3	2.79	1.37	1.33
31	CA	2457	PSU	O5'-C5'	-2.77	1.38	1.44
1	AA	1516	2MG	C6-C5	2.67	1.46	1.41
1	BA	1516	2MG	C6-C5	2.65	1.45	1.41
1	AA	1207	2MG	C6-C5	2.62	1.45	1.41
1	AA	527	7MG	C6-C5	2.61	1.45	1.41
31	CA	746	PSU	O4'-C1'	-2.61	1.40	1.44
1	AA	516	PSU	C5-C1'	-2.57	1.50	1.52
55	DA	1917	PSU	C5-C1'	-2.56	1.50	1.52
55	DA	2552	OMU	C6-N1	2.52	1.38	1.35
1	BA	1498	UR3	C6-N1	2.49	1.38	1.35
55	DA	745	1MG	C6-C5	2.42	1.45	1.41
31	CA	2251	OMG	C6-C5	2.40	1.45	1.41
31	CA	2552	OMU	C6-N1	2.39	1.38	1.35
55	DA	2604	PSU	O3'-C3'	-2.39	1.37	1.43
55	DA	2604	PSU	C6-C5	-2.36	1.35	1.38
41	CN	81	4D4	CZ-NH1	2.36	1.44	1.34
55	DA	955	PSU	C6-C5	-2.35	1.35	1.38
55	DA	1962	5MC	O5'-C5'	-2.34	1.39	1.44
31	CA	1915	3TD	C4-N3	2.31	1.41	1.38
55	DA	2457	PSU	C5-C1'	-2.29	1.50	1.52
55	DA	2504	PSU	C4-C5	2.26	1.46	1.41
31	CA	1915	3TD	C6-C5	-2.26	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	516	PSU	C5-C1'	-2.25	1.50	1.52
55	DA	1911	PSU	C6-C5	-2.24	1.35	1.38
55	DA	2457	PSU	C6-C5	-2.24	1.35	1.38
55	DA	1915	3TD	C6-C5	-2.24	1.35	1.38
1	BA	516	PSU	C6-C5	-2.22	1.35	1.38
31	CA	2580	PSU	O4'-C1'	-2.22	1.41	1.44
31	CA	2498	OMC	C6-N1	2.20	1.38	1.35
41	DN	81[B]	4D4	CZ-NH1	2.20	1.43	1.34
31	CA	1917	PSU	C6-C5	-2.20	1.35	1.38
31	CA	1911	PSU	C6-C5	-2.20	1.35	1.38
1	AA	516	PSU	C6-C5	-2.17	1.35	1.38
31	CA	2069	7MG	C6-C5	2.15	1.44	1.41
55	DA	2504	PSU	C6-C5	-2.15	1.35	1.38
31	CA	1618	6MZ	O5'-C5'	-2.14	1.39	1.44
31	CA	2457	PSU	C6-C5	-2.14	1.35	1.38
55	DA	1917	PSU	C6-C5	-2.14	1.35	1.38
55	DA	2605	PSU	C6-C5	-2.13	1.35	1.38
31	CA	2605	PSU	C6-C5	-2.13	1.35	1.38
55	DA	747	5MU	C6-C5	-2.13	1.34	1.40
55	DA	745	1MG	C8-N7	-2.12	1.30	1.34
31	CA	2457	PSU	C5-C1'	-2.12	1.50	1.52
55	DA	2498	OMC	C6-N1	2.10	1.38	1.35
31	CA	745	1MG	C6-N1	2.10	1.41	1.38
31	CA	2504	PSU	C6-C5	-2.09	1.35	1.38
31	CA	1915	3TD	C5-C1'	-2.09	1.50	1.52
31	CA	955	PSU	C6-C5	-2.09	1.35	1.38
55	DA	955	PSU	C2'-C1'	-2.07	1.51	1.54
31	CA	2504	PSU	C4-C5	2.06	1.45	1.41
55	DA	2580	PSU	C6-C5	-2.06	1.35	1.38
31	CA	1835	2MG	C6-C5	2.05	1.44	1.41
55	DA	1962	5MC	C6-C5	-2.05	1.34	1.40
1	AA	1519	MA6	C8-N7	-2.03	1.31	1.34
55	DA	746	PSU	C6-C5	-2.03	1.35	1.38
1	BA	1402	4OC	C6-N1	2.02	1.38	1.35
31	CA	2580	PSU	C6-C5	-2.02	1.35	1.38
31	CA	1939	5MU	C4-C5	2.02	1.45	1.41
31	CA	746	PSU	C4-C5	2.02	1.45	1.41
1	AA	1407	5MC	C6-C5	-2.01	1.34	1.40
1	AA	967	5MC	O4'-C1'	2.00	1.43	1.41
1	AA	1402	4OC	C6-N1	2.00	1.38	1.35

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	955	PSU	N1-C2-N3	-17.20	114.76	128.43
31	CA	2605	PSU	N1-C2-N3	-17.19	114.76	128.43
31	CA	1917	PSU	N1-C2-N3	-17.17	114.78	128.43
1	AA	516	PSU	N1-C2-N3	-17.17	114.78	128.43
31	CA	746	PSU	N1-C2-N3	-17.15	114.79	128.43
31	CA	2504	PSU	N1-C2-N3	-17.15	114.80	128.43
31	CA	1911	PSU	N1-C2-N3	-17.15	114.80	128.43
31	CA	955	PSU	N1-C2-N3	-17.11	114.82	128.43
1	BA	516	PSU	N1-C2-N3	-17.10	114.84	128.43
55	DA	2580	PSU	N1-C2-N3	-17.07	114.86	128.43
55	DA	2605	PSU	N1-C2-N3	-17.04	114.88	128.43
55	DA	1917	PSU	N1-C2-N3	-17.04	114.88	128.43
55	DA	746	PSU	N1-C2-N3	-17.04	114.89	128.43
55	DA	2504	PSU	N1-C2-N3	-17.02	114.90	128.43
55	DA	2604	PSU	N1-C2-N3	-17.02	114.90	128.43
31	CA	2457	PSU	N1-C2-N3	-17.02	114.90	128.43
55	DA	1911	PSU	N1-C2-N3	-16.98	114.93	128.43
55	DA	2457	PSU	N1-C2-N3	-16.98	114.93	128.43
31	CA	2580	PSU	N1-C2-N3	-16.97	114.94	128.43
55	DA	747	5MU	C4-N3-C2	14.45	127.34	115.14
31	CA	747	5MU	C4-N3-C2	14.37	127.27	115.14
55	DA	1939	5MU	C4-N3-C2	14.28	127.20	115.14
31	CA	1939	5MU	C4-N3-C2	14.24	127.17	115.14
55	DA	2580	PSU	C4-N3-C2	13.59	126.61	115.14
31	CA	1917	PSU	C4-N3-C2	13.54	126.57	115.14
55	DA	2504	PSU	C4-N3-C2	13.49	126.53	115.14
31	CA	2504	PSU	C4-N3-C2	13.48	126.53	115.14
31	CA	2605	PSU	C4-N3-C2	13.48	126.52	115.14
31	CA	2457	PSU	C4-N3-C2	13.45	126.50	115.14
55	DA	746	PSU	C4-N3-C2	13.43	126.48	115.14
31	CA	2580	PSU	C4-N3-C2	13.43	126.48	115.14
31	CA	746	PSU	C4-N3-C2	13.43	126.48	115.14
1	AA	516	PSU	C4-N3-C2	13.43	126.48	115.14
55	DA	2604	PSU	C4-N3-C2	13.42	126.47	115.14
31	CA	1911	PSU	C4-N3-C2	13.41	126.47	115.14
55	DA	1917	PSU	C4-N3-C2	13.38	126.44	115.14
31	CA	955	PSU	C4-N3-C2	13.37	126.43	115.14
1	BA	516	PSU	C4-N3-C2	13.35	126.41	115.14
55	DA	2457	PSU	C4-N3-C2	13.29	126.36	115.14
55	DA	1911	PSU	C4-N3-C2	13.28	126.35	115.14
55	DA	955	PSU	C4-N3-C2	13.23	126.31	115.14
55	DA	2605	PSU	C4-N3-C2	13.16	126.25	115.14
55	DA	1835	2MG	C5-C6-N1	-8.54	111.75	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	1835	2MG	C5-C6-N1	-8.27	112.12	123.43
1	AA	1207	2MG	C5-C6-N1	-8.18	112.24	123.43
31	CA	2445	2MG	C5-C6-N1	-8.14	112.30	123.43
31	CA	2251	OMG	C5-C6-N1	-8.13	112.31	123.43
1	BA	1516	2MG	C5-C6-N1	-8.13	112.32	123.43
1	BA	966	2MG	C5-C6-N1	-8.09	112.36	123.43
31	CA	2457	PSU	C5-C4-N3	-8.00	115.05	125.36
1	BA	1207	2MG	C5-C6-N1	-7.98	112.51	123.43
31	CA	2504	PSU	C5-C4-N3	-7.98	115.07	125.36
55	DA	2445	2MG	C5-C6-N1	-7.97	112.54	123.43
55	DA	2251	OMG	C5-C6-N1	-7.96	112.54	123.43
55	DA	2504	PSU	C5-C4-N3	-7.96	115.11	125.36
55	DA	1917	PSU	C5-C4-N3	-7.94	115.13	125.36
1	AA	1516	2MG	C5-C6-N1	-7.93	112.58	123.43
1	AA	966	2MG	C5-C6-N1	-7.92	112.60	123.43
31	CA	1917	PSU	C5-C4-N3	-7.91	115.16	125.36
31	CA	2580	PSU	C5-C4-N3	-7.90	115.18	125.36
1	AA	516	PSU	C5-C4-N3	-7.89	115.19	125.36
31	CA	746	PSU	C5-C4-N3	-7.88	115.21	125.36
55	DA	1911	PSU	C5-C4-N3	-7.86	115.23	125.36
31	CA	1911	PSU	C5-C4-N3	-7.83	115.27	125.36
31	CA	2605	PSU	C5-C4-N3	-7.83	115.27	125.36
55	DA	2604	PSU	C5-C4-N3	-7.81	115.30	125.36
1	BA	516	PSU	C5-C4-N3	-7.80	115.31	125.36
31	CA	955	PSU	C5-C4-N3	-7.80	115.31	125.36
55	DA	2580	PSU	C5-C4-N3	-7.78	115.33	125.36
55	DA	2457	PSU	C5-C4-N3	-7.78	115.34	125.36
55	DA	746	PSU	C5-C4-N3	-7.76	115.36	125.36
55	DA	2605	PSU	C5-C4-N3	-7.75	115.37	125.36
55	DA	955	PSU	C5-C4-N3	-7.68	115.46	125.36
31	CA	2503	2MA	C5-C6-N1	-7.32	115.38	123.06
55	DA	1618	6MZ	C9-N6-C6	-7.16	116.70	122.87
55	DA	2503	2MA	C5-C6-N1	-7.06	115.65	123.06
41	DN	81[A]	4D4	NE-CZ-NH2	6.55	132.21	120.70
31	CA	2069	7MG	C5-C6-N1	-6.22	110.36	123.14
1	AA	527	7MG	C5-C6-N1	-6.07	110.67	123.14
55	DA	2069	7MG	C5-C6-N1	-5.93	110.95	123.14
1	BA	527	7MG	C5-C6-N1	-5.88	111.05	123.14
55	DA	2251	OMG	C6-N1-C2	5.84	125.20	115.93
31	CA	2251	OMG	C6-N1-C2	5.81	125.15	115.93
1	BA	527	7MG	O4'-C1'-N9	5.57	116.87	109.35
1	AA	527	7MG	C6-N1-C2	5.46	124.61	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	2445	2MG	C6-N1-C2	5.38	124.81	115.18
55	DA	1835	2MG	C6-N1-C2	5.37	124.80	115.18
1	AA	1207	2MG	C6-N1-C2	5.35	124.77	115.18
1	BA	1207	2MG	C6-N1-C2	5.35	124.76	115.18
1	BA	1516	2MG	C6-N1-C2	5.35	124.76	115.18
31	CA	1835	2MG	C6-N1-C2	5.35	124.75	115.18
1	BA	966	2MG	C6-N1-C2	5.34	124.74	115.18
1	AA	1516	2MG	C6-N1-C2	5.30	124.68	115.18
1	BA	527	7MG	C6-N1-C2	5.17	124.14	115.93
41	CN	81	4D4	NE-CZ-NH2	5.15	129.75	120.70
1	AA	527	7MG	O4'-C1'-N9	5.15	116.30	109.35
55	DA	2069	7MG	C6-N1-C2	5.14	124.10	115.93
55	DA	2069	7MG	C5-C4-N3	-5.13	118.11	126.49
1	AA	527	7MG	C5-C4-N3	-5.13	118.12	126.49
31	CA	2069	7MG	C6-N1-C2	5.12	124.06	115.93
1	AA	966	2MG	C6-N1-C2	5.09	124.29	115.18
31	CA	2445	2MG	C6-N1-C2	5.08	124.28	115.18
31	CA	2069	7MG	N7-C8-N9	5.08	110.64	103.38
31	CA	1915	3TD	C6-N1-C2	5.05	123.69	115.36
55	DA	2069	7MG	O4'-C1'-N9	5.04	116.16	109.35
55	DA	1915	3TD	C6-N1-C2	4.95	123.53	115.36
1	AA	527	7MG	N7-C8-N9	4.86	110.33	103.38
41	DN	81[B]	4D4	NE-CZ-NH2	4.85	129.22	120.70
1	BA	1518	MA6	N1-C6-N6	-4.84	111.97	117.06
55	DA	1911	PSU	C6-N1-C2	4.51	122.79	115.36
31	CA	2605	PSU	C6-N1-C2	4.50	122.78	115.36
55	DA	955	PSU	C6-N1-C2	4.49	122.78	115.36
41	DN	81[A]	4D4	NH1-CZ-NE	-4.49	108.84	119.19
1	AA	516	PSU	C6-N1-C2	4.47	122.74	115.36
31	CA	1911	PSU	C6-N1-C2	4.47	122.74	115.36
1	BA	516	PSU	C6-N1-C2	4.47	122.73	115.36
55	DA	746	PSU	C6-N1-C2	4.47	122.73	115.36
55	DA	2605	PSU	C6-N1-C2	4.46	122.72	115.36
31	CA	746	PSU	C6-N1-C2	4.46	122.72	115.36
31	CA	2504	PSU	C6-N1-C2	4.45	122.70	115.36
55	DA	2504	PSU	C6-N1-C2	4.45	122.70	115.36
31	CA	955	PSU	C6-N1-C2	4.45	122.70	115.36
31	CA	1917	PSU	C6-N1-C2	4.45	122.70	115.36
55	DA	2457	PSU	C6-N1-C2	4.44	122.69	115.36
31	CA	2457	PSU	C6-N1-C2	4.44	122.68	115.36
1	BA	527	7MG	C6-C5-C4	-4.44	110.43	115.20
55	DA	2604	PSU	C6-N1-C2	4.43	122.67	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2580	PSU	C6-N1-C2	4.43	122.67	115.36
55	DA	2580	PSU	C6-N1-C2	4.42	122.66	115.36
55	DA	1917	PSU	C6-N1-C2	4.42	122.65	115.36
31	CA	2069	7MG	O4'-C1'-N9	4.41	115.30	109.35
1	BA	527	7MG	N7-C8-N9	4.28	109.50	103.38
1	AA	1518	MA6	N1-C6-N6	-4.26	112.57	117.06
31	CA	745	1MG	C6-C5-C4	-4.26	117.23	119.96
31	CA	2498	OMC	C2-N3-C4	4.24	120.64	116.34
1	BA	527	7MG	C5-C4-N3	-4.22	119.60	126.49
55	DA	2069	7MG	N7-C8-N9	4.22	109.41	103.38
55	DA	2498	OMC	C2-N3-C4	4.16	120.56	116.34
31	CA	1962	5MC	C2-N3-C4	4.15	121.03	116.02
1	AA	1407	5MC	C2-N3-C4	4.14	121.02	116.02
1	BA	1407	5MC	C2-N3-C4	4.08	120.95	116.02
1	BA	967	5MC	C2-N3-C4	4.08	120.94	116.02
1	AA	967	5MC	C2-N3-C4	4.07	120.93	116.02
55	DA	1962	5MC	C2-N3-C4	4.07	120.93	116.02
31	CA	2552	OMU	C5-C4-N3	-3.95	114.62	123.31
55	DA	2552	OMU	C5-C4-N3	-3.83	114.88	123.31
31	CA	2069	7MG	C5-C4-N3	-3.70	120.45	126.49
1	AA	966	2MG	C6-C5-C4	-3.64	117.33	120.80
1	AA	1516	2MG	C6-C5-C4	-3.53	117.43	120.80
1	AA	527	7MG	C4-C5-N7	-3.46	101.69	106.98
1	BA	966	2MG	C6-C5-C4	-3.40	117.55	120.80
1	BA	1516	2MG	C6-C5-C4	-3.40	117.55	120.80
1	BA	1207	2MG	C6-C5-C4	-3.40	117.56	120.80
31	CA	2069	7MG	C4-C5-N7	-3.34	101.87	106.98
55	DA	2445	2MG	C6-C5-C4	-3.31	117.63	120.80
32	DD	150[B]	MEQ	CB-CG-CD	3.25	120.29	113.04
55	DA	745	1MG	C5-C6-N1	-3.24	114.75	118.20
55	DA	2069	7MG	C4-C5-N7	-3.20	102.08	106.98
1	BA	527	7MG	C4-C5-N7	-3.19	102.10	106.98
31	CA	2069	7MG	C6-C5-C4	-3.19	111.78	115.20
55	DA	2251	OMG	N3-C2-N1	-3.13	123.05	127.22
1	AA	1207	2MG	C6-C5-C4	-3.11	117.83	120.80
31	CA	1915	3TD	C5-C4-N3	-3.09	116.16	118.66
55	DA	1915	3TD	C5-C4-N3	-3.05	116.19	118.66
1	BA	1207	2MG	N2-C2-N3	3.05	119.89	116.96
1	BA	1402	4OC	CM4-N4-C4	3.01	125.55	122.97
31	CA	2445	2MG	C6-C5-C4	-2.99	117.95	120.80
1	BA	966	2MG	N2-C2-N3	2.92	119.77	116.96
31	CA	2251	OMG	C6-C5-C4	-2.92	118.01	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	1835	2MG	C6-C5-C4	-2.91	118.02	120.80
31	CA	1835	2MG	C6-C5-C4	-2.90	118.02	120.80
1	AA	1402	4OC	CM4-N4-C4	2.89	125.45	122.97
31	CA	2251	OMG	N3-C2-N1	-2.88	123.38	127.22
1	AA	1207	2MG	N2-C2-N3	2.76	119.61	116.96
31	CA	745	1MG	C5-C6-N1	-2.74	115.27	118.20
1	AA	1516	2MG	N2-C2-N3	2.74	119.59	116.96
55	DA	746	PSU	C4-C5-C1'	-2.71	116.00	121.12
55	DA	2445	2MG	N2-C2-N3	2.70	119.55	116.96
41	DN	81[B]	4D4	NH1-CZ-NE	-2.64	113.09	119.19
1	BA	1516	2MG	N2-C2-N3	2.63	119.49	116.96
31	CA	1835	2MG	N2-C2-N3	2.61	119.47	116.96
55	DA	1835	2MG	N2-C2-N3	2.57	119.43	116.96
55	DA	2251	OMG	C6-C5-C4	-2.46	118.45	120.80
31	CA	1618	6MZ	C4-C5-N7	2.39	111.89	109.40
55	DA	1618	6MZ	O4'-C1'-C2'	-2.39	103.44	106.93
55	DA	745	1MG	C6-C5-C4	-2.38	118.43	119.96
55	DA	955	PSU	C4-C5-C1'	-2.31	116.77	121.12
41	CN	81	4D4	NH1-CZ-NE	-2.29	113.90	119.19
55	DA	2251	OMG	C2-N3-C4	-2.28	112.75	115.36
31	CA	955	PSU	C3'-C2'-C1'	-2.27	99.32	101.93
55	DA	2030	6MZ	C9-N6-C6	2.26	124.82	122.87
31	CA	2503	2MA	CM2-C2-N3	2.26	120.68	117.16
1	AA	1519	MA6	N1-C6-N6	-2.25	114.69	117.06
31	CA	2503	2MA	N3-C2-N1	-2.22	121.64	125.72
31	CA	1962	5MC	CM5-C5-C6	2.21	123.35	118.68
31	CA	2503	2MA	C6-C5-C4	-2.21	115.12	119.63
1	AA	1407	5MC	CM5-C5-C6	2.20	123.33	118.68
55	DA	2503	2MA	CM2-C2-N3	2.18	120.56	117.16
55	DA	1962	5MC	CM5-C5-C6	2.15	123.22	118.68
1	BA	527	7MG	N1-C2-N3	-2.15	122.05	125.42
55	DA	1939	5MU	C5M-C5-C6	2.13	123.18	118.68
1	AA	967	5MC	CM5-C5-C6	2.13	123.17	118.68
1	BA	967	5MC	CM5-C5-C6	2.12	123.16	118.68
55	DA	2503	2MA	N3-C2-N1	-2.12	121.82	125.72
1	AA	527	7MG	N1-C2-N3	-2.12	122.09	125.42
31	CA	2580	PSU	O4'-C1'-C2'	2.12	108.09	104.66
55	DA	2503	2MA	C6-C5-C4	-2.05	115.44	119.63
31	CA	2030	6MZ	C2-N1-C6	2.04	118.34	116.59
1	BA	1407	5MC	CM5-C5-C6	2.03	122.96	118.68
31	CA	747	5MU	C5M-C5-C6	2.02	122.95	118.68

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	CA	2498	OMC	C2'-C1'-N1-C6
41	DN	81[B]	4D4	CA-CB-CG-CD
41	DN	81[A]	4D4	O-C-CA-CB
32	DD	150[B]	MEQ	N-CA-CB-CG
12	BL	89	D2T	O-C-CA-CB
12	BL	89	D2T	CA-CB-SB-CB1
32	DD	150[A]	MEQ	N-CA-CB-CG
32	DD	150[A]	MEQ	C-CA-CB-CG
32	DD	150[A]	MEQ	O-C-CA-CB
41	CN	81	4D4	O-C-CA-CB
55	DA	1962	5MC	O4'-C1'-N1-C6
55	DA	1962	5MC	C2'-C1'-N1-C6
55	DA	746	PSU	O4'-C1'-C5-C4
55	DA	746	PSU	O4'-C1'-C5-C6
12	AL	89	D2T	O-C-CA-CB
12	AL	89	D2T	CG-CB-SB-CB1
31	CA	2030	6MZ	O4'-C4'-C5'-O5'
31	CA	2030	6MZ	C3'-C4'-C5'-O5'
1	BA	1519	MA6	O4'-C4'-C5'-O5'
1	BA	527	7MG	C3'-C4'-C5'-O5'
1	AA	527	7MG	C3'-C4'-C5'-O5'
1	BA	1519	MA6	C3'-C4'-C5'-O5'
1	BA	527	7MG	O4'-C4'-C5'-O5'
1	AA	527	7MG	O4'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
55	DA	2445	2MG	C3'-C4'-C5'-O5'
41	DN	81[B]	4D4	OB-CB-CG-CD
32	DD	150[B]	MEQ	C-CA-CB-CG
1	BA	1519	MA6	C5-C6-N6-C9
1	AA	1519	MA6	C5-C6-N6-C9
55	DA	2030	6MZ	O4'-C4'-C5'-O5'
55	DA	2504	PSU	O4'-C4'-C5'-O5'
55	DA	2604	PSU	O4'-C4'-C5'-O5'
55	DA	746	PSU	C2'-C1'-C5-C6
31	CA	2504	PSU	O4'-C4'-C5'-O5'
32	DD	150[B]	MEQ	CA-CB-CG-CD
55	DA	2069	7MG	C4'-C5'-O5'-P
55	DA	2503	2MA	O4'-C4'-C5'-O5'
31	CA	2503	2MA	O4'-C4'-C5'-O5'
31	CA	1618	6MZ	C4'-C5'-O5'-P
41	DN	81[B]	4D4	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
31	CA	746	PSU	O4'-C1'-C5-C4
12	AL	89	D2T	CA-CB-SB-CB1
55	DA	2580	PSU	C2'-C1'-C5-C6
55	DA	2580	PSU	O4'-C4'-C5'-O5'
32	DD	150[A]	MEQ	OE1-CD-CG-CB
55	DA	2503	2MA	C4'-C5'-O5'-P
55	DA	2445	2MG	O4'-C4'-C5'-O5'
31	CA	2498	OMC	O4'-C4'-C5'-O5'
55	DA	2069	7MG	O4'-C4'-C5'-O5'
55	DA	2030	6MZ	C3'-C4'-C5'-O5'
12	BL	89	D2T	CG-CB-SB-CB1
31	CA	2503	2MA	C4'-C5'-O5'-P
55	DA	2504	PSU	C3'-C4'-C5'-O5'
31	CA	2504	PSU	C3'-C4'-C5'-O5'
31	CA	1939	5MU	C3'-C4'-C5'-O5'
31	CA	1939	5MU	O4'-C4'-C5'-O5'
31	CA	2069	7MG	O4'-C4'-C5'-O5'
41	DN	81[B]	4D4	O-C-CA-CB
55	DA	2449	H2U	C4'-C5'-O5'-P

There are no ring outliers.

16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1518	MA6	1	0
1	BA	1402	4OC	1	0
55	DA	2030	6MZ	2	0
1	BA	1519	MA6	1	0
32	DD	150[B]	MEQ	1	0
55	DA	2498	OMC	1	0
32	DD	150[A]	MEQ	2	0
1	BA	1518	MA6	1	0
55	DA	747	5MU	1	0
31	CA	1939	5MU	1	0
31	CA	2030	6MZ	5	0
1	AA	1519	MA6	1	0
31	CA	745	1MG	1	0
1	AA	1402	4OC	1	0
31	CA	747	5MU	1	0
1	BA	967	5MC	3	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	GUN	DA	3211	-	9,12,12	1.55	2 (22%)	8,17,17	3.91	4 (50%)
61	PEG	DL	201	-	6,6,6	0.10	0	5,5,5	0.07	0
59	PUT	AA	1672	-	5,5,5	0.08	0	4,4,4	0.14	0
62	EDO	DA	3003	-	3,3,3	0.68	0	2,2,2	0.32	0
59	PUT	DA	3213	-	5,5,5	0.24	0	4,4,4	0.18	0
59	PUT	AA	1675	-	5,5,5	0.18	0	4,4,4	0.08	0
65	1PE	DA	3185	-	15,15,15	0.20	0	14,14,14	0.16	0
59	PUT	DM	201	-	5,5,5	0.22	0	4,4,4	0.27	0
59	PUT	AA	1674	-	5,5,5	0.15	0	4,4,4	0.12	0
58	MPD	DA	3204	-	7,7,7	0.71	0	9,10,10	0.51	0
59	PUT	DA	3222	-	5,5,5	0.27	0	4,4,4	0.50	0
57	PG4	DA	3216	-	12,12,12	0.14	0	11,11,11	0.15	0
62	EDO	DA	3197	-	3,3,3	0.67	0	2,2,2	0.16	0
57	PG4	AA	1670	-	12,12,12	0.18	0	11,11,11	0.20	0
62	EDO	D1	101	-	3,3,3	0.68	0	2,2,2	0.22	0
64	SPD	DA	3187	-	9,9,9	0.12	0	8,8,8	0.21	0
63	PGE	D1	102	-	9,9,9	0.11	0	8,8,8	0.13	0
62	EDO	DA	3002	-	3,3,3	0.63	0	2,2,2	0.15	0
57	PG4	DA	3193	-	12,12,12	0.28	0	11,11,11	0.26	0
66	ACY	DA	3191	-	1,3,3	2.03	1 (100%)	0,3,3	0.00	-
57	PG4	BA	1642	-	12,12,12	0.23	0	11,11,11	0.19	0
62	EDO	DA	3215	-	3,3,3	0.72	0	2,2,2	0.23	0
63	PGE	DA	3214	-	9,9,9	0.24	0	8,8,8	0.34	0
61	PEG	DP	201	-	6,6,6	0.16	0	5,5,5	0.13	0
64	SPD	DA	3224	-	9,9,9	0.13	0	8,8,8	0.23	0
66	ACY	DA	3202	-	1,3,3	0.01	0	0,3,3	0.00	-
57	PG4	DS	202	-	12,12,12	0.19	0	11,11,11	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	PEG	DA	3218	-	6,6,6	0.15	0	5,5,5	0.08	0
57	PG4	DQ	202	-	12,12,12	0.13	0	11,11,11	0.15	0
68	TRS	DA	3220	-	7,7,7	0.23	0	9,9,9	0.22	0
61	PEG	DA	3200	-	6,6,6	0.23	0	5,5,5	0.09	0
59	PUT	DA	3189	-	5,5,5	0.09	0	4,4,4	0.22	0
61	PEG	DA	3201	-	6,6,6	0.14	0	5,5,5	0.15	0
58	MPD	DA	3207	-	7,7,7	0.37	0	9,10,10	0.52	0
61	PEG	DQ	201	-	6,6,6	0.22	0	5,5,5	0.12	0
65	1PE	DA	3203	-	15,15,15	0.21	0	14,14,14	0.25	0
58	MPD	DA	3210	-	7,7,7	0.82	0	9,10,10	0.34	0
62	EDO	DA	3209	-	3,3,3	0.53	0	2,2,2	0.33	0
59	PUT	DA	3188	-	5,5,5	0.12	0	4,4,4	0.17	0
58	MPD	DN	201	-	7,7,7	1.17	1 (14%)	9,10,10	0.51	0
63	PGE	DA	3225	-	9,9,9	0.26	0	8,8,8	0.31	0
63	PGE	DA	3217	-	9,9,9	0.22	0	8,8,8	0.19	0
59	PUT	DA	3223	-	5,5,5	0.20	0	4,4,4	0.17	0
58	MPD	DT	202	-	7,7,7	0.78	0	9,10,10	0.50	0
59	PUT	DA	3221	-	5,5,5	0.25	0	4,4,4	0.13	0
63	PGE	DS	201	-	9,9,9	0.22	0	8,8,8	0.18	0
59	PUT	DA	3184	-	5,5,5	0.17	0	4,4,4	0.21	0
61	PEG	DA	3199	-	6,6,6	0.18	0	5,5,5	0.12	0
66	ACY	DA	3196	-	1,3,3	4.11	1 (100%)	0,3,3	0.00	-
61	PEG	DA	3226	-	6,6,6	0.20	0	5,5,5	0.06	0
63	PGE	DD	301	-	9,9,9	0.21	0	8,8,8	0.16	0
58	MPD	DE	301	-	7,7,7	0.67	0	9,10,10	0.43	0
63	PGE	D3	101	-	9,9,9	0.22	0	8,8,8	0.11	0
58	MPD	DA	3190	-	7,7,7	0.53	0	9,10,10	0.45	0
59	PUT	DA	3205	-	5,5,5	0.18	0	4,4,4	0.16	0
62	EDO	DA	3194	-	3,3,3	0.74	0	2,2,2	0.13	0
59	PUT	DA	3212	-	5,5,5	0.25	0	4,4,4	0.13	0
59	PUT	DA	3219	-	5,5,5	0.21	0	4,4,4	0.16	0
62	EDO	DA	3198	-	3,3,3	0.76	0	2,2,2	0.25	0
61	PEG	AL	201	-	6,6,6	0.19	0	5,5,5	0.15	0
62	EDO	DB	210	-	3,3,3	0.69	0	2,2,2	0.15	0
57	PG4	DR	201	-	12,12,12	0.22	0	11,11,11	0.25	0
62	EDO	DB	211	-	3,3,3	0.59	0	2,2,2	0.31	0
62	EDO	D0	101	-	3,3,3	0.63	0	2,2,2	0.55	0
58	MPD	DK	201	-	7,7,7	1.02	1 (14%)	9,10,10	0.37	0
61	PEG	D3	102	-	6,6,6	0.21	0	5,5,5	0.20	0
59	PUT	DA	3195	-	5,5,5	0.28	0	4,4,4	0.25	0
58	MPD	DT	201	-	7,7,7	0.76	0	9,10,10	0.30	0
58	MPD	DA	3192	-	7,7,7	0.84	0	9,10,10	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	MPD	DE	302	-	7,7,7	0.96	1 (14%)	9,10,10	0.72	0
62	EDO	DA	3208	-	3,3,3	0.59	0	2,2,2	0.31	0
64	SPD	DA	3183	-	9,9,9	0.22	0	8,8,8	0.34	0
58	MPD	AA	1676	-	7,7,7	0.74	0	9,10,10	0.54	0
63	PGE	DU	201	-	9,9,9	0.32	0	8,8,8	0.29	0
59	PUT	AA	1673	-	5,5,5	0.14	0	4,4,4	0.09	0
63	PGE	DA	3186	-	9,9,9	0.33	0	8,8,8	0.35	0
58	MPD	DS	203	-	7,7,7	0.36	0	9,10,10	0.38	0
64	SPD	DA	3206	-	9,9,9	0.23	0	8,8,8	0.21	0
58	MPD	AA	1671	-	7,7,7	0.43	0	9,10,10	0.49	0
61	PEG	DA	3227	-	6,6,6	0.24	0	5,5,5	0.16	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
67	GUN	DA	3211	-	-	-	0/2/2/2
61	PEG	DL	201	-	-	3/4/4/4	-
59	PUT	AA	1672	-	-	0/3/3/3	-
62	EDO	DA	3003	-	-	1/1/1/1	-
59	PUT	DA	3213	-	-	1/3/3/3	-
59	PUT	AA	1675	-	-	1/3/3/3	-
65	1PE	DA	3185	-	-	4/13/13/13	-
59	PUT	DM	201	-	-	0/3/3/3	-
59	PUT	AA	1674	-	-	0/3/3/3	-
58	MPD	DA	3204	-	-	2/5/5/5	-
59	PUT	DA	3222	-	-	0/3/3/3	-
57	PG4	DA	3216	-	-	5/10/10/10	-
62	EDO	DA	3197	-	-	0/1/1/1	-
57	PG4	AA	1670	-	-	6/10/10/10	-
62	EDO	D1	101	-	-	0/1/1/1	-
64	SPD	DA	3187	-	-	2/7/7/7	-
63	PGE	D1	102	-	-	5/7/7/7	-
62	EDO	DA	3002	-	-	0/1/1/1	-
57	PG4	DA	3193	-	-	4/10/10/10	-
57	PG4	BA	1642	-	-	5/10/10/10	-
62	EDO	DA	3215	-	-	0/1/1/1	-
63	PGE	DA	3214	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PEG	DP	201	-	-	1/4/4/4	-
64	SPD	DA	3224	-	-	3/7/7/7	-
57	PG4	DS	202	-	-	4/10/10/10	-
61	PEG	DA	3218	-	-	1/4/4/4	-
57	PG4	DQ	202	-	-	1/10/10/10	-
68	TRS	DA	3220	-	-	0/9/9/9	-
61	PEG	DA	3200	-	-	1/4/4/4	-
59	PUT	DA	3189	-	-	0/3/3/3	-
61	PEG	DA	3201	-	-	1/4/4/4	-
58	MPD	DA	3207	-	-	2/5/5/5	-
61	PEG	DQ	201	-	-	2/4/4/4	-
65	1PE	DA	3203	-	-	5/13/13/13	-
58	MPD	DA	3210	-	-	2/5/5/5	-
62	EDO	DA	3209	-	-	0/1/1/1	-
59	PUT	DA	3188	-	-	0/3/3/3	-
58	MPD	DN	201	-	-	0/5/5/5	-
63	PGE	DA	3225	-	-	4/7/7/7	-
63	PGE	DA	3217	-	-	3/7/7/7	-
59	PUT	DA	3223	-	-	1/3/3/3	-
58	MPD	DT	202	-	-	1/5/5/5	-
59	PUT	DA	3221	-	-	0/3/3/3	-
63	PGE	DS	201	-	-	4/7/7/7	-
59	PUT	DA	3184	-	-	1/3/3/3	-
61	PEG	DA	3199	-	-	2/4/4/4	-
61	PEG	DA	3226	-	-	0/4/4/4	-
63	PGE	DD	301	-	-	5/7/7/7	-
58	MPD	DE	301	-	-	2/5/5/5	-
63	PGE	D3	101	-	-	4/7/7/7	-
58	MPD	DA	3190	-	-	1/5/5/5	-
59	PUT	DA	3205	-	-	0/3/3/3	-
62	EDO	DA	3194	-	-	0/1/1/1	-
59	PUT	DA	3212	-	-	0/3/3/3	-
59	PUT	DA	3219	-	-	0/3/3/3	-
62	EDO	DA	3198	-	-	1/1/1/1	-
61	PEG	AL	201	-	-	2/4/4/4	-
62	EDO	DB	210	-	-	1/1/1/1	-
57	PG4	DR	201	-	-	4/10/10/10	-
62	EDO	DB	211	-	-	0/1/1/1	-
62	EDO	D0	101	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	MPD	DK	201	-	-	5/5/5/5	-
61	PEG	D3	102	-	-	1/4/4/4	-
59	PUT	DA	3195	-	-	0/3/3/3	-
58	MPD	DT	201	-	-	1/5/5/5	-
58	MPD	DA	3192	-	-	2/5/5/5	-
58	MPD	DE	302	-	-	3/5/5/5	-
62	EDO	DA	3208	-	-	0/1/1/1	-
64	SPD	DA	3183	-	-	3/7/7/7	-
58	MPD	AA	1676	-	-	1/5/5/5	-
63	PGE	DU	201	-	-	4/7/7/7	-
59	PUT	AA	1673	-	-	0/3/3/3	-
63	PGE	DA	3186	-	-	2/7/7/7	-
58	MPD	DS	203	-	-	1/5/5/5	-
64	SPD	DA	3206	-	-	2/7/7/7	-
58	MPD	AA	1671	-	-	0/5/5/5	-
61	PEG	DA	3227	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	DA	3196	ACY	CH3-C	4.11	1.54	1.48
67	DA	3211	GUN	C6-N1	3.70	1.39	1.33
58	DN	201	MPD	C3-C2	2.72	1.61	1.53
58	DK	201	MPD	C3-C2	2.38	1.60	1.53
58	DE	302	MPD	C3-C2	2.25	1.59	1.53
67	DA	3211	GUN	C6-C5	2.09	1.45	1.41
66	DA	3191	ACY	CH3-C	2.03	1.51	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	DA	3211	GUN	C5-C6-N1	-8.01	112.48	123.43
67	DA	3211	GUN	C6-N1-C2	5.91	125.32	115.93
67	DA	3211	GUN	N3-C2-N1	-3.30	122.82	127.22
67	DA	3211	GUN	C6-C5-C4	-2.97	117.96	120.80

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	DE	302	MPD	C1-C2-C3-C4
58	DE	302	MPD	O2-C2-C3-C4
57	BA	1642	PG4	O4-C7-C8-O5
63	DA	3225	PGE	O2-C3-C4-O3
63	DS	201	PGE	O2-C3-C4-O3
57	DA	3193	PG4	O3-C5-C6-O4
65	DA	3185	1PE	OH2-C12-C22-OH3
63	DA	3214	PGE	O2-C3-C4-O3
64	DA	3224	SPD	C3-C4-C5-N6
63	DA	3214	PGE	O3-C5-C6-O4
63	DA	3225	PGE	O1-C1-C2-O2
57	DS	202	PG4	O1-C1-C2-O2
57	DR	201	PG4	O2-C3-C4-O3
64	DA	3183	SPD	C8-C7-N6-C5
63	DU	201	PGE	O3-C5-C6-O4
61	DA	3199	PEG	O2-C3-C4-O4
63	DA	3214	PGE	O1-C1-C2-O2
57	AA	1670	PG4	O4-C7-C8-O5
59	DA	3213	PUT	C1-C2-C3-C4
62	DA	3198	EDO	O1-C1-C2-O2
62	DB	210	EDO	O1-C1-C2-O2
63	D1	102	PGE	O3-C5-C6-O4
63	DU	201	PGE	O1-C1-C2-O2
61	DL	201	PEG	O2-C3-C4-O4
61	DQ	201	PEG	O2-C3-C4-O4
57	AA	1670	PG4	O1-C1-C2-O2
57	BA	1642	PG4	O2-C3-C4-O3
61	DL	201	PEG	O1-C1-C2-O2
65	DA	3203	1PE	OH4-C13-C23-OH3
63	D1	102	PGE	O2-C3-C4-O3
65	DA	3203	1PE	OH5-C14-C24-OH4
59	DA	3184	PUT	C1-C2-C3-C4
57	DR	201	PG4	O3-C5-C6-O4
64	DA	3183	SPD	C4-C5-N6-C7
64	DA	3206	SPD	C8-C7-N6-C5
63	DA	3186	PGE	C6-C5-O3-C4
57	DA	3193	PG4	C4-C3-O2-C2
63	DD	301	PGE	C3-C4-O3-C5
63	DS	201	PGE	C4-C3-O2-C2
61	DA	3201	PEG	C1-C2-O2-C3
61	DA	3218	PEG	C1-C2-O2-C3
63	DA	3225	PGE	C3-C4-O3-C5
61	DA	3200	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
65	DA	3185	1PE	C14-C24-OH4-C13
63	D3	101	PGE	C1-C2-O2-C3
57	DA	3216	PG4	C3-C4-O3-C5
63	D1	102	PGE	C4-C3-O2-C2
57	BA	1642	PG4	C1-C2-O2-C3
63	DS	201	PGE	C6-C5-O3-C4
57	DA	3193	PG4	C8-C7-O4-C6
57	DA	3216	PG4	C4-C3-O2-C2
57	DA	3216	PG4	C8-C7-O4-C6
57	DR	201	PG4	C8-C7-O4-C6
63	DA	3214	PGE	C4-C3-O2-C2
63	DA	3217	PGE	C4-C3-O2-C2
57	DQ	202	PG4	O1-C1-C2-O2
57	AA	1670	PG4	C5-C6-O4-C7
63	DA	3217	PGE	C6-C5-O3-C4
61	DP	201	PEG	C1-C2-O2-C3
65	DA	3203	1PE	C12-C22-OH3-C23
58	DT	202	MPD	C2-C3-C4-C5
58	DA	3192	MPD	C2-C3-C4-C5
58	DA	3190	MPD	C2-C3-C4-C5
58	DE	301	MPD	C2-C3-C4-C5
58	DK	201	MPD	C2-C3-C4-C5
58	DA	3204	MPD	C2-C3-C4-C5
63	DA	3217	PGE	C3-C4-O3-C5
63	DD	301	PGE	O3-C5-C6-O4
63	DS	201	PGE	O3-C5-C6-O4
57	BA	1642	PG4	C8-C7-O4-C6
57	DS	202	PG4	C1-C2-O2-C3
64	DA	3224	SPD	C8-C7-N6-C5
57	DA	3216	PG4	C1-C2-O2-C3
63	DU	201	PGE	C3-C4-O3-C5
57	DS	202	PG4	C3-C4-O3-C5
57	AA	1670	PG4	C3-C4-O3-C5
63	D3	101	PGE	O3-C5-C6-O4
58	DT	201	MPD	C1-C2-C3-C4
58	DA	3210	MPD	C1-C2-C3-C4
58	DK	201	MPD	C1-C2-C3-C4
58	DK	201	MPD	CM-C2-C3-C4
58	DE	302	MPD	CM-C2-C3-C4
63	D3	101	PGE	C3-C4-O3-C5
63	DA	3225	PGE	C1-C2-O2-C3
59	DA	3223	PUT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
65	DA	3185	1PE	C16-C26-OH6-C15
61	AL	201	PEG	C1-C2-O2-C3
57	AA	1670	PG4	C4-C3-O2-C2
61	AL	201	PEG	C4-C3-O2-C2
57	DS	202	PG4	C4-C3-O2-C2
61	DA	3199	PEG	C4-C3-O2-C2
63	D1	102	PGE	C1-C2-O2-C3
65	DA	3203	1PE	OH2-C12-C22-OH3
61	DQ	201	PEG	C1-C2-O2-C3
64	DA	3183	SPD	C2-C3-C4-C5
65	DA	3203	1PE	C14-C24-OH4-C13
63	DD	301	PGE	O2-C3-C4-O3
63	D1	102	PGE	C3-C4-O3-C5
63	DD	301	PGE	C1-C2-O2-C3
61	D3	102	PEG	C4-C3-O2-C2
63	DD	301	PGE	C4-C3-O2-C2
59	AA	1675	PUT	C1-C2-C3-C4
63	DA	3186	PGE	O3-C5-C6-O4
57	DR	201	PG4	C5-C6-O4-C7
64	DA	3224	SPD	C4-C5-N6-C7
61	DL	201	PEG	C4-C3-O2-C2
58	DA	3210	MPD	O2-C2-C3-C4
58	DK	201	MPD	O2-C2-C3-C4
63	D3	101	PGE	C4-C3-O2-C2
57	DA	3193	PG4	O2-C3-C4-O3
65	DA	3185	1PE	C24-C14-OH5-C25
57	BA	1642	PG4	C3-C4-O3-C5
57	AA	1670	PG4	C1-C2-O2-C3
63	DU	201	PGE	C1-C2-O2-C3
64	DA	3187	SPD	C2-C3-C4-C5
64	DA	3187	SPD	C7-C8-C9-N10
64	DA	3206	SPD	C3-C4-C5-N6
57	DA	3216	PG4	O4-C7-C8-O5
58	DA	3207	MPD	C2-C3-C4-C5
62	DA	3003	EDO	O1-C1-C2-O2
58	DA	3192	MPD	C2-C3-C4-O4
58	DE	301	MPD	C2-C3-C4-O4
58	DK	201	MPD	C2-C3-C4-O4
58	DA	3204	MPD	C2-C3-C4-O4
58	AA	1676	MPD	C2-C3-C4-O4
58	DA	3207	MPD	C2-C3-C4-O4
58	DS	203	MPD	C2-C3-C4-O4

There are no ring outliers.

19 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	DA	3213	PUT	1	0
65	DA	3185	1PE	1	0
62	DA	3002	EDO	1	0
57	BA	1642	PG4	1	0
63	DA	3214	PGE	1	0
66	DA	3202	ACY	2	0
68	DA	3220	TRS	1	0
61	DA	3201	PEG	1	0
61	DQ	201	PEG	1	0
63	DA	3225	PGE	4	0
59	DA	3223	PUT	1	0
62	DA	3194	EDO	3	0
59	DA	3212	PUT	1	0
59	DA	3219	PUT	1	0
57	DR	201	PG4	1	0
61	D3	102	PEG	1	0
58	DA	3192	MPD	2	0
63	DU	201	PGE	1	0
58	DS	203	MPD	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1523/1534 (99%)	0.32	109 (7%) 15 16	65, 138, 270, 291	0
1	BA	1522/1534 (99%)	0.84	261 (17%) 1 1	86, 162, 293, 294	0
2	AB	224/224 (100%)	1.18	57 (25%) 0 0	108, 156, 231, 272	0
2	BB	224/224 (100%)	1.03	44 (19%) 1 0	138, 181, 229, 262	0
3	AC	206/206 (100%)	1.32	56 (27%) 0 0	138, 174, 208, 228	0
3	BC	206/206 (100%)	3.38	125 (60%) 0 0	223, 253, 269, 279	0
4	AD	205/205 (100%)	0.24	4 (1%) 65 64	100, 145, 174, 190	0
4	BD	205/205 (100%)	-0.21	0 100 100	71, 100, 137, 174	0
5	AE	155/155 (100%)	0.39	7 (4%) 33 33	83, 119, 150, 176	0
5	BE	150/155 (96%)	0.43	12 (8%) 12 12	92, 125, 168, 236	0
6	AF	106/106 (100%)	0.01	5 (4%) 31 31	89, 126, 149, 187	0
6	BF	100/106 (94%)	0.73	14 (14%) 2 2	135, 162, 188, 196	0
7	AG	151/151 (100%)	1.99	70 (46%) 0 0	159, 186, 216, 229	0
7	BG	151/151 (100%)	4.00	108 (71%) 0 0	198, 247, 263, 268	0
8	AH	129/129 (100%)	0.48	10 (7%) 13 13	89, 122, 148, 158	0
8	BH	129/129 (100%)	0.33	11 (8%) 10 11	119, 151, 179, 192	0
9	AI	127/127 (100%)	2.23	51 (40%) 0 0	168, 196, 251, 270	0
9	BI	127/127 (100%)	2.80	63 (49%) 0 0	198, 234, 277, 283	0
10	AJ	99/99 (100%)	2.36	44 (44%) 0 0	169, 190, 228, 238	0
10	BJ	98/99 (98%)	4.87	73 (74%) 0 0	209, 248, 280, 287	0
11	AK	117/129 (90%)	0.76	18 (15%) 2 1	77, 139, 174, 190	0
11	BK	117/129 (90%)	1.20	28 (23%) 0 0	111, 166, 186, 202	0
12	AL	122/123 (99%)	0.47	11 (9%) 9 10	78, 112, 137, 178	0
12	BL	122/123 (99%)	0.62	12 (9%) 7 7	96, 121, 148, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	2.14	53 (46%) 0 0	167, 198, 220, 233	0
13	BM	114/114 (100%)	4.71	103 (90%) 0 0	254, 271, 288, 292	0
14	AN	100/100 (100%)	2.49	51 (51%) 0 0	166, 188, 252, 260	0
14	BN	100/100 (100%)	4.56	77 (77%) 0 0	226, 252, 282, 288	0
15	AO	88/88 (100%)	0.30	7 (7%) 12 12	75, 109, 142, 169	0
15	BO	88/88 (100%)	0.94	17 (19%) 1 0	127, 160, 180, 197	0
16	AP	82/82 (100%)	1.41	28 (34%) 0 0	88, 128, 168, 195	0
16	BP	82/82 (100%)	1.12	21 (25%) 0 0	106, 136, 168, 184	0
17	AQ	80/80 (100%)	0.57	10 (12%) 3 3	86, 115, 149, 157	0
17	BQ	80/80 (100%)	1.41	25 (31%) 0 0	120, 159, 182, 197	0
18	AR	55/55 (100%)	0.71	8 (14%) 2 2	86, 116, 172, 194	0
18	BR	55/55 (100%)	1.75	19 (34%) 0 0	126, 143, 173, 216	0
19	AS	79/79 (100%)	1.36	25 (31%) 0 0	180, 201, 215, 222	0
19	BS	79/79 (100%)	4.58	55 (69%) 0 0	229, 265, 274, 278	0
20	AT	86/86 (100%)	0.24	3 (3%) 44 42	91, 122, 151, 161	0
20	BT	85/86 (98%)	1.67	26 (30%) 0 0	136, 157, 183, 193	0
21	AU	56/56 (100%)	1.15	7 (12%) 3 3	114, 146, 208, 223	0
21	BU	56/56 (100%)	0.65	8 (14%) 2 2	112, 151, 191, 204	0
22	C1	56/56 (100%)	1.67	18 (32%) 0 0	131, 187, 206, 219	0
22	D1	56/56 (100%)	-0.35	0 100 100	31, 57, 81, 120	0
23	C2	50/51 (98%)	3.48	37 (74%) 0 0	179, 197, 215, 237	0
23	D2	51/51 (100%)	0.18	0 100 100	81, 98, 130, 145	0
24	C3	46/46 (100%)	1.91	20 (43%) 0 0	129, 153, 170, 177	0
24	D3	46/46 (100%)	-0.11	0 100 100	42, 51, 71, 143	0
25	C4	64/64 (100%)	1.43	23 (35%) 0 0	145, 165, 182, 187	0
25	D4	64/64 (100%)	-0.18	0 100 100	51, 64, 78, 105	0
26	C5	38/38 (100%)	1.26	6 (15%) 2 1	126, 153, 166, 174	0
26	D5	38/38 (100%)	0.07	1 (2%) 56 53	52, 68, 95, 120	0
27	C0	58/58 (100%)	1.24	15 (25%) 0 0	123, 142, 171, 180	0
27	D0	58/58 (100%)	-0.34	0 100 100	36, 49, 85, 112	0
28	CB	118/120 (98%)	0.58	7 (5%) 22 23	134, 208, 253, 258	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	-0.18	0 100 100	45, 87, 138, 167	0
29	CC	271/272 (99%)	0.70	35 (12%) 3 3	102, 130, 160, 176	0
29	DC	271/272 (99%)	-0.18	0 100 100	42, 75, 106, 142	0
30	CD	209/209 (100%)	1.64	75 (35%) 0 0	100, 154, 179, 193	0
31	CA	2876/2904 (99%)	0.63	271 (9%) 8 9	92, 184, 267, 286	0
32	DD	208/209 (99%)	-0.24	0 100 100	27, 55, 93, 121	0
33	CE	201/201 (100%)	1.60	68 (33%) 0 0	133, 193, 233, 243	0
33	DE	201/201 (100%)	-0.06	0 100 100	30, 82, 132, 150	0
34	CF	177/178 (99%)	2.60	109 (61%) 0 0	212, 233, 249, 254	0
34	DF	177/178 (99%)	0.33	10 (5%) 24 24	79, 120, 170, 188	0
35	CG	176/176 (100%)	2.55	100 (56%) 0 0	168, 196, 232, 244	0
35	DG	176/176 (100%)	0.08	9 (5%) 28 27	57, 93, 122, 156	0
36	CH	149/149 (100%)	1.57	52 (34%) 0 0	131, 172, 197, 208	0
36	DH	149/149 (100%)	1.18	30 (20%) 1 0	83, 173, 211, 231	0
37	CJ	134/135 (99%)	5.46	110 (82%) 0 0	259, 279, 289, 291	0
37	DJ	134/135 (99%)	3.81	92 (68%) 0 0	228, 249, 266, 272	0
38	CK	142/142 (100%)	0.65	9 (6%) 20 21	115, 144, 168, 182	0
38	DK	142/142 (100%)	-0.32	0 100 100	28, 49, 82, 106	0
39	CL	122/123 (99%)	0.68	16 (13%) 3 3	105, 133, 168, 181	0
39	DL	123/123 (100%)	-0.23	0 100 100	43, 62, 95, 135	0
40	CM	144/144 (100%)	2.54	69 (47%) 0 0	131, 195, 243, 260	0
40	DM	144/144 (100%)	-0.18	1 (0%) 87 89	26, 78, 114, 152	0
41	CN	135/136 (99%)	0.88	19 (14%) 2 2	107, 145, 176, 205	0
41	DN	135/136 (99%)	-0.38	0 100 100	36, 59, 90, 112	0
42	CO	120/127 (94%)	1.25	25 (20%) 1 0	127, 158, 186, 233	0
42	DO	125/127 (98%)	-0.26	0 100 100	33, 52, 96, 155	0
43	CP	116/117 (99%)	2.36	60 (51%) 0 0	165, 195, 217, 223	0
43	DP	117/117 (100%)	-0.09	0 100 100	56, 84, 121, 136	0
44	CQ	114/114 (100%)	1.49	38 (33%) 0 0	124, 150, 174, 186	0
44	DQ	114/114 (100%)	-0.22	1 (0%) 84 85	47, 72, 105, 135	0
45	CR	117/117 (100%)	1.35	31 (26%) 0 0	117, 144, 166, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	DR	117/117 (100%)	-0.17	0 100 100	24, 41, 63, 114	0
46	CS	103/103 (100%)	1.93	38 (36%) 0 0	117, 159, 195, 202	0
46	DS	103/103 (100%)	-0.24	0 100 100	30, 55, 92, 126	0
47	CT	110/110 (100%)	1.58	38 (34%) 0 0	140, 171, 196, 207	0
47	DT	110/110 (100%)	-0.28	0 100 100	26, 45, 79, 128	0
48	CU	93/100 (93%)	2.62	54 (58%) 0 0	159, 194, 219, 229	0
48	DU	93/100 (93%)	0.26	2 (2%) 62 60	51, 73, 136, 154	0
49	CV	102/103 (99%)	3.12	70 (68%) 0 0	157, 198, 231, 242	0
49	DV	102/103 (99%)	0.08	5 (4%) 29 29	57, 82, 126, 156	0
50	CW	94/94 (100%)	1.56	34 (36%) 0 0	133, 172, 186, 192	0
50	DW	94/94 (100%)	-0.30	0 100 100	43, 73, 110, 119	0
51	CX	75/76 (98%)	1.94	31 (41%) 0 0	129, 161, 175, 206	0
51	DX	76/76 (100%)	-0.35	0 100 100	36, 62, 92, 157	0
52	CY	77/77 (100%)	0.86	14 (18%) 1 1	120, 145, 173, 185	0
52	DY	77/77 (100%)	-0.10	1 (1%) 77 77	56, 76, 111, 130	0
53	CZ	62/62 (100%)	2.61	38 (61%) 0 0	177, 199, 210, 217	0
53	DZ	62/62 (100%)	0.33	2 (3%) 47 46	65, 97, 136, 174	0
54	DI	135/135 (100%)	1.29	39 (28%) 0 0	104, 179, 244, 266	1 (0%)
55	DA	2873/2904 (98%)	0.06	78 (2%) 54 53	29, 65, 231, 294	0
All	All	20634/20795 (99%)	0.86	3537 (17%) 1 1	24, 144, 266, 294	1 (0%)

All (3537) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	CJ	13	VAL	34.4
9	BI	126	GLN	26.3
9	BI	128	SER	23.0
37	DJ	54	PRO	20.5
1	BA	1302	C	20.3
10	BJ	41	PRO	19.5
3	BC	197	GLY	19.0
10	BJ	74	VAL	18.6
10	BJ	75	ASP	18.1
3	BC	196	ILE	17.9
37	CJ	14	ALA	17.3

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Mol	Chain	Res	Type	RSRZ
3	BC	198	VAL	17.0
3	BC	195	VAL	16.7
37	DJ	53	LEU	16.7
1	BA	985	C	16.6
37	CJ	12	GLN	16.3
9	BI	127	PHE	16.2
1	BA	1242	G	16.0
19	BS	29	LYS	16.0
10	BJ	77	VAL	15.7
10	BJ	8	ILE	15.6
7	BG	42	ILE	15.6
1	BA	1241	G	15.5
7	BG	39	ALA	15.4
37	CJ	23	PRO	15.1
10	BJ	73	LEU	15.1
55	DA	2120	G	15.1
37	CJ	69	PHE	15.0
7	BG	38	THR	14.5
3	BC	159	GLY	14.5
14	BN	37	SER	14.2
9	AI	127	PHE	14.1
1	BA	1305	G	14.0
14	BN	36	ALA	13.8
19	BS	66	MET	13.7
19	BS	30	PRO	13.7
14	AN	21	PHE	13.5
3	BC	193	TYR	13.5
13	BM	95	LEU	13.3
35	CG	32	GLU	13.3
31	CA	1068	G	13.2
37	DJ	13	VAL	13.1
37	CJ	57	VAL	13.1
31	CA	1067	A	12.9
9	AI	130	ARG	12.6
13	BM	45	ILE	12.5
14	BN	55	SER	12.5
18	BR	20	GLU	12.5
37	CJ	87	LYS	12.4
37	CJ	54	PRO	12.3
7	BG	112	GLY	12.2
7	BG	45	SER	12.2
30	CD	6	GLY	12.1

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Mol	Chain	Res	Type	RSRZ
10	BJ	9	ARG	12.1
40	CM	81	ASP	12.1
7	BG	43	VAL	12.0
9	BI	31	ASN	12.0
19	BS	60	VAL	11.9
37	DJ	79	LEU	11.9
37	CJ	88	SER	11.7
1	BA	1016	A	11.6
13	BM	104	THR	11.6
37	CJ	20	PRO	11.5
37	CJ	51	LYS	11.3
10	BJ	72	ARG	11.3
1	BA	983	A	11.3
37	DJ	76	ALA	11.2
37	CJ	11	LEU	11.1
37	CJ	55	ILE	11.1
13	BM	83	LEU	11.1
37	CJ	42	PHE	11.1
13	BM	108	THR	11.0
1	BA	1201	A	10.9
37	CJ	53	LEU	10.8
13	BM	40	ALA	10.8
55	DA	2116	G	10.8
46	CS	50	GLY	10.7
1	BA	1274	A	10.7
1	BA	1243	C	10.7
19	BS	61	PHE	10.7
37	CJ	71	THR	10.5
43	CP	64	TYR	10.5
1	BA	1049	U	10.5
9	AI	128	SER	10.5
37	CJ	24	VAL	10.4
13	BM	33	ILE	10.4
14	BN	72	GLY	10.4
3	BC	181	ASP	10.4
10	BJ	26	VAL	10.3
37	DJ	59	ILE	10.3
34	CF	153	ASP	10.3
31	CA	2126	A	10.3
7	BG	65	ALA	10.3
1	BA	986	U	10.3
31	CA	331	C	10.1

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Mol	Chain	Res	Type	RSRZ
19	BS	48	THR	10.1
13	BM	39	ILE	10.0
7	BG	62	PHE	10.0
13	BM	84	GLY	10.0
35	CG	2	SER	10.0
37	DJ	12	GLN	10.0
1	BA	987	G	10.0
31	CA	2172	U	10.0
3	BC	128	VAL	10.0
10	BJ	22	THR	9.9
9	AI	126	GLN	9.9
10	BJ	40	ILE	9.8
37	CJ	21	SER	9.8
10	BJ	7	ARG	9.8
37	DJ	23	PRO	9.8
14	BN	67	THR	9.8
14	BN	54	ASP	9.8
7	BG	49	THR	9.8
51	CX	54	GLY	9.8
1	BA	954	G	9.7
9	BI	17	ALA	9.7
3	BC	192	THR	9.7
1	BA	984	C	9.7
31	CA	1087	G	9.7
37	DJ	21	SER	9.6
13	BM	10	PRO	9.6
23	C2	52	ALA	9.6
14	AN	24	ARG	9.5
37	DJ	67	PHE	9.5
19	BS	49	ILE	9.4
10	BJ	10	LEU	9.4
49	CV	89	ASP	9.4
14	BN	4	GLN	9.4
37	DJ	80	LEU	9.3
10	BJ	76	ILE	9.3
14	BN	60	GLN	9.2
1	BA	1196	A	9.2
7	BG	41	SER	9.2
40	CM	120	VAL	9.2
1	BA	1024	G	9.2
31	CA	1537	G	9.1
3	BC	156	ARG	9.1

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Mol	Chain	Res	Type	RSRZ
7	BG	69	VAL	9.1
7	BG	116	MET	9.1
37	CJ	22	PRO	9.0
37	CJ	116	ASP	9.0
1	BA	1022	A	9.0
37	DJ	20	PRO	9.0
55	DA	2110	G	9.0
48	CU	15	HIS	9.0
10	BJ	35	GLN	9.0
48	CU	83	ALA	8.9
54	DI	131	THR	8.9
37	CJ	83	ALA	8.9
14	AN	55	SER	8.9
23	C2	21	TYR	8.9
37	DJ	55	ILE	8.9
37	CJ	126	THR	8.8
1	BA	1307	U	8.8
1	BA	955	U	8.8
7	BG	66	LEU	8.8
1	BA	1331	G	8.8
31	CA	2402	U	8.8
10	BJ	42	LEU	8.7
14	BN	13	ARG	8.7
3	BC	157	LEU	8.7
7	BG	73	VAL	8.7
10	BJ	6	ILE	8.6
37	CJ	86	ILE	8.6
13	BM	24	GLY	8.6
37	CJ	77	ALA	8.6
37	CJ	60	THR	8.6
34	CF	128	TYR	8.6
1	BA	1020	G	8.6
3	BC	71	ALA	8.5
1	BA	962	C	8.5
14	BN	15	ALA	8.5
9	AI	90	TYR	8.5
14	BN	6	MET	8.5
55	DA	2111	U	8.4
14	BN	35	ASN	8.4
1	BA	1025	U	8.4
21	AU	2	PRO	8.4
14	BN	2	ALA	8.4

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Mol	Chain	Res	Type	RSRZ
43	CP	66	GLY	8.4
3	BC	164	ARG	8.4
1	BA	1244	G	8.4
13	BM	64	VAL	8.3
37	CJ	82	LYS	8.3
37	CJ	52	GLY	8.3
13	BM	105	ASN	8.3
37	CJ	80	LEU	8.3
1	BA	958	A	8.3
43	CP	65	THR	8.3
1	BA	1306	A	8.2
19	BS	24	GLU	8.2
1	AA	1030	U	8.2
37	DJ	88	SER	8.2
14	BN	44	ALA	8.2
3	BC	172	ARG	8.2
10	BJ	23	ALA	8.2
7	BG	148	ASN	8.2
13	BM	29	ARG	8.2
10	AJ	75	ASP	8.2
19	BS	63	THR	8.1
14	AN	25	ALA	8.1
1	BA	1219	A	8.1
7	BG	18	PHE	8.1
37	CJ	73	THR	8.1
40	CM	80	SER	8.1
31	CA	2174	C	8.1
37	DJ	135	SER	8.1
19	BS	75	ALA	8.1
43	CP	63	LYS	8.1
14	BN	5	SER	8.1
9	AI	89	GLU	8.1
14	BN	22	ALA	8.0
40	CM	78	ARG	8.0
43	CP	52	SER	8.0
1	BA	1217	C	8.0
31	CA	931	U	8.0
19	BS	41	PHE	8.0
1	BA	1240	U	8.0
13	BM	32	ALA	8.0
31	CA	1066	U	8.0
37	DJ	24	VAL	8.0

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Mol	Chain	Res	Type	RSRZ
13	BM	96	PRO	8.0
31	CA	2123	G	8.0
51	CX	56	ASP	8.0
7	BG	111	ARG	7.9
35	CG	111	HIS	7.9
7	AG	50	LEU	7.9
9	BI	16	ALA	7.9
37	DJ	14	ALA	7.9
7	BG	91	VAL	7.9
40	CM	113	ALA	7.8
14	BN	68	GLY	7.8
1	BA	953	G	7.8
10	BJ	37	ARG	7.8
10	AJ	8	ILE	7.8
37	DJ	77	ALA	7.8
1	BA	1204	A	7.7
40	CM	77	ILE	7.7
7	BG	54	SER	7.7
3	BC	174	PRO	7.7
44	CQ	110	ILE	7.7
23	C2	36	LEU	7.7
7	BG	107	ALA	7.6
49	CV	36	VAL	7.6
1	BA	981	U	7.6
31	CA	1084	A	7.6
46	CS	20	VAL	7.6
19	BS	76	PRO	7.6
54	DI	130	PRO	7.6
3	BC	155	GLY	7.6
14	BN	58	SER	7.5
7	BG	72	THR	7.5
46	CS	96	VAL	7.5
49	CV	18	ASP	7.5
36	DH	87	GLU	7.5
49	CV	69	ASN	7.5
37	DJ	22	PRO	7.5
1	BA	1296	C	7.5
10	BJ	71	LEU	7.5
19	BS	65	GLU	7.5
49	CV	35	ILE	7.5
9	BI	130	ARG	7.4
37	CJ	45	LYS	7.4

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Mol	Chain	Res	Type	RSRZ
14	AN	23	LYS	7.4
10	BJ	39	PRO	7.4
10	AJ	36	VAL	7.4
9	AI	125	PRO	7.4
55	DA	2121	G	7.4
19	BS	59	PRO	7.4
31	CA	2125	G	7.4
14	BN	28	LYS	7.4
1	AA	1032	G	7.3
7	BG	15	ASP	7.3
3	BC	78	GLY	7.3
7	AG	54	SER	7.3
3	BC	158	GLY	7.2
34	CF	85	ILE	7.2
14	BN	8	ALA	7.2
49	CV	3	ALA	7.2
9	BI	125	PRO	7.2
1	AA	1031	C	7.2
1	BA	1028	C	7.2
7	BG	52	GLN	7.2
10	AJ	91	ASP	7.2
14	BN	20	TYR	7.1
19	BS	37	ARG	7.1
13	BM	23	TYR	7.1
13	BM	63	PHE	7.1
1	BA	1031	C	7.1
37	CJ	33	VAL	7.1
54	DI	2	ALA	7.1
40	CM	115	GLU	7.1
9	AI	20	PHE	7.1
37	CJ	46	THR	7.1
9	AI	18	ARG	7.1
13	AM	30	SER	7.1
37	CJ	59	ILE	7.0
13	BM	94	GLY	7.0
13	AM	64	VAL	7.0
48	CU	60	THR	7.0
14	BN	32	SER	7.0
55	DA	2172	U	7.0
3	BC	206	GLU	7.0
7	BG	2	PRO	7.0
49	CV	29	LEU	7.0

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Mol	Chain	Res	Type	RSRZ
14	BN	52	PRO	7.0
13	BM	58	ASP	6.9
37	CJ	50	GLU	6.9
31	CA	1175	A	6.9
1	BA	1032	G	6.9
19	BS	43	ASN	6.9
1	BA	1218	C	6.9
19	BS	67	VAL	6.8
7	BG	8	GLY	6.8
13	BM	11	ASP	6.8
14	BN	51	LEU	6.8
55	DA	2127	G	6.8
10	BJ	25	ILE	6.8
37	CJ	56	PRO	6.8
35	CG	107	LEU	6.8
10	AJ	43	PRO	6.8
1	BA	988	G	6.7
46	CS	27	ILE	6.7
7	AG	49	THR	6.7
19	BS	62	VAL	6.7
7	BG	71	PRO	6.7
23	C2	42	VAL	6.7
7	BG	105	VAL	6.7
13	BM	48	LEU	6.7
43	CP	40	ILE	6.7
7	BG	103	TRP	6.7
9	AI	104	VAL	6.7
42	CO	118	ARG	6.7
1	BA	209	U	6.7
55	DA	896	A	6.7
40	CM	82	LEU	6.7
1	BA	1030	U	6.7
10	AJ	74	VAL	6.7
37	CJ	68	THR	6.6
31	CA	2110	G	6.6
14	BN	3	LYS	6.6
14	AN	32	SER	6.6
37	CJ	61	VAL	6.6
1	BA	1033	G	6.6
23	C2	24	THR	6.6
33	CE	143	LEU	6.6
37	CJ	63	ALA	6.6

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Mol	Chain	Res	Type	RSRZ
19	BS	71	LEU	6.6
10	AJ	76	ILE	6.6
49	CV	31	SER	6.6
53	CZ	29	ARG	6.6
19	BS	39	THR	6.5
43	CP	53	THR	6.5
40	CM	79	LEU	6.5
10	BJ	70	HIS	6.5
3	BC	53	SER	6.5
9	AI	17	ALA	6.5
1	BA	982	U	6.5
19	BS	12	ASP	6.5
48	CU	55	VAL	6.5
9	BI	66	THR	6.5
3	BC	79	LYS	6.5
10	AJ	35	GLN	6.5
55	DA	884	U	6.5
30	CD	200	ASP	6.5
43	CP	51	ALA	6.5
30	CD	26	VAL	6.5
14	AN	67	THR	6.5
40	CM	114	GLY	6.5
3	BC	127	ARG	6.5
31	CA	1104	C	6.5
34	CF	27	GLN	6.5
35	CG	103	ILE	6.4
48	CU	43	ILE	6.4
9	BI	20	PHE	6.4
7	BG	82	GLY	6.4
1	AA	984	C	6.4
49	CV	33	LYS	6.4
1	BA	1019	A	6.4
10	BJ	12	ALA	6.4
48	CU	61	LEU	6.4
55	DA	2125	G	6.4
37	DJ	42	PHE	6.4
49	CV	13	VAL	6.4
19	BS	23	VAL	6.4
1	BA	959	A	6.4
1	BA	1304	G	6.4
23	C2	37	LYS	6.4
37	CJ	47	ASP	6.3

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Mol	Chain	Res	Type	RSRZ
49	CV	80	ALA	6.3
49	CV	83	VAL	6.3
13	BM	17	ILE	6.3
14	BN	59	ARG	6.3
1	BA	1048	G	6.3
31	CA	2127	G	6.3
1	AA	1125	U	6.3
54	DI	136	ILE	6.3
48	CU	59	ASN	6.3
1	BA	1021	A	6.3
9	AI	21	ILE	6.3
10	AJ	73	LEU	6.3
49	CV	32	GLY	6.3
1	BA	1023	U	6.3
22	C1	57	LYS	6.3
7	AG	58	GLU	6.3
10	AJ	6	ILE	6.3
37	CJ	81	LYS	6.3
19	BS	50	ALA	6.3
7	BG	131	LYS	6.3
9	AI	6	TYR	6.2
13	AM	24	GLY	6.2
37	CJ	28	LEU	6.2
19	BS	28	LYS	6.2
19	BS	40	ILE	6.2
37	CJ	67	PHE	6.2
14	BN	78	GLY	6.2
7	BG	16	PRO	6.2
13	AM	40	ALA	6.2
13	BM	41	GLU	6.2
37	CJ	75	PRO	6.2
7	BG	30	LEU	6.2
1	AA	1286	U	6.2
55	DA	2124	G	6.2
19	BS	32	ARG	6.2
40	CM	101	ILE	6.2
13	BM	46	SER	6.2
7	AG	62	PHE	6.2
3	BC	168	TYR	6.2
14	BN	30	ILE	6.1
31	CA	2124	G	6.1
49	CV	40	ASN	6.1

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Mol	Chain	Res	Type	RSRZ
31	CA	2797	U	6.1
10	BJ	38	GLY	6.1
35	CG	52	PHE	6.1
10	AJ	56	HIS	6.1
1	BA	1026	G	6.1
2	BB	213	TYR	6.1
20	BT	4	ILE	6.1
55	DA	2175	C	6.1
13	BM	36	ALA	6.1
55	DA	2174	C	6.1
3	BC	160	ALA	6.1
55	DA	2118	U	6.1
3	BC	170	GLU	6.0
49	CV	87	PHE	6.0
31	CA	1103	A	6.0
37	CJ	76	ALA	6.0
14	BN	16	LEU	6.0
19	BS	31	LEU	6.0
35	CG	105	LEU	6.0
35	CG	151	TYR	6.0
7	BG	133	THR	6.0
9	BI	9	THR	6.0
43	CP	50	ALA	6.0
54	DI	134	GLU	6.0
37	DJ	68	THR	6.0
37	CJ	138	LEU	6.0
23	C2	47	VAL	6.0
37	DJ	52	GLY	6.0
14	BN	48	LEU	6.0
1	AA	87	C	6.0
37	CJ	25	GLY	6.0
40	CM	92	LEU	6.0
14	BN	61	ARG	6.0
34	CF	84	PRO	6.0
33	CE	200	LEU	6.0
37	CJ	121	ASP	6.0
10	AJ	101	SER	6.0
15	BO	17	ARG	5.9
30	CD	4	LEU	5.9
30	CD	199	SER	5.9
2	BB	67	ILE	5.9
3	BC	194	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
43	CP	29	HIS	5.9
34	CF	152	LEU	5.9
1	BA	1015	G	5.9
13	BM	54	ASP	5.9
3	BC	73	PRO	5.9
40	CM	132	ARG	5.9
10	BJ	97	ASP	5.9
49	CV	70	VAL	5.9
34	CF	91	LEU	5.9
35	CG	33	LEU	5.9
1	BA	1210	C	5.9
14	AN	50	THR	5.9
7	BG	150	ALA	5.9
40	CM	102	GLY	5.8
13	BM	34	LEU	5.8
3	AC	68	ILE	5.8
10	AJ	5	ARG	5.8
33	CE	172	ALA	5.8
1	BA	980	C	5.8
7	AG	7	ILE	5.8
13	AM	33	ILE	5.8
3	BC	43	LEU	5.8
7	AG	61	ALA	5.8
1	BA	1029	U	5.8
18	BR	51	TYR	5.8
7	BG	132	GLY	5.8
1	AA	1025	U	5.8
1	BA	1126	U	5.8
9	BI	67	VAL	5.8
31	CA	2667	C	5.8
49	CV	88	GLU	5.8
51	CX	55	ARG	5.8
10	BJ	19	ASP	5.8
14	BN	43	ASN	5.8
14	AN	20	TYR	5.8
19	BS	72	GLY	5.8
13	AM	15	ALA	5.8
3	BC	171	GLY	5.8
37	DJ	11	LEU	5.8
40	CM	130	GLY	5.8
7	BG	53	ARG	5.7
1	BA	1208	C	5.7

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Mol	Chain	Res	Type	RSRZ
30	CD	9	VAL	5.7
13	BM	109	ARG	5.7
37	CJ	129	ILE	5.7
13	BM	13	LYS	5.7
31	CA	2168	G	5.7
10	AJ	34	ALA	5.7
35	CG	131	ILE	5.7
13	AM	41	GLU	5.7
3	BC	179	ARG	5.7
33	CE	14	VAL	5.7
37	CJ	62	TYR	5.7
3	BC	116	VAL	5.7
37	CJ	10	LYS	5.7
13	AM	32	ALA	5.7
31	CA	1057	A	5.7
37	CJ	38	PHE	5.7
35	CG	40	ALA	5.7
13	BM	97	VAL	5.7
1	BA	1237	C	5.7
7	BG	106	GLU	5.7
1	BA	1221	G	5.7
3	BC	120	ILE	5.7
37	CJ	58	VAL	5.7
46	CS	88	GLY	5.7
13	BM	35	ALA	5.6
10	BJ	102	LEU	5.6
23	C2	46	HIS	5.6
34	CF	23	ASN	5.6
44	CQ	91	ALA	5.6
3	BC	80	LYS	5.6
3	BC	36	ASP	5.6
48	CU	8	LEU	5.6
40	CM	131	ALA	5.6
10	BJ	11	LYS	5.6
35	CG	9	VAL	5.6
23	C2	43	VAL	5.6
1	BA	1018	G	5.6
19	BS	74	PHE	5.6
37	CJ	41	ALA	5.6
47	CT	97	LEU	5.6
10	AJ	29	ALA	5.6
10	BJ	21	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
53	CZ	56	LEU	5.6
31	CA	2173	A	5.6
13	BM	6	GLY	5.6
13	BM	18	ALA	5.6
37	CJ	17	MET	5.6
19	BS	22	ALA	5.5
50	CW	43	ASP	5.5
19	BS	38	SER	5.5
37	DJ	73	THR	5.5
11	AK	19	GLY	5.5
1	BA	1038	C	5.5
33	CE	128	ALA	5.5
10	BJ	50	THR	5.5
19	BS	26	GLY	5.5
2	AB	123	ASP	5.5
23	C2	40	ASP	5.5
31	CA	1083	U	5.5
49	CV	12	ILE	5.5
2	AB	36	ASN	5.5
14	BN	18	ASP	5.5
3	AC	77	ILE	5.5
9	BI	117	GLY	5.5
3	BC	109	PRO	5.5
14	AN	54	ASP	5.5
37	CJ	74	PRO	5.5
37	DJ	38	PHE	5.5
48	CU	47	VAL	5.5
30	CD	186	LEU	5.5
38	CK	142	ILE	5.5
7	BG	4	ARG	5.5
3	AC	103	ILE	5.5
11	BK	110	ILE	5.5
3	AC	82	GLU	5.5
14	AN	31	ILE	5.5
34	CF	144	ASP	5.5
35	CG	104	ASN	5.5
37	CJ	19	ASN	5.5
55	DA	879	G	5.5
10	BJ	91	ASP	5.4
37	CJ	18	ALA	5.4
45	CR	29	SER	5.4
40	CM	117	THR	5.4

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Mol	Chain	Res	Type	RSRZ
30	CD	8	LYS	5.4
37	DJ	78	VAL	5.4
40	CM	121	THR	5.4
34	CF	173	PHE	5.4
53	CZ	45	GLN	5.4
7	BG	152	ALA	5.4
17	AQ	53	CYS	5.4
37	CJ	31	GLN	5.4
31	CA	2666	C	5.4
51	CX	53	CYS	5.4
13	BM	16	VAL	5.4
20	BT	3	ASN	5.4
50	CW	28	ALA	5.4
31	CA	345	A	5.4
33	CE	144	GLU	5.4
25	C4	61	CYS	5.4
30	CD	10	GLY	5.4
31	CA	2120	G	5.4
54	DI	128	THR	5.4
13	AM	29	ARG	5.4
31	CA	1085	A	5.4
9	BI	38	TYR	5.4
37	CJ	78	VAL	5.4
1	AA	86	G	5.4
9	AI	129	LYS	5.4
51	CX	26	PHE	5.4
1	BA	1148	U	5.4
1	BA	976	G	5.4
33	CE	126	VAL	5.4
41	CN	136	MET	5.4
34	CF	105	THR	5.4
13	BM	56	LEU	5.3
3	BC	119	SER	5.3
34	CF	34	ILE	5.3
34	CF	155	THR	5.3
1	BA	1273	C	5.3
48	CU	2	ILE	5.3
13	BM	30	SER	5.3
1	BA	1125	U	5.3
1	BA	1276	G	5.3
10	AJ	25	ILE	5.3
49	CV	72	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
50	CW	45	ASP	5.3
23	C2	39	PHE	5.3
14	BN	66	GLN	5.3
3	BC	84	VAL	5.3
34	CF	95	ARG	5.3
3	AC	105	GLU	5.3
48	CU	75	GLY	5.3
42	CO	25	ALA	5.3
34	CF	67	ILE	5.3
40	CM	100	ILE	5.3
27	C0	10	THR	5.3
3	BC	39	VAL	5.3
13	AM	19	LEU	5.3
37	CJ	96	ASP	5.3
3	AC	81	GLY	5.3
33	CE	103	GLY	5.3
9	AI	123	ARG	5.3
13	BM	103	LYS	5.3
53	CZ	15	ASN	5.3
48	CU	10	VAL	5.3
20	BT	76	LYS	5.2
10	BJ	87	LEU	5.2
14	AN	37	SER	5.2
9	AI	19	VAL	5.2
1	BA	1017	U	5.2
37	DJ	71	THR	5.2
9	AI	95	ARG	5.2
31	CA	75	G	5.2
7	BG	17	LYS	5.2
43	CP	38	GLN	5.2
42	CO	26	GLY	5.2
23	C2	41	PRO	5.2
31	CA	1105	U	5.2
34	CF	130	MET	5.2
10	BJ	15	HIS	5.2
14	AN	28	LYS	5.2
13	BM	21	SER	5.2
9	BI	103	PHE	5.2
55	DA	883	G	5.2
37	DJ	28	LEU	5.2
19	BS	27	ASP	5.2
49	CV	28	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
14	AN	9	ARG	5.2
3	BC	8	ASN	5.2
22	C1	36	GLU	5.2
24	C3	17	GLY	5.2
40	CM	142	ILE	5.2
43	CP	117	PHE	5.2
43	CP	46	GLU	5.2
31	CA	1065	U	5.2
7	BG	37	SER	5.2
7	AG	53	ARG	5.2
30	CD	198	GLY	5.1
14	BN	31	ILE	5.1
13	AM	25	VAL	5.1
48	CU	58	VAL	5.1
37	DJ	40	LYS	5.1
35	CG	110	SER	5.1
40	CM	126	ARG	5.1
37	DJ	137	GLY	5.1
1	BA	973	G	5.1
55	DA	2109	U	5.1
37	DJ	19	ASN	5.1
3	BC	35	SER	5.1
35	CG	57	GLY	5.1
33	CE	157	LEU	5.1
51	CX	59	LEU	5.1
47	CT	94	ASP	5.1
35	CG	94	TYR	5.1
19	BS	25	SER	5.1
34	CF	24	SER	5.1
19	AS	33	THR	5.1
29	CC	18	LYS	5.1
37	DJ	87	LYS	5.1
7	BG	109	ARG	5.1
13	BM	22	ILE	5.1
13	BM	2	ALA	5.1
47	CT	5	ALA	5.1
1	BA	1003	G	5.1
14	BN	27	LEU	5.1
17	BQ	70	THR	5.1
1	BA	1275	A	5.1
35	CG	108	GLY	5.1
37	DJ	116	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
25	C4	36	LYS	5.1
3	AC	168	TYR	5.0
49	CV	39	ILE	5.0
37	DJ	96	ASP	5.0
14	BN	71	HIS	5.0
1	BA	1297	G	5.0
10	BJ	56	HIS	5.0
2	BB	14	VAL	5.0
20	BT	35	VAL	5.0
33	CE	127	GLU	5.0
19	BS	47	LEU	5.0
1	BA	1270	G	5.0
31	CA	2162	G	5.0
23	C2	29	THR	5.0
33	CE	153	LEU	5.0
13	AM	11	ASP	5.0
1	BA	1205	U	5.0
7	BG	151	PHE	5.0
9	BI	32	GLN	5.0
11	BK	112	ASP	5.0
1	AA	1127	G	5.0
1	BA	211	G	5.0
2	AB	30	PHE	5.0
30	CD	75	ALA	5.0
55	DA	885	C	5.0
36	CH	142	VAL	5.0
37	CJ	43	ASN	5.0
47	CT	103	ILE	5.0
7	BG	34	GLY	5.0
13	AM	63	PHE	5.0
48	CU	35	ALA	5.0
49	CV	78	GLY	5.0
9	BI	39	PHE	5.0
12	AL	124	ALA	5.0
3	BC	165	THR	5.0
22	C1	55	ILE	5.0
9	BI	90	TYR	5.0
34	CF	92	ARG	5.0
37	CJ	72	LYS	5.0
3	BC	180	ALA	5.0
7	AG	6	VAL	5.0
1	AA	1126	U	5.0

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Mol	Chain	Res	Type	RSRZ
35	CG	109	PHE	5.0
7	BG	48	GLU	4.9
20	BT	59	ASP	4.9
14	BN	56	SER	4.9
7	BG	55	GLY	4.9
2	AB	46	THR	4.9
29	CC	232	HIS	4.9
10	AJ	24	GLU	4.9
7	BG	51	ALA	4.9
31	CA	2111	U	4.9
40	CM	75	ALA	4.9
3	AC	79	LYS	4.9
11	BK	109	ASN	4.9
23	C2	53	LYS	4.9
35	CG	58	TYR	4.9
37	CJ	89	GLY	4.9
13	AM	115	PRO	4.9
13	BM	37	ALA	4.9
26	C5	1	MET	4.9
37	DJ	138	LEU	4.9
7	AG	4	ARG	4.9
37	CJ	130	GLU	4.9
42	CO	120	GLU	4.9
3	BC	177	THR	4.9
30	CD	31	ALA	4.9
33	CE	173	THR	4.9
1	BA	1245	C	4.9
40	CM	89	VAL	4.9
16	BP	52	LEU	4.9
14	BN	9	ARG	4.9
36	CH	132	PHE	4.9
1	BA	956	U	4.9
14	BN	53	ARG	4.9
55	DA	2163	A	4.9
37	CJ	8	TYR	4.9
10	BJ	101	SER	4.9
49	CV	77	THR	4.9
13	AM	34	LEU	4.9
30	CD	96	ILE	4.9
2	AB	131	LYS	4.9
46	CS	32	THR	4.9
30	CD	180	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
13	BM	38	GLY	4.9
1	BA	1309	G	4.9
46	CS	52	PRO	4.9
7	BG	113	ASP	4.9
34	CF	106	ILE	4.9
13	AM	99	GLY	4.9
31	CA	2171	A	4.9
43	CP	36	TYR	4.9
14	BN	49	GLN	4.8
53	CZ	36	GLN	4.8
31	CA	2128	G	4.8
29	CC	241	GLY	4.8
7	AG	52	GLN	4.8
44	CQ	43	PHE	4.8
1	BA	1220	G	4.8
49	CV	5	ILE	4.8
7	AG	123	GLU	4.8
11	BK	96	THR	4.8
39	CL	110	GLU	4.8
44	CQ	9	GLU	4.8
3	AC	78	GLY	4.8
34	CF	119	ALA	4.8
35	CG	84	THR	4.8
1	BA	1004	A	4.8
33	CE	119	ILE	4.8
14	BN	17	ALA	4.8
46	CS	24	LYS	4.8
19	BS	14	HIS	4.8
11	AK	111	THR	4.8
13	BM	77	ILE	4.8
10	AJ	7	ARG	4.8
48	CU	40	LYS	4.8
53	CZ	22	LEU	4.8
1	BA	82	G	4.8
35	CG	56	ASP	4.8
50	CW	7	GLU	4.8
9	BI	40	GLY	4.8
24	C3	42	LEU	4.8
35	CG	106	SER	4.8
29	CC	242	LYS	4.8
37	DJ	82	LYS	4.8
43	CP	27	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
39	CL	83	ALA	4.7
1	BA	1027	C	4.7
13	BM	31	LYS	4.7
14	BN	21	PHE	4.7
54	DI	132	TYR	4.7
37	DJ	25	GLY	4.7
11	BK	64	GLN	4.7
42	CO	29	VAL	4.7
3	BC	85	GLU	4.7
35	CG	26	ILE	4.7
31	CA	846	U	4.7
36	DH	137	GLU	4.7
48	CU	71	GLY	4.7
14	AN	8	ALA	4.7
41	CN	80	VAL	4.7
43	CP	37	ALA	4.7
14	BN	50	THR	4.7
27	C0	8	THR	4.7
3	BC	207	ILE	4.7
3	BC	154	SER	4.7
7	BG	35	LYS	4.7
19	BS	35	SER	4.7
37	DJ	36	MET	4.7
51	CX	63	ALA	4.7
3	AC	166	GLU	4.7
37	DJ	8	TYR	4.7
40	CM	144	GLU	4.7
7	AG	122	ASN	4.7
44	CQ	111	LYS	4.7
1	BA	1271	A	4.7
7	AG	110	LYS	4.7
19	BS	81	ARG	4.7
25	C4	64	TYR	4.7
35	CG	126	PRO	4.7
13	BM	101	ARG	4.7
35	CG	152	ARG	4.7
49	CV	81	ASP	4.7
9	BI	21	ILE	4.7
14	BN	24	ARG	4.7
10	BJ	80	THR	4.7
52	CY	78	TYR	4.7
34	CF	35	THR	4.6

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Mol	Chain	Res	Type	RSRZ
3	BC	205	GLY	4.6
9	BI	123	ARG	4.6
53	CZ	18	LEU	4.6
1	BA	948	C	4.6
9	BI	65	ILE	4.6
42	CO	28	LEU	4.6
1	AA	1281	C	4.6
2	AB	37	LYS	4.6
3	AC	47	LEU	4.6
14	BN	79	LEU	4.6
7	AG	48	GLU	4.6
14	AN	22	ALA	4.6
43	CP	92	PHE	4.6
3	AC	110	GLU	4.6
30	CD	77	ARG	4.6
37	DJ	89	GLY	4.6
23	C2	20	PHE	4.6
1	BA	79	G	4.6
37	DJ	133	ALA	4.6
55	DA	2132	U	4.6
33	CE	47	LYS	4.6
9	BI	44	ALA	4.6
43	CP	39	VAL	4.6
13	BM	111	GLY	4.6
54	DI	3	LEU	4.6
31	CA	1536	C	4.6
53	CZ	49	ASP	4.6
13	BM	12	HIS	4.6
34	CF	69	LYS	4.6
31	CA	2150	C	4.5
2	BB	37	LYS	4.5
17	BQ	46	VAL	4.5
43	CP	93	ASP	4.5
7	AG	46	ALA	4.5
13	BM	51	GLY	4.5
13	BM	67	GLY	4.5
9	BI	41	ARG	4.5
31	CA	329	G	4.5
55	DA	2123	G	4.5
13	BM	89	LEU	4.5
31	CA	1213	A	4.5
7	BG	126	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
27	C0	56	LYS	4.5
37	CJ	44	ALA	4.5
37	CJ	26	PRO	4.5
9	BI	11	ARG	4.5
34	CF	86	GLY	4.5
7	BG	134	ALA	4.5
35	CG	43	VAL	4.5
37	DJ	83	ALA	4.5
40	CM	116	VAL	4.5
22	C1	34	SER	4.5
48	CU	84	TYR	4.5
37	CJ	91	GLY	4.5
55	DA	2115	G	4.5
7	BG	31	MET	4.5
7	BG	79	ARG	4.5
13	AM	48	LEU	4.5
24	C3	35	ARG	4.5
1	BA	1303	C	4.5
44	CQ	3	ASN	4.5
2	BB	201	PRO	4.5
23	C2	25	LYS	4.5
34	CF	31	VAL	4.5
43	CP	103	VAL	4.5
11	BK	111	THR	4.5
37	CJ	79	LEU	4.5
10	BJ	58	ASN	4.5
37	DJ	9	VAL	4.5
1	BA	996	A	4.5
1	BA	1050	G	4.5
3	AC	83	ASP	4.5
6	BF	8	PHE	4.5
10	BJ	20	GLN	4.5
31	CA	1064	C	4.5
55	DA	2106	U	4.5
1	AA	1285	A	4.5
7	BG	78	ARG	4.5
34	CF	76	GLY	4.5
40	CM	28	GLY	4.5
1	BA	1001	C	4.5
10	BJ	90	LEU	4.4
47	CT	44	ALA	4.4
3	BC	51	SER	4.4

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Mol	Chain	Res	Type	RSRZ
37	DJ	131	GLY	4.4
51	CX	23	VAL	4.4
3	BC	191	THR	4.4
7	BG	115	SER	4.4
10	BJ	36	VAL	4.4
13	AM	16	VAL	4.4
17	BQ	24	ALA	4.4
31	CA	2122	U	4.4
44	CQ	97	LEU	4.4
55	DA	2167	U	4.4
19	AS	68	GLY	4.4
34	CF	104	ILE	4.4
45	CR	74	ILE	4.4
43	CP	107	ALA	4.4
1	BA	1039	G	4.4
3	BC	77	ILE	4.4
7	BG	77	SER	4.4
37	CJ	117	MET	4.4
10	BJ	100	ILE	4.4
20	BT	49	LYS	4.4
31	CA	1082	U	4.4
29	CC	244	PRO	4.4
41	CN	72	PRO	4.4
11	BK	67	ALA	4.4
36	CH	11	ASN	4.4
55	DA	880	G	4.4
48	CU	42	GLU	4.4
17	BQ	21	ILE	4.4
7	AG	57	SER	4.4
19	BS	44	MET	4.4
22	C1	27	SER	4.4
16	AP	47	GLU	4.4
55	DA	2108	A	4.4
53	CZ	59	GLU	4.4
11	AK	110	ILE	4.4
29	CC	233	GLY	4.4
2	AB	32	PHE	4.4
10	BJ	27	GLU	4.4
14	BN	10	GLU	4.4
31	CA	2665	A	4.4
47	CT	47	VAL	4.4
37	CJ	64	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
49	CV	86	ARG	4.4
17	BQ	47	HIS	4.4
37	CJ	131	GLY	4.4
13	BM	19	LEU	4.3
21	AU	16	LEU	4.3
34	CF	175	PHE	4.3
3	BC	129	MET	4.3
19	BS	42	PRO	4.3
47	CT	82	MET	4.3
48	CU	46	ALA	4.3
1	BA	1341	U	4.3
1	BA	1280	A	4.3
3	BC	46	GLU	4.3
10	BJ	81	GLU	4.3
47	CT	43	ALA	4.3
3	BC	15	VAL	4.3
35	CG	24	ILE	4.3
3	BC	122	SER	4.3
21	BU	12	PHE	4.3
13	AM	7	ILE	4.3
23	C2	19	HIS	4.3
55	DA	1729	U	4.3
9	AI	63	LEU	4.3
7	BG	26	PHE	4.3
34	CF	177	PHE	4.3
31	CA	1086	A	4.3
55	DA	882	G	4.3
31	CA	2175	C	4.3
3	AC	43	LEU	4.3
3	BC	173	VAL	4.3
49	CV	90	GLY	4.3
35	CG	112	PRO	4.3
2	AB	139	ARG	4.3
11	BK	85	MET	4.3
31	CA	2383	G	4.3
47	CT	48	LYS	4.3
37	DJ	58	VAL	4.3
1	BA	977	A	4.3
2	AB	35	ARG	4.3
41	CN	84	LYS	4.3
10	BJ	63	ASP	4.3
31	CA	12	U	4.3

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Mol	Chain	Res	Type	RSRZ
31	CA	1870	C	4.3
37	CJ	136	MET	4.3
54	DI	129	LEU	4.3
45	CR	71	GLN	4.3
31	CA	1078	U	4.3
7	BG	46	ALA	4.3
1	BA	1047	G	4.3
2	BB	89	GLN	4.3
34	CF	97	TRP	4.3
13	BM	14	HIS	4.3
3	BC	14	ILE	4.3
37	CJ	32	GLY	4.3
53	CZ	11	VAL	4.3
49	CV	52	LEU	4.2
22	C1	46	ASP	4.2
31	CA	2627	G	4.2
13	BM	5	ALA	4.2
13	BM	8	ASN	4.2
37	CJ	34	ASN	4.2
37	DJ	94	ASN	4.2
14	AN	66	GLN	4.2
31	CA	2181	U	4.2
13	BM	74	SER	4.2
13	AM	18	ALA	4.2
35	CG	4	VAL	4.2
49	CV	42	VAL	4.2
10	AJ	39	PRO	4.2
33	CE	201	ALA	4.2
49	CV	51	ALA	4.2
1	BA	1035	A	4.2
37	CJ	85	GLY	4.2
13	BM	9	ILE	4.2
37	CJ	120	ALA	4.2
42	CO	24	MET	4.2
43	CP	87	ILE	4.2
45	CR	79	PHE	4.2
11	BK	63	ALA	4.2
36	CH	12	LEU	4.2
55	DA	881	G	4.2
1	BA	1209	C	4.2
1	BA	1317	C	4.2
14	AN	78	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
14	BN	69	ARG	4.2
37	DJ	16	GLY	4.2
1	BA	1212	U	4.2
2	AB	135	LEU	4.2
31	CA	879	G	4.2
31	CA	1106	G	4.2
1	BA	998	C	4.2
7	BG	147	ALA	4.2
24	C3	32	ALA	4.2
33	CE	131	THR	4.2
39	CL	14	SER	4.2
13	BM	68	ASP	4.2
51	CX	25	ARG	4.2
23	C2	18	GLY	4.2
40	CM	90	VAL	4.2
40	CM	127	VAL	4.2
30	CD	44	GLY	4.2
36	CH	122	LEU	4.2
9	BI	64	TYR	4.2
35	CG	25	THR	4.2
1	BA	968	A	4.2
7	AG	137	LYS	4.2
30	CD	55	LYS	4.2
50	CW	42	LEU	4.2
37	DJ	49	ILE	4.2
34	CF	36	LEU	4.1
36	CH	130	VAL	4.1
13	AM	45	ILE	4.1
24	C3	33	ARG	4.1
37	CJ	115	ALA	4.1
14	BN	47	LYS	4.1
37	DJ	69	PHE	4.1
55	DA	2122	U	4.1
1	BA	1037	C	4.1
3	BC	153	VAL	4.1
14	BN	14	VAL	4.1
19	BS	58	VAL	4.1
34	CF	151	GLY	4.1
34	CF	96	MET	4.1
51	CX	58	THR	4.1
19	BS	51	VAL	4.1
10	AJ	40	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
31	CA	878	A	4.1
20	BT	47	ALA	4.1
20	BT	87	ALA	4.1
30	CD	151	THR	4.1
37	CJ	27	ALA	4.1
24	C3	18	PHE	4.1
7	AG	45	SER	4.1
1	BA	1034	G	4.1
9	BI	30	ILE	4.1
35	CG	148	LEU	4.1
55	DA	2169	A	4.1
24	C3	28	ARG	4.1
49	CV	6	ARG	4.1
3	BC	204	LYS	4.1
16	AP	38	PHE	4.1
29	CC	2	ALA	4.1
1	BA	946	A	4.1
10	BJ	60	ASP	4.1
53	CZ	6	LEU	4.1
7	BG	127	ALA	4.1
1	BA	1044	A	4.1
13	BM	65	VAL	4.1
16	AP	17	TYR	4.1
30	CD	27	ILE	4.1
37	DJ	134	ARG	4.1
35	CG	89	LEU	4.1
33	CE	23	PHE	4.1
34	CF	40	VAL	4.1
37	DJ	104	ALA	4.1
22	C1	33	THR	4.1
2	AB	9	MET	4.1
3	AC	80	LYS	4.1
23	C2	38	LYS	4.1
1	AA	1000	A	4.1
7	AG	38	THR	4.0
7	BG	36	LYS	4.0
14	BN	38	ASP	4.0
37	CJ	48	SER	4.0
9	AI	5	GLN	4.0
34	CF	154	ILE	4.0
36	CH	72	ILE	4.0
31	CA	1167	C	4.0

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Mol	Chain	Res	Type	RSRZ
29	CC	3	VAL	4.0
36	CH	148	ALA	4.0
40	CM	108	ALA	4.0
42	CO	116	VAL	4.0
10	AJ	42	LEU	4.0
35	CG	7	ALA	4.0
36	CH	84	ALA	4.0
1	AA	1196	A	4.0
9	AI	91	ASP	4.0
31	CA	877	A	4.0
3	BC	103	ILE	4.0
34	CF	29	PRO	4.0
34	CF	136	ILE	4.0
3	BC	126	ARG	4.0
16	AP	39	PHE	4.0
2	AB	12	ALA	4.0
35	CG	65	ALA	4.0
51	CX	52	GLY	4.0
7	AG	111	ARG	4.0
30	CD	38	LYS	4.0
14	BN	100	SER	4.0
31	CA	1524	G	4.0
47	CT	7	HIS	4.0
48	CU	63	VAL	4.0
9	BI	121	ALA	4.0
17	BQ	73	TRP	4.0
7	AG	106	GLU	4.0
17	BQ	23	VAL	4.0
46	CS	63	VAL	4.0
49	CV	37	GLU	4.0
34	CF	26	MET	4.0
34	CF	37	ASN	4.0
2	BB	187	VAL	4.0
40	CM	70	LYS	4.0
14	BN	57	PRO	4.0
31	CA	546	U	4.0
1	BA	1322	C	4.0
12	BL	124	ALA	4.0
33	CE	199	MET	4.0
35	CG	83	PHE	4.0
1	BA	1236	A	4.0
30	CD	154	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
31	CA	2800	A	4.0
46	CS	31	GLU	4.0
13	BM	99	GLY	4.0
14	AN	68	GLY	4.0
1	AA	1148	U	4.0
1	BA	1330	U	4.0
44	CQ	85	SER	4.0
9	BI	37	GLN	4.0
48	CU	14	PRO	4.0
3	BC	112	ASP	4.0
37	CJ	99	GLY	4.0
13	BM	52	GLN	4.0
1	BA	979	C	4.0
37	DJ	57	VAL	4.0
30	CD	76	GLY	4.0
7	AG	140	ASP	4.0
18	AR	23	TYR	3.9
3	BC	185	ASN	3.9
16	BP	54	LEU	3.9
53	CZ	28	LEU	3.9
53	CZ	42	LEU	3.9
7	BG	144	MET	3.9
40	CM	76	GLU	3.9
50	CW	69	GLU	3.9
53	CZ	17	GLU	3.9
2	AB	43	LEU	3.9
3	BC	102	ASN	3.9
40	CM	8	PRO	3.9
53	CZ	58	ASN	3.9
25	C4	37	ALA	3.9
34	CF	83	TYR	3.9
30	CD	203	VAL	3.9
37	CJ	66	SER	3.9
47	CT	98	LYS	3.9
49	CV	84	GLY	3.9
31	CA	2149	U	3.9
18	BR	74	HIS	3.9
37	CJ	113	LYS	3.9
40	CM	118	THR	3.9
46	CS	19	THR	3.9
1	BA	1295	U	3.9
16	BP	57	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
33	CE	104	ALA	3.9
49	CV	71	ALA	3.9
53	CZ	24	GLU	3.9
1	AA	1320	C	3.9
1	BA	1203	C	3.9
37	DJ	81	LYS	3.9
1	AA	1033	G	3.9
48	CU	87	LEU	3.9
7	BG	29	ILE	3.9
34	CF	71	ARG	3.9
7	BG	87	VAL	3.9
9	BI	7	TYR	3.9
1	BA	1239	A	3.9
2	BB	21	ARG	3.9
10	AJ	100	ILE	3.9
24	C3	30	VAL	3.9
1	BA	989	U	3.9
22	C1	4	GLN	3.9
34	CF	100	PHE	3.9
3	AC	134	MET	3.9
14	AN	57	PRO	3.9
39	CL	111	LYS	3.9
13	AM	17	ILE	3.9
37	DJ	63	ALA	3.9
9	BI	104	VAL	3.9
16	AP	20	VAL	3.9
35	CG	27	LYS	3.9
2	BB	208	ARG	3.9
3	AC	74	GLY	3.9
34	CF	107	ALA	3.9
18	BR	48	ARG	3.9
49	CV	15	THR	3.9
35	CG	62	TRP	3.9
10	BJ	24	GLU	3.9
11	BK	94	GLU	3.9
36	CH	94	ILE	3.9
1	BA	999	C	3.8
31	CA	2118	U	3.8
48	CU	72	GLN	3.8
2	BB	159	ASP	3.8
1	BA	842	U	3.8
2	AB	44	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
7	BG	137	LYS	3.8
24	C3	22	MET	3.8
21	BU	2	PRO	3.8
34	CF	158	THR	3.8
2	AB	6	MET	3.8
2	AB	47	VAL	3.8
3	AC	157	LEU	3.8
31	CA	1538	G	3.8
55	DA	2162	G	3.8
9	BI	108	ALA	3.8
35	CG	10	VAL	3.8
14	BN	23	LYS	3.8
30	CD	185	ASN	3.8
19	BS	73	GLU	3.8
22	C1	3	VAL	3.8
43	CP	110	ALA	3.8
1	AA	1260	G	3.8
31	CA	289	G	3.8
7	AG	59	LEU	3.8
7	BG	141	VAL	3.8
51	CX	51	VAL	3.8
53	CZ	37	LEU	3.8
18	AR	24	LYS	3.8
31	CA	2154	A	3.8
35	CG	44	LYS	3.8
55	DA	1064	C	3.8
17	BQ	61	ILE	3.8
42	CO	52	ILE	3.8
1	AA	1138	G	3.8
49	CV	26	LYS	3.8
3	BC	133	ALA	3.8
30	CD	166	GLY	3.8
37	CJ	15	ALA	3.8
45	CR	99	ALA	3.8
31	CA	1048	A	3.8
14	BN	19	LYS	3.8
37	DJ	113	LYS	3.8
14	BN	11	VAL	3.8
7	AG	133	THR	3.8
1	BA	997	U	3.8
3	BC	101	ILE	3.8
13	AM	54	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
31	CA	613	A	3.8
55	DA	2117	A	3.8
35	CG	132	VAL	3.8
50	CW	27	PRO	3.8
18	AR	20	GLU	3.8
47	CT	3	THR	3.8
13	BM	71	ARG	3.8
43	CP	30	ARG	3.8
13	BM	43	VAL	3.8
14	AN	6	MET	3.8
49	CV	95	PHE	3.8
31	CA	1075	C	3.8
7	BG	99	LEU	3.8
45	CR	117	LEU	3.8
39	CL	15	GLY	3.8
7	BG	50	LEU	3.8
9	AI	66	THR	3.8
43	CP	26	LEU	3.8
31	CA	33	C	3.8
35	CG	102	VAL	3.8
1	BA	1211	U	3.7
3	BC	161	GLU	3.7
30	CD	45	TYR	3.7
1	AA	1020	G	3.7
36	CH	108	VAL	3.7
43	CP	88	LYS	3.7
48	CU	67	VAL	3.7
2	BB	123	ASP	3.7
14	BN	65	ARG	3.7
16	AP	41	PRO	3.7
16	BP	42	ILE	3.7
52	CY	49	LEU	3.7
35	CG	162	VAL	3.7
31	CA	1731	G	3.7
31	CA	2803	G	3.7
34	CF	164	GLU	3.7
9	AI	62	ASP	3.7
40	CM	91	ASP	3.7
1	AA	1008	U	3.7
19	AS	25	SER	3.7
21	AU	26	ALA	3.7
42	CO	119	SER	3.7

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Mol	Chain	Res	Type	RSRZ
35	CG	133	LEU	3.7
3	AC	53	SER	3.7
30	CD	49	GLN	3.7
37	DJ	61	VAL	3.7
7	AG	144	MET	3.7
11	BK	29	ASN	3.7
26	C5	32	LYS	3.7
29	CC	100	GLU	3.7
35	CG	5	ALA	3.7
9	BI	43	THR	3.7
13	BM	90	ARG	3.7
37	CJ	35	ILE	3.7
3	BC	200	VAL	3.7
10	BJ	78	GLU	3.7
33	CE	152	GLU	3.7
13	BM	57	ARG	3.7
2	AB	186	ILE	3.7
20	BT	80	THR	3.7
31	CA	1168	G	3.7
34	CF	132	VAL	3.7
14	AN	33	ASP	3.7
44	CQ	24	ASP	3.7
3	BC	104	ALA	3.7
1	AA	1049	U	3.7
31	CA	2119	A	3.7
34	DF	83	TYR	3.7
10	BJ	98	VAL	3.7
36	DH	142	VAL	3.7
30	CD	184	ARG	3.7
40	CM	133	ALA	3.7
13	BM	85	CYS	3.7
29	CC	102	ARG	3.7
37	DJ	114	ALA	3.7
31	CA	2801	G	3.7
33	CE	175	ILE	3.7
17	AQ	9	GLN	3.7
24	C3	13	ASN	3.7
7	BG	119	ARG	3.7
30	CD	28	GLU	3.7
35	CG	130	GLU	3.7
3	BC	201	TRP	3.7
29	CC	33	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
34	CF	117	LEU	3.7
31	CA	32	C	3.7
43	CP	99	TYR	3.7
13	BM	93	ARG	3.7
47	CT	84	ARG	3.7
18	BR	67	LEU	3.6
8	BH	2	SER	3.6
14	AN	5	SER	3.6
54	DI	104	ALA	3.6
31	CA	101	A	3.6
31	CA	1535	A	3.6
47	CT	105	VAL	3.6
35	CG	22	GLN	3.6
1	BA	1308	U	3.6
8	BH	55	THR	3.6
13	AM	46	SER	3.6
37	CJ	132	THR	3.6
31	CA	2819	G	3.6
41	CN	6	ARG	3.6
2	AB	65	GLY	3.6
55	DA	2164	C	3.6
14	BN	29	ALA	3.6
15	BO	15	PHE	3.6
1	BA	1235	U	3.6
9	AI	9	THR	3.6
34	CF	156	ILE	3.6
7	BG	63	GLU	3.6
14	AN	40	ASP	3.6
1	BA	1006	G	3.6
48	CU	76	ARG	3.6
55	DA	1067	A	3.6
55	DA	2126	A	3.6
7	AG	69	VAL	3.6
1	BA	1121	U	3.6
10	BJ	16	ARG	3.6
53	CZ	31	GLN	3.6
48	CU	82	LYS	3.6
7	BG	123	GLU	3.6
46	CS	30	GLY	3.6
13	AM	5	ALA	3.6
14	BN	25	ALA	3.6
30	CD	2	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
53	CZ	47	ARG	3.6
54	DI	6	GLN	3.6
14	BN	45	VAL	3.6
36	CH	137	GLU	3.6
37	CJ	98	VAL	3.6
2	AB	201	PRO	3.6
9	BI	6	TYR	3.6
35	CG	54	PRO	3.6
1	AA	844	G	3.6
1	BA	1002	G	3.6
1	BA	1222	G	3.6
33	CE	186	VAL	3.6
3	BC	178	LEU	3.6
8	AH	122	GLY	3.6
44	CQ	8	LEU	3.6
20	BT	51	PHE	3.6
13	AM	39	ILE	3.6
13	BM	59	GLU	3.6
24	C3	1	MET	3.6
36	CH	143	ILE	3.6
37	CJ	139	VAL	3.6
44	CQ	84	ILE	3.6
17	BQ	8	LEU	3.6
53	CZ	26	PHE	3.6
54	DI	55	VAL	3.6
1	BA	1007	U	3.6
34	CF	22	TYR	3.6
14	AN	52	PRO	3.6
19	BS	19	VAL	3.6
37	DJ	51	LYS	3.6
39	CL	2	ILE	3.6
40	CM	136	GLU	3.6
3	BC	70	THR	3.6
37	DJ	46	THR	3.6
9	AI	7	TYR	3.6
31	CA	1534	U	3.5
1	AA	1128	C	3.5
33	CE	148	ILE	3.5
53	CZ	20	ASN	3.5
16	AP	22	ALA	3.5
9	BI	81	HIS	3.5
30	CD	95	SER	3.5

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Mol	Chain	Res	Type	RSRZ
34	CF	126	GLY	3.5
40	CM	94	THR	3.5
9	BI	68	LYS	3.5
10	BJ	30	LYS	3.5
3	BC	106	VAL	3.5
31	CA	2245	U	3.5
36	CH	110	VAL	3.5
40	CM	110	VAL	3.5
47	CT	66	ILE	3.5
1	AA	1243	C	3.5
7	AG	39	ALA	3.5
37	CJ	119	GLY	3.5
40	CM	125	LEU	3.5
1	AA	959	A	3.5
3	BC	147	LYS	3.5
7	AG	56	LYS	3.5
7	BG	140	ASP	3.5
37	DJ	66	SER	3.5
1	BA	1124	G	3.5
3	AC	66	VAL	3.5
13	BM	7	ILE	3.5
19	AS	67	VAL	3.5
34	CF	32	GLU	3.5
35	CG	41	VAL	3.5
1	AA	1029	U	3.5
2	AB	225	ARG	3.5
14	AN	51	LEU	3.5
19	AS	74	PHE	3.5
1	AA	977	A	3.5
1	BA	975	A	3.5
9	AI	92	GLU	3.5
55	DA	1175	A	3.5
10	AJ	37	ARG	3.5
11	BK	93	ARG	3.5
34	CF	112	ARG	3.5
53	CZ	14	LEU	3.5
5	BE	120	VAL	3.5
34	CF	170	LEU	3.5
47	CT	87	PRO	3.5
2	BB	206	ALA	3.5
14	BN	73	PHE	3.5
14	BN	64	CYS	3.5

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Mol	Chain	Res	Type	RSRZ
25	C4	24	HIS	3.5
30	CD	29	VAL	3.5
34	CF	28	VAL	3.5
36	CH	144	VAL	3.5
2	BB	34	ALA	3.5
3	BC	7	PRO	3.5
25	C4	2	PRO	3.5
1	BA	1238	A	3.5
1	BA	957	U	3.5
6	BF	10	VAL	3.5
3	AC	101	ILE	3.5
3	BC	190	HIS	3.5
50	CW	89	ILE	3.5
6	BF	39	LEU	3.5
21	AU	12	PHE	3.5
1	BA	1367	C	3.5
13	BM	98	ARG	3.5
1	BA	1046	A	3.5
33	CE	33	VAL	3.5
14	AN	71	HIS	3.5
37	CJ	49	ILE	3.5
29	CC	47	GLY	3.5
13	BM	70	ARG	3.5
30	CD	152	PRO	3.5
41	CN	69	PRO	3.5
53	CZ	33	ALA	3.5
27	C0	55	VAL	3.5
2	BB	33	GLY	3.5
10	BJ	34	ALA	3.5
1	BA	1314	C	3.5
22	C1	15	MET	3.5
37	CJ	97	LYS	3.5
7	BG	86	GLN	3.5
16	AP	81	ALA	3.5
27	C0	9	GLN	3.5
10	BJ	55	PRO	3.5
37	DJ	39	CYS	3.5
40	CM	135	ILE	3.5
17	AQ	47	HIS	3.5
45	CR	26	GLY	3.5
46	CS	35	PHE	3.5
13	AM	8	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
22	C1	5	GLN	3.4
40	CM	134	ALA	3.5
1	BA	952	U	3.4
37	DJ	33	VAL	3.4
3	BC	144	LEU	3.4
9	BI	98	LEU	3.4
27	C0	48	ILE	3.4
37	CJ	125	MET	3.4
29	CC	245	VAL	3.4
30	CD	5	VAL	3.4
13	BM	4	ILE	3.4
23	C2	23	THR	3.4
34	CF	129	SER	3.4
44	CQ	4	ILE	3.4
1	BA	1014	A	3.4
31	CA	2156	G	3.4
3	AC	170	GLU	3.4
7	BG	108	ALA	3.4
12	BL	70	GLU	3.4
3	BC	111	LEU	3.4
10	AJ	90	LEU	3.4
11	BK	84	VAL	3.4
35	CG	6	LYS	3.4
44	CQ	115	ASN	3.4
2	BB	156	GLY	3.4
55	DA	2165	C	3.4
41	CN	79	ALA	3.4
49	CV	79	LYS	3.4
39	CL	89	ASN	3.4
1	BA	1364	U	3.4
9	BI	129	LYS	3.4
31	CA	2109	U	3.4
37	DJ	17	MET	3.4
1	AA	1022	A	3.4
52	CY	46	PHE	3.4
55	DA	2170	A	3.4
49	CV	27	ASN	3.4
1	BA	1013	G	3.4
13	BM	62	LYS	3.4
55	DA	2152	G	3.4
44	CQ	28	VAL	3.4
19	AS	49	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
19	BS	69	HIS	3.4
14	BN	95	GLY	3.4
20	BT	60	ARG	3.4
1	BA	1036	A	3.4
7	BG	90	GLU	3.4
21	AU	9	ASN	3.4
31	CA	501	A	3.4
31	CA	896	A	3.4
46	CS	61	ALA	3.4
54	DI	5	LEU	3.4
13	BM	100	GLN	3.4
36	DH	47	PHE	3.4
3	BC	105	GLU	3.4
24	C3	31	LEU	3.4
31	CA	344	A	3.4
3	BC	40	ARG	3.4
7	AG	26	PHE	3.4
9	BI	18	ARG	3.4
31	CA	476	G	3.4
12	AL	67	ILE	3.4
23	C2	49	TYR	3.4
1	AA	1280	A	3.4
13	BM	47	GLU	3.4
30	CD	30	GLU	3.4
35	CG	169	VAL	3.4
48	DU	92	ASN	3.4
15	BO	25	THR	3.4
29	CC	251	GLN	3.4
1	AA	1332	A	3.4
37	CJ	95	LYS	3.4
3	BC	124	LEU	3.4
7	BG	32	VAL	3.4
54	DI	84	TYR	3.4
1	BA	1356	G	3.4
2	BB	145	GLU	3.4
34	CF	42	GLU	3.4
49	CV	22	ARG	3.4
13	BM	81	MET	3.4
40	CM	83	ALA	3.3
45	CR	116	ALA	3.3
3	BC	74	GLY	3.3
14	BN	39	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
37	CJ	16	GLY	3.3
19	AS	32	ARG	3.3
31	CA	2628	C	3.3
33	CE	17	THR	3.3
7	AG	43	VAL	3.3
33	CE	193	VAL	3.3
44	CQ	92	VAL	3.3
3	BC	50	ALA	3.3
7	BG	145	ALA	3.3
30	CD	101	PHE	3.3
31	CA	2802	G	3.3
16	BP	60	TRP	3.3
31	CA	2449	U	3.3
43	CP	58	ILE	3.3
1	AA	1044	A	3.3
1	BA	1246	A	3.3
37	DJ	50	GLU	3.3
7	BG	23	LEU	3.3
13	BM	55	THR	3.3
13	AM	35	ALA	3.3
30	CD	90	PHE	3.3
52	CY	45	ARG	3.3
49	DV	56	GLY	3.3
7	BG	75	VAL	3.3
9	AI	67	VAL	3.3
4	AD	154	ARG	3.3
7	AG	136	LYS	3.3
10	AJ	28	THR	3.3
35	CG	86	LYS	3.3
44	CQ	2	SER	3.3
43	CP	35	ILE	3.3
7	AG	55	GLY	3.3
40	CM	22	GLY	3.3
46	CS	25	LEU	3.3
55	DA	1065	U	3.3
1	BA	1316	G	3.3
42	CO	96	ARG	3.3
47	CT	86	MET	3.3
1	BA	1216	A	3.3
55	DA	892	A	3.3
10	BJ	79	PRO	3.3
29	CC	93	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
33	CE	154	ASP	3.3
53	CZ	60	LYS	3.3
7	BG	68	ASN	3.3
1	BA	1363	A	3.3
9	BI	122	ARG	3.3
43	CP	54	VAL	3.3
2	BB	9	MET	3.3
3	AC	104	ALA	3.3
3	BC	166	GLU	3.3
6	BF	5	GLU	3.3
20	AT	2	ALA	3.3
31	CA	2796	U	3.3
25	C4	25	LYS	3.3
7	AG	109	ARG	3.3
10	BJ	89	ARG	3.3
49	CV	85	PHE	3.3
7	BG	60	GLU	3.3
20	BT	75	HIS	3.3
31	CA	646	U	3.3
31	CA	2151	U	3.3
48	CU	32	LEU	3.3
49	CV	50	PRO	3.3
29	CC	30	PHE	3.3
1	AA	1042	A	3.3
13	AM	4	ILE	3.3
13	BM	44	LYS	3.3
19	AS	24	GLU	3.3
41	CN	73	ILE	3.3
3	BC	148	GLY	3.3
14	AN	41	ARG	3.3
31	CA	1058	U	3.3
33	CE	24	ASN	3.3
40	DM	104	GLN	3.3
51	CX	85	GLU	3.3
36	DH	86	ASP	3.3
40	CM	112	LEU	3.3
2	AB	16	PHE	3.3
7	BG	80	VAL	3.3
29	CC	94	VAL	3.3
16	AP	46	LYS	3.3
31	CA	880	G	3.3
31	CA	930	G	3.3

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Mol	Chain	Res	Type	RSRZ
31	CA	1862	G	3.3
55	DA	2133	G	3.3
55	DA	2149	U	3.3
35	CG	35	ARG	3.3
16	BP	53	ASP	3.3
20	BT	72	ALA	3.3
7	BG	5	ARG	3.2
31	CA	2177	C	3.2
53	CZ	32	ALA	3.2
7	BG	44	TYR	3.2
43	CP	34	HIS	3.2
51	CX	69	PHE	3.2
7	BG	7	ILE	3.2
31	CA	138	U	3.2
35	CG	127	THR	3.2
7	BG	76	LYS	3.2
19	AS	21	LYS	3.2
48	CU	44	LYS	3.2
17	BQ	53	CYS	3.2
23	C2	6	ARG	3.2
37	DJ	47	ASP	3.2
31	CA	81	G	3.2
7	AG	127	ALA	3.2
39	CL	16	ALA	3.2
44	CQ	95	ALA	3.2
3	BC	42	TYR	3.2
3	BC	72	ARG	3.2
18	BR	23	TYR	3.2
9	BI	58	VAL	3.2
16	AP	16	PHE	3.2
54	DI	106	PHE	3.2
14	BN	33	ASP	3.2
2	AB	15	HIS	3.2
9	AI	37	GLN	3.2
18	BR	39	ILE	3.2
35	CG	141	ILE	3.2
49	CV	21	LYS	3.2
50	CW	46	LYS	3.2
16	AP	78	VAL	3.2
21	AU	3	VAL	3.2
1	AA	997	U	3.2
31	CA	431	U	3.2

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Mol	Chain	Res	Type	RSRZ
48	CU	5	GLU	3.2
19	BS	21	LYS	3.2
3	AC	144	LEU	3.2
3	BC	81	GLY	3.2
16	AP	6	LEU	3.2
31	CA	1076	C	3.2
45	CR	75	SER	3.2
1	BA	1312	G	3.2
7	BG	129	GLU	3.2
55	DA	1731	G	3.2
7	AG	66	LEU	3.2
9	AI	94	LEU	3.2
9	BI	94	LEU	3.2
13	BM	53	ILE	3.2
14	BN	42	TRP	3.2
18	BR	35	GLU	3.2
34	CF	159	THR	3.2
1	AA	973	G	3.2
3	BC	33	LEU	3.2
36	DH	12	LEU	3.2
7	AG	51	ALA	3.2
54	DI	135	ALA	3.2
1	BA	1146	A	3.2
36	CH	103	VAL	3.2
1	AA	962	C	3.2
1	AA	1001	C	3.2
30	CD	201	LEU	3.2
45	CR	98	ILE	3.2
15	BO	21	ASP	3.2
17	BQ	45	HIS	3.2
36	CH	67	ALA	3.2
43	CP	61	GLN	3.2
11	BK	86	VAL	3.2
3	BC	107	ARG	3.2
30	CD	89	GLU	3.2
37	CJ	94	ASN	3.2
1	BA	995	C	3.2
55	DA	893	C	3.2
11	BK	66	ALA	3.2
16	BP	9	HIS	3.2
12	BL	50	ARG	3.2
47	CT	36	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
51	CX	37	ILE	3.2
36	CH	91	PHE	3.2
50	CW	26	PHE	3.2
11	BK	24	HIS	3.2
13	BM	3	ARG	3.2
43	CP	28	VAL	3.2
1	BA	1366	C	3.2
3	BC	87	LEU	3.2
19	BS	11	ILE	3.2
35	DG	103	ILE	3.2
40	CM	73	ILE	3.2
40	CM	88	GLY	3.2
42	CO	83	LEU	3.2
25	C4	49	MET	3.2
3	AC	70	THR	3.2
11	BK	30	THR	3.2
34	CF	68	THR	3.2
49	CV	76	ALA	3.2
35	CG	157	TYR	3.2
55	DA	1068	G	3.2
7	AG	71	PRO	3.1
31	CA	102	U	3.1
31	CA	850	U	3.1
35	CG	121	ILE	3.1
37	DJ	106	LEU	3.1
45	CR	65	ILE	3.1
55	DA	2153	C	3.1
33	CE	100	MET	3.1
11	AK	21	ALA	3.1
37	CJ	124	ALA	3.1
2	AB	64	LYS	3.1
2	AB	130	THR	3.1
51	CX	57	HIS	3.1
40	CM	119	PRO	3.1
1	AA	971	G	3.1
1	BA	1257	A	3.1
31	CA	2799	A	3.1
1	BA	1086	U	3.1
31	CA	885	C	3.1
31	CA	1044	C	3.1
21	BU	5	LYS	3.1
29	CC	92	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
54	DI	28	ALA	3.1
25	C4	43	HIS	3.1
39	CL	56	ASP	3.1
48	CU	12	ARG	3.1
36	DH	88	GLY	3.1
39	CL	99	ILE	3.1
13	BM	25	VAL	3.1
14	BN	12	LYS	3.1
13	AM	23	TYR	3.1
31	CA	336	C	3.1
36	CH	133	GLN	3.1
55	DA	897	C	3.1
33	CE	15	SER	3.1
10	BJ	57	VAL	3.1
46	CS	1	MET	3.1
51	CX	70	GLU	3.1
45	CR	30	ARG	3.1
3	BC	47	LEU	3.1
10	BJ	52	LEU	3.1
31	CA	2170	A	3.1
29	CC	240	PHE	3.1
52	CY	47	VAL	3.1
13	BM	61	ALA	3.1
35	CG	96	ALA	3.1
53	DZ	3	ALA	3.1
2	AB	217	VAL	3.1
9	AI	88	MET	3.1
34	CF	46	ASP	3.1
40	CM	122	VAL	3.1
1	BA	844	G	3.1
11	BK	62	ALA	3.1
43	CP	113	ALA	3.1
50	CW	94	ALA	3.1
14	BN	7	LYS	3.1
1	AA	991	U	3.1
1	BA	1315	U	3.1
7	AG	5	ARG	3.1
7	BG	70	ARG	3.1
34	CF	165	GLU	3.1
34	CF	176	PRO	3.1
36	CH	82	SER	3.1
1	AA	974	A	3.1

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Mol	Chain	Res	Type	RSRZ
30	CD	46	ARG	3.1
3	AC	151	VAL	3.1
35	CG	113	VAL	3.1
7	AG	108	ALA	3.1
10	AJ	30	LYS	3.1
13	AM	104	THR	3.1
14	AN	19	LYS	3.1
53	CZ	40	SER	3.1
33	CE	12	LEU	3.1
43	CP	62	LEU	3.1
38	CK	55	ILE	3.1
2	BB	40	ILE	3.1
16	AP	57	ILE	3.1
21	BU	28	VAL	3.1
31	CA	316	C	3.1
34	CF	89	VAL	3.1
10	AJ	102	LEU	3.1
2	BB	36	ASN	3.1
1	BA	1347	G	3.1
28	CB	23	G	3.1
34	CF	82	GLY	3.1
35	CG	66	GLY	3.1
44	CQ	23	GLY	3.1
1	AA	1028	C	3.1
1	BA	1362	A	3.1
14	AN	13	ARG	3.1
10	BJ	18	ILE	3.0
51	CX	64	ASP	3.0
48	CU	31	VAL	3.0
18	AR	29	LEU	3.0
23	C2	34	LEU	3.0
35	DG	105	LEU	3.0
33	CE	161	ALA	3.0
55	DA	2119	A	3.0
30	CD	88	GLU	3.0
47	CT	101	SER	3.0
6	BF	96	VAL	3.0
12	BL	93	VAL	3.0
31	CA	1174	U	3.0
2	AB	213	TYR	3.0
14	BN	70	PRO	3.0
31	CA	2152	G	3.0

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Mol	Chain	Res	Type	RSRZ
1	BA	1000	A	3.0
3	BC	118	ASP	3.0
16	AP	21	VAL	3.0
31	CA	2169	A	3.0
34	CF	147	ASP	3.0
14	AN	16	LEU	3.0
29	CC	202	LEU	3.0
33	CE	43	THR	3.0
36	DH	5	LEU	3.0
37	DJ	92	LYS	3.0
14	AN	72	GLY	3.0
13	BM	107	ARG	3.0
40	CM	21	ARG	3.0
1	BA	1310	G	3.0
11	BK	21	ALA	3.0
36	CH	74	ALA	3.0
50	CW	6	ALA	3.0
2	BB	35	ARG	3.0
9	BI	124	ARG	3.0
36	DH	123	ARG	3.0
14	AN	34	VAL	3.0
1	BA	1230	C	3.0
33	CE	45	ALA	3.0
3	BC	28	GLU	3.0
31	CA	312	G	3.0
31	CA	1210	G	3.0
31	CA	1732	C	3.0
31	CA	2891	U	3.0
36	CH	149	GLU	3.0
37	CJ	123	GLU	3.0
44	CQ	27	GLU	3.0
2	BB	4	VAL	3.0
33	CE	32	VAL	3.0
18	BR	55	LEU	3.0
35	CG	50	LEU	3.0
6	AF	42	TRP	3.0
17	AQ	4	LYS	3.0
18	BR	33	ILE	3.0
23	C2	32	GLU	3.0
34	CF	54	ALA	3.0
30	CD	155	VAL	3.0
37	CJ	70	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	BA	1186	G	3.0
1	BA	1272	G	3.0
19	BS	56	GLN	3.0
31	CA	502	A	3.0
31	CA	513	A	3.0
55	DA	1063	G	3.0
14	BN	63	ARG	3.0
34	CF	122	PHE	3.0
14	AN	47	LYS	3.0
1	AA	1322	C	3.0
3	AC	107	ARG	3.0
14	BN	41	ARG	3.0
55	DA	2131	U	3.0
1	BA	1145	A	3.0
9	AI	8	GLY	3.0
13	BM	50	GLU	3.0
46	CS	67	GLY	3.0
3	BC	76	VAL	3.0
7	BG	89	VAL	3.0
20	BT	84	ASN	3.0
25	C4	28	ASN	3.0
49	CV	94	ARG	3.0
3	BC	123	GLN	3.0
36	CH	107	GLY	3.0
16	BP	17	TYR	3.0
23	C2	48	ILE	3.0
3	BC	151	VAL	3.0
48	CU	79	ASP	3.0
13	BM	80	LEU	3.0
1	AA	1220	G	3.0
1	AA	1244	G	3.0
11	BK	46	THR	3.0
31	CA	1407	G	3.0
37	DJ	60	THR	3.0
17	BQ	17	MET	3.0
23	C2	31	PRO	3.0
7	AG	132	GLY	3.0
35	CG	61	GLY	3.0
2	AB	31	ILE	3.0
3	BC	75	ILE	3.0
21	BU	15	ALA	3.0
47	CT	96	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
31	CA	1278	C	3.0
3	AC	130	PHE	3.0
45	CR	106	PHE	3.0
27	C0	39	GLU	3.0
7	AG	79	ARG	2.9
17	BQ	76	VAL	2.9
47	CT	6	LYS	2.9
48	CU	68	LYS	2.9
45	CR	81	ASN	2.9
31	CA	508	A	2.9
31	CA	1551	A	2.9
2	AB	14	VAL	2.9
13	BM	86	TYR	2.9
20	BT	50	ALA	2.9
40	CM	103	ILE	2.9
53	CZ	9	LYS	2.9
55	DA	546	U	2.9
55	DA	2166	U	2.9
1	BA	1112	C	2.9
29	CC	234	GLY	2.9
48	CU	1	MET	2.9
8	AH	56	LYS	2.9
55	DA	1170	C	2.9
13	BM	60	VAL	2.9
35	CG	37	LEU	2.9
47	CT	45	VAL	2.9
55	DA	2171	A	2.9
1	BA	991	U	2.9
14	AN	18	ASP	2.9
3	BC	41	GLN	2.9
3	BC	145	GLY	2.9
8	BH	120	GLY	2.9
31	CA	2136	G	2.9
36	DH	18	GLN	2.9
3	AC	149	ILE	2.9
54	DI	103	ASN	2.9
11	AK	84	VAL	2.9
14	AN	27	LEU	2.9
24	C3	7	PRO	2.9
33	CE	101	TYR	2.9
1	AA	994	A	2.9
24	C3	37	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
30	CD	7	LYS	2.9
34	DF	72	LYS	2.9
49	CV	20	GLY	2.9
3	BC	32	ASN	2.9
14	BN	34	VAL	2.9
20	BT	79	LEU	2.9
30	CD	40	LEU	2.9
35	CG	68	ALA	2.9
43	CP	41	ALA	2.9
1	BA	1187	G	2.9
1	BA	1334	G	2.9
40	CM	107	PHE	2.9
48	CU	80	TRP	2.9
13	AM	44	LYS	2.9
31	CA	228	C	2.9
31	CA	2161	C	2.9
35	CG	172	LYS	2.9
36	DH	16	GLY	2.9
39	CL	1	MET	2.9
51	CX	34	GLY	2.9
31	CA	505	A	2.9
31	CA	2346	A	2.9
2	BB	38	VAL	2.9
35	CG	79	VAL	2.9
30	CD	97	SER	2.9
34	CF	30	ARG	2.9
45	CR	118	ALA	2.9
3	BC	203	PHE	2.9
54	DI	96	PHE	2.9
1	BA	275	G	2.9
1	BA	1139	G	2.9
51	CX	42	GLY	2.9
9	BI	118	LEU	2.9
29	CC	19	VAL	2.9
48	CU	30	ILE	2.9
35	CG	125	CYS	2.9
1	BA	1005	A	2.9
14	AN	2	ALA	2.9
31	CA	975	A	2.9
31	CA	1095	A	2.9
42	CO	23	ASN	2.9
43	CP	67	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
50	CW	37	PRO	2.9
23	C2	7	GLU	2.9
2	AB	17	GLY	2.9
30	CD	3	GLY	2.9
6	BF	62	MET	2.9
13	BM	73	ILE	2.9
13	BM	75	MET	2.9
36	CH	75	LEU	2.9
40	CM	1	MET	2.9
1	BA	1265	C	2.9
14	AN	60	GLN	2.9
31	CA	876	C	2.9
44	CQ	7	GLN	2.9
1	BA	102	G	2.9
14	BN	26	GLU	2.9
2	BB	212	LEU	2.9
7	AG	91	VAL	2.9
18	BR	50	LYS	2.9
20	BT	34	LYS	2.9
50	CW	8	VAL	2.9
10	BJ	86	ALA	2.9
30	CD	39	ASP	2.9
34	CF	172	ALA	2.9
37	CJ	30	GLN	2.9
53	DZ	63	ALA	2.9
6	BF	58	HIS	2.9
23	C2	16	GLY	2.9
36	CH	136	SER	2.9
31	CA	72	U	2.9
31	CA	1026	G	2.9
31	CA	2107	G	2.9
31	CA	2155	U	2.9
31	CA	2180	U	2.9
37	CJ	29	GLY	2.9
37	DJ	48	SER	2.9
23	C2	22	THR	2.9
49	CV	34	VAL	2.9
8	AH	130	ALA	2.9
1	BA	1045	C	2.9
10	AJ	92	LEU	2.9
31	CA	1049	C	2.9
36	DH	4	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
9	AI	64	TYR	2.9
30	CD	132	ALA	2.9
36	CH	140	ALA	2.9
13	BM	42	ASP	2.9
45	CR	92	ARG	2.9
11	AK	113	VAL	2.8
1	BA	990	C	2.8
2	AB	21	ARG	2.8
3	AC	191	THR	2.8
9	BI	113	ARG	2.8
31	CA	1533	C	2.8
18	BR	38	LYS	2.8
23	C2	45	GLN	2.8
43	CP	55	GLU	2.8
50	CW	10	LYS	2.8
1	AA	412	A	2.8
31	CA	1107	G	2.8
31	CA	1214	A	2.8
43	CP	106	LEU	2.8
46	CS	12	HIS	2.8
7	AG	151	PHE	2.8
10	BJ	5	ARG	2.8
16	BP	35	ARG	2.8
37	DJ	103	ARG	2.8
7	BG	110	LYS	2.8
13	AM	36	ALA	2.8
31	CA	405	U	2.8
31	CA	2300	C	2.8
35	CG	31	GLY	2.8
53	CZ	21	LEU	2.8
13	AM	22	ILE	2.8
1	BA	1339	A	2.8
16	AP	51	ARG	2.8
31	CA	1532	A	2.8
9	BI	15	SER	2.8
31	CA	1047	G	2.8
31	CA	1166	G	2.8
20	BT	36	TYR	2.8
36	CH	127	GLU	2.8
44	CQ	99	TYR	2.8
46	CS	62	GLU	2.8
49	DV	46	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	BA	84	U	2.8
31	CA	2165	C	2.8
31	CA	2313	C	2.8
19	AS	59	PRO	2.8
37	DJ	97	LYS	2.8
44	CQ	22	PRO	2.8
3	AC	188	GLU	2.8
7	BG	98	ALA	2.8
9	BI	112	GLU	2.8
9	BI	5	GLN	2.8
17	BQ	7	THR	2.8
26	C5	19	ARG	2.8
31	CA	409	G	2.8
34	CF	157	THR	2.8
1	BA	208	U	2.8
13	AM	43	VAL	2.8
17	AQ	46	VAL	2.8
34	DF	80	ARG	2.8
35	CG	17	VAL	2.8
40	CM	111	ILE	2.8
49	CV	67	VAL	2.8
9	BI	91	ASP	2.8
31	CA	2153	C	2.8
49	CV	48	PRO	2.8
23	C2	35	GLU	2.8
9	BI	10	GLY	2.8
13	AM	56	LEU	2.8
37	DJ	105	GLN	2.8
1	BA	1360	A	2.8
34	CF	137	ILE	2.8
31	CA	549	G	2.8
31	CA	2148	G	2.8
31	CA	2286	G	2.8
34	CF	113	ASP	2.8
9	AI	32	GLN	2.8
41	CN	8	LYS	2.8
8	BH	107	SER	2.8
1	AA	1188	A	2.8
1	AA	1321	U	2.8
7	AG	143	ARG	2.8
34	CF	65	PRO	2.8
35	CG	95	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
42	CO	117	ASP	2.8
9	AI	24	GLY	2.8
31	CA	2892	G	2.8
49	CV	38	GLY	2.8
37	CJ	140	VAL	2.8
36	CH	70	GLU	2.8
37	DJ	136	MET	2.8
9	AI	107	ASP	2.8
55	DA	2114	A	2.8
15	BO	16	GLY	2.8
10	AJ	98	VAL	2.8
37	DJ	140	VAL	2.8
2	AB	5	SER	2.8
13	AM	85	CYS	2.8
51	CX	36	ILE	2.8
1	AA	951	G	2.8
1	BA	1190	G	2.8
25	C4	26	HIS	2.8
33	CE	91	ASP	2.8
42	CO	94	TYR	2.8
45	CR	91	ASP	2.8
17	BQ	78	VAL	2.8
16	BP	8	ARG	2.8
1	AA	972	C	2.8
1	AA	999	C	2.8
1	AA	1140	C	2.8
55	DA	2161	C	2.8
1	AA	134	G	2.8
1	BA	202	G	2.8
4	AD	18	ASP	2.8
29	CC	98	ASP	2.8
3	BC	108	LYS	2.8
9	AI	22	LYS	2.8
9	AI	119	ARG	2.8
1	AA	121	U	2.8
1	BA	1224	U	2.8
2	BB	17	GLY	2.8
18	BR	32	TYR	2.8
29	CC	101	ARG	2.8
2	AB	40	ILE	2.7
7	AG	126	ASP	2.8
31	CA	1211	C	2.8

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Mol	Chain	Res	Type	RSRZ
10	AJ	78	GLU	2.7
1	AA	433	G	2.7
5	AE	96	MET	2.7
31	CA	2877	G	2.7
1	AA	1319	A	2.7
2	BB	69	PHE	2.7
3	BC	146	ALA	2.7
34	CF	33	LYS	2.7
34	CF	47	LYS	2.7
34	CF	62	GLY	2.7
40	CM	129	LYS	2.7
7	BG	122	ASN	2.7
49	CV	82	ARG	2.7
46	CS	14	VAL	2.7
14	BN	40	ASP	2.7
18	AR	22	ASP	2.7
19	AS	27	ASP	2.7
37	DJ	10	LYS	2.7
42	CO	63	ARG	2.7
48	CU	11	LEU	2.7
31	CA	2904	U	2.7
3	AC	187	SER	2.7
9	BI	111	VAL	2.7
16	BP	39	PHE	2.7
28	CB	24	G	2.7
31	CA	881	G	2.7
43	CP	78	VAL	2.7
11	AK	97	ILE	2.7
31	CA	2860	A	2.7
36	DH	94	ILE	2.7
33	CE	18	THR	2.7
8	AH	127	CYS	2.7
11	BK	100	LEU	2.7
17	BQ	44	LEU	2.7
1	BA	1149	C	2.7
1	BA	1320	C	2.7
49	CV	56	GLY	2.7
50	CW	65	VAL	2.7
30	CD	48	ILE	2.7
14	AN	70	PRO	2.7
20	BT	48	GLN	2.7
3	AC	89	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
19	BS	18	LYS	2.7
35	DG	115	HIS	2.7
43	CP	56	LYS	2.7
48	CU	81	LYS	2.7
1	BA	1318	A	2.7
3	AC	180	ALA	2.7
12	AL	68	GLY	2.7
1	BA	1335	U	2.7
40	CM	7	SER	2.7
55	DA	1066	U	2.7
51	CX	32	LEU	2.7
54	DI	124	ASP	2.7
1	AA	1272	G	2.7
31	CA	1046	A	2.7
31	CA	1112	G	2.7
31	CA	1548	A	2.7
33	CE	174	GLY	2.7
46	CS	5	PHE	2.7
8	BH	130	ALA	2.7
18	AR	32	TYR	2.7
11	BK	97	ILE	2.7
1	BA	1336	C	2.7
17	BQ	72	SER	2.7
26	C5	10	LEU	2.7
47	CT	37	THR	2.7
31	CA	1090	A	2.7
1	BA	107	G	2.7
44	CQ	12	GLN	2.7
46	CS	22	LEU	2.7
55	DA	2140	G	2.7
1	AA	88	U	2.7
1	BA	961	U	2.7
1	BA	1054	C	2.7
2	BB	13	GLY	2.7
55	DA	1172	C	2.7
2	AB	159	ASP	2.7
10	AJ	22	THR	2.7
11	AK	18	ASP	2.7
34	CF	80	ARG	2.7
7	BG	47	LEU	2.7
9	BI	87	LEU	2.7
46	CS	18	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
9	AI	103	PHE	2.7
10	BJ	54	SER	2.7
19	AS	44	MET	2.7
30	CD	19	GLY	2.7
31	CA	1238	G	2.7
35	CG	28	GLY	2.7
35	DG	177	LYS	2.7
38	CK	40	HIS	2.7
54	DI	38	MET	2.7
1	BA	945	G	2.7
7	BG	61	ALA	2.7
9	AI	83	ILE	2.7
31	CA	2143	C	2.7
9	AI	98	LEU	2.7
10	AJ	10	LEU	2.7
18	BR	29	LEU	2.7
2	BB	131	LYS	2.7
1	BA	325	A	2.7
1	BA	974	A	2.7
31	CA	1077	A	2.7
2	AB	42	ASN	2.7
31	CA	1212	G	2.7
43	CP	115	LEU	2.7
55	DA	2178	C	2.7
3	AC	127	ARG	2.7
3	BC	54	ARG	2.7
9	AI	124	ARG	2.7
34	CF	93	GLY	2.7
34	DF	81	GLN	2.7
36	DH	13	GLY	2.7
49	CV	25	VAL	2.7
2	BB	164	ILE	2.7
21	BU	4	ILE	2.7
44	DQ	2	SER	2.7
19	BS	6	LYS	2.7
29	CC	90	ASN	2.7
53	CZ	4	LYS	2.7
15	BO	88	ARG	2.7
15	BO	89	ARG	2.7
1	BA	1132	C	2.7
1	AA	1323	G	2.7
5	BE	38	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
7	AG	105	VAL	2.7
11	BK	20	VAL	2.7
31	CA	474	G	2.7
31	CA	2121	G	2.7
37	CJ	122	ILE	2.7
16	AP	40	ASN	2.6
54	DI	36	ASP	2.6
1	BA	1248	A	2.6
14	AN	49	GLN	2.6
37	DJ	115	ALA	2.6
46	CS	49	ILE	2.6
31	CA	1863	G	2.6
35	DG	107	LEU	2.6
27	C0	54	MET	2.6
47	CT	49	LYS	2.6
1	BA	1319	A	2.6
8	AH	121	LEU	2.6
27	C0	24	LEU	2.6
29	CC	210	ALA	2.6
44	CQ	59	PHE	2.6
46	CS	7	SER	2.6
34	DF	37	ASN	2.6
36	DH	19	VAL	2.6
41	CN	17	ASN	2.6
13	AM	57	ARG	2.6
42	CO	36	THR	2.6
3	AC	87	LEU	2.6
6	BF	36	ILE	2.6
33	CE	105	LEU	2.6
35	CG	72	LEU	2.6
37	DJ	41	ALA	2.6
1	AA	1201	A	2.6
31	CA	330	A	2.6
31	CA	1089	A	2.6
30	CD	153	GLY	2.6
31	CA	2078	C	2.6
37	CJ	92	LYS	2.6
2	AB	136	MET	2.6
33	CE	25	GLU	2.6
33	CE	171	ASP	2.6
47	CT	50	VAL	2.6
9	BI	63	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
16	AP	50	THR	2.6
2	BB	76	ALA	2.6
31	CA	1216	G	2.6
13	BM	27	LYS	2.6
1	AA	1216	A	2.6
7	AG	103	TRP	2.6
12	BL	71	GLY	2.6
31	CA	1073	A	2.6
31	CA	2287	A	2.6
36	CH	134	VAL	2.6
51	CX	38	VAL	2.6
54	DI	98	GLU	2.6
1	BA	83	C	2.6
9	BI	107	ASP	2.6
2	BB	135	LEU	2.6
31	CA	183	C	2.6
13	AM	110	LYS	2.6
27	C0	43	ALA	2.6
1	BA	92	U	2.6
19	BS	55	ARG	2.6
43	CP	111	ARG	2.6
1	AA	1026	G	2.6
1	BA	944	G	2.6
26	D5	38	GLY	2.6
31	CA	2895	G	2.6
33	CE	28	VAL	2.6
48	CU	85	VAL	2.6
13	BM	76	SER	2.6
52	CY	56	MET	2.6
1	BA	1340	A	2.6
11	AK	82	LEU	2.6
1	AA	1027	C	2.6
1	AA	1119	C	2.6
34	CF	75	ALA	2.6
46	CS	93	PHE	2.6
11	BK	92	GLY	2.6
16	AP	49	GLY	2.6
36	CH	141	LYS	2.6
1	BA	108	G	2.6
10	BJ	29	ALA	2.6
29	CC	182	ARG	2.6
1	BA	1141	C	2.6

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Mol	Chain	Res	Type	RSRZ
2	AB	4	VAL	2.6
2	AB	156	GLY	2.6
5	BE	123	VAL	2.6
17	AQ	10	GLY	2.6
19	AS	46	GLY	2.6
19	AS	57	HIS	2.6
1	AA	1121	U	2.6
1	BA	950	U	2.6
49	CV	4	LYS	2.6
16	AP	52	LEU	2.6
34	CF	169	LEU	2.6
10	AJ	86	ALA	2.6
24	C3	36	ALA	2.6
34	CF	94	GLU	2.6
42	CO	49	GLU	2.6
54	DI	4	ASN	2.6
10	BJ	83	THR	2.6
2	BB	39	HIS	2.6
1	AA	1147	C	2.6
31	CA	2129	C	2.6
35	CG	3	ARG	2.6
2	AB	84	ALA	2.6
2	BB	188	ASP	2.6
7	BG	125	SER	2.6
12	BL	65	SER	2.6
22	C1	18	SER	2.6
16	AP	19	VAL	2.6
25	C4	58	VAL	2.6
36	CH	15	LEU	2.6
37	CJ	118	THR	2.6
1	AA	1019	A	2.6
1	BA	78	A	2.6
1	BA	1188	A	2.6
15	BO	43	PHE	2.6
31	CA	1530	G	2.6
43	CP	97	PHE	2.6
55	DA	2176	A	2.6
43	CP	109	ALA	2.6
51	CX	61	ALA	2.6
25	C4	41	LYS	2.6
35	CG	85	LYS	2.6
5	BE	96	MET	2.6

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Mol	Chain	Res	Type	RSRZ
10	AJ	55	PRO	2.6
20	BT	56	PRO	2.6
22	C1	8	PRO	2.6
42	CO	98	LEU	2.6
50	CW	84	PRO	2.6
34	CF	60	ILE	2.6
52	CY	34	HIS	2.6
5	BE	127	ALA	2.5
1	AA	958	A	2.5
7	BG	40	GLU	2.5
7	BG	85	TYR	2.5
10	BJ	99	GLN	2.5
22	C1	56	ALA	2.5
9	BI	92	GLU	2.5
1	BA	942	G	2.5
1	BA	1247	U	2.5
9	AI	58	VAL	2.5
13	BM	87	ARG	2.5
16	BP	36	VAL	2.5
35	DG	113	VAL	2.5
36	CH	123	ARG	2.5
43	CP	25	ARG	2.5
35	CG	87	LEU	2.5
2	AB	27	MET	2.5
7	AG	131	LYS	2.5
7	BG	56	LYS	2.5
14	AN	64	CYS	2.5
36	CH	27	ARG	2.5
50	CW	41	GLU	2.5
40	CM	20	GLY	2.5
40	CM	85	VAL	2.5
8	BH	121	LEU	2.5
33	CE	118	LEU	2.5
1	BA	947	G	2.5
1	BA	993	G	2.5
26	C5	13	ASN	2.5
51	CX	60	PHE	2.5
13	BM	28	THR	2.5
14	AN	63	ARG	2.5
34	CF	135	GLN	2.5
34	CF	143	TYR	2.5
35	CG	116	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
37	DJ	107	GLN	2.5
48	CU	86	THR	2.5
52	DY	78	TYR	2.5
54	DI	114	GLU	2.5
5	AE	124	LEU	2.5
37	DJ	100	LYS	2.5
34	CF	121	SER	2.5
36	CH	99	ILE	2.5
9	AI	4	ASN	2.5
55	DA	1847	A	2.5
48	CU	70	HIS	2.5
1	BA	1144	G	2.5
2	AB	13	GLY	2.5
3	AC	148	GLY	2.5
35	CG	129	THR	2.5
50	CW	67	GLY	2.5
23	C2	9	ILE	2.5
44	CQ	74	PHE	2.5
14	AN	100	SER	2.5
10	AJ	27	GLU	2.5
17	BQ	63	GLU	2.5
2	AB	134	ALA	2.5
1	BA	81	A	2.5
1	BA	1325	C	2.5
2	AB	221	VAL	2.5
30	CD	32	ASN	2.5
30	CD	104	VAL	2.5
49	CV	66	GLN	2.5
53	CZ	41	HIS	2.5
33	CE	150	THR	2.5
40	CM	74	THR	2.5
7	AG	104	ILE	2.5
9	BI	33	ARG	2.5
13	AM	101	ARG	2.5
45	CR	90	ILE	2.5
47	CT	95	ARG	2.5
50	CW	29	ILE	2.5
46	CS	26	ASP	2.5
16	AP	82	ALA	2.5
18	BR	40	VAL	2.5
33	CE	120	VAL	2.5
43	CP	47	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
44	CQ	26	VAL	2.5
48	CU	41	ALA	2.5
53	CZ	35	GLY	2.5
5	AE	81	LEU	2.5
54	DI	126	LEU	2.5
9	AI	33	ARG	2.5
30	CD	179	ARG	2.5
18	AR	21	ILE	2.5
44	CQ	34	GLU	2.5
3	BC	183	ASP	2.5
1	BA	933	G	2.5
1	BA	1266	G	2.5
29	CC	78	VAL	2.5
33	CE	121	VAL	2.5
43	CP	71	ALA	2.5
43	CP	95	SER	2.5
6	BF	47	LEU	2.5
31	CA	767	U	2.5
16	AP	42	ILE	2.5
34	CF	99	PHE	2.5
35	CG	51	THR	2.5
51	CX	24	LYS	2.5
1	BA	250	A	2.5
31	CA	357	C	2.5
31	CA	1143	A	2.5
2	AB	57	LEU	2.5
3	AC	73	PRO	2.5
13	BM	115	PRO	2.5
19	BS	46	GLY	2.5
48	CU	50	LEU	2.5
48	CU	65	GLY	2.5
50	CW	60	VAL	2.5
53	CZ	63	ALA	2.5
7	BG	57	SER	2.5
10	BJ	82	LYS	2.5
31	CA	1171	G	2.5
35	CG	67	THR	2.5
49	CV	62	GLU	2.5
33	CE	37	ALA	2.5
48	CU	62	VAL	2.5
1	BA	1140	C	2.5
31	CA	262	A	2.5

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Mol	Chain	Res	Type	RSRZ
31	CA	1043	C	2.5
41	CN	106	ASP	2.5
43	CP	108	ASP	2.5
49	CV	30	SER	2.5
53	CZ	25	GLN	2.5
50	CW	1	MET	2.5
35	CG	69	ARG	2.5
52	CY	18	ARG	2.5
1	BA	1043	G	2.5
4	AD	2	ALA	2.5
30	CD	37	VAL	2.5
30	CD	188	LEU	2.5
31	CA	315	G	2.5
31	CA	2668	G	2.5
41	CN	78	LEU	2.5
35	CG	128	GLN	2.5
53	CZ	44	LYS	2.5
31	CA	2163	A	2.5
36	CH	76	GLU	2.5
36	CH	114	GLU	2.5
9	AI	54	LEU	2.5
55	DA	1060	U	2.5
13	BM	106	ALA	2.5
34	CF	81	GLN	2.5
1	BA	1057	G	2.5
24	C3	16	HIS	2.5
31	CA	317	G	2.5
31	CA	561	G	2.5
31	CA	1215	G	2.5
44	CQ	19	SER	2.5
31	CA	1874	C	2.4
31	CA	2045	C	2.4
30	CD	53	GLY	2.4
31	CA	311	A	2.4
43	CP	114	GLY	2.4
1	AA	981	U	2.4
1	BA	1202	U	2.4
3	AC	50	ALA	2.4
23	C2	15	ALA	2.4
25	C4	14	PHE	2.4
43	CP	33	ARG	2.4
2	AB	132	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
23	C2	12	VAL	2.4
25	C4	44	LEU	2.4
1	AA	135	C	2.4
1	AA	985	C	2.4
31	CA	1984	G	2.4
20	BT	45	ALA	2.4
37	DJ	27	ALA	2.4
1	BA	1189	U	2.4
31	CA	1880	U	2.4
2	AB	164	ILE	2.4
9	AI	65	ILE	2.4
13	BM	112	PRO	2.4
43	CP	60	GLU	2.4
54	DI	122	GLN	2.4
2	AB	45	LYS	2.4
2	AB	214	LEU	2.4
3	BC	6	HIS	2.4
36	DH	35	LYS	2.4
2	BB	155	GLY	2.4
7	AG	64	VAL	2.4
17	BQ	22	VAL	2.4
1	AA	980	C	2.4
1	AA	998	C	2.4
35	CG	19	ILE	2.4
35	CG	42	GLU	2.4
31	CA	2176	A	2.4
35	CG	134	LYS	2.4
7	AG	15	ASP	2.4
8	BH	99	LEU	2.4
42	CO	115	LEU	2.4
3	BC	88	ARG	2.4
49	CV	57	GLY	2.4
3	AC	133	ALA	2.4
7	AG	128	ALA	2.4
14	AN	36	ALA	2.4
19	AS	75	ALA	2.4
30	CD	41	ALA	2.4
3	BC	199	LYS	2.4
5	BE	13	GLU	2.4
11	AK	107	ILE	2.4
34	DF	85	ILE	2.4
40	CM	86	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
46	CS	11	GLN	2.4
6	AF	61	LEU	2.4
1	BA	68	G	2.4
1	BA	94	G	2.4
1	BA	203	G	2.4
1	BA	969	A	2.4
47	CT	99	ARG	2.4
3	AC	93	ASP	2.4
31	CA	2138	G	2.4
15	BO	19	ALA	2.4
36	CH	102	ALA	2.4
45	CR	68	ALA	2.4
52	CY	76	GLU	2.4
54	DI	133	GLU	2.4
38	CK	22	GLY	2.4
51	CX	65	GLY	2.4
31	CA	545	U	2.4
49	CV	44	LYS	2.4
1	AA	1021	A	2.4
1	BA	1311	A	2.4
2	BB	75	ALA	2.4
14	AN	10	GLU	2.4
43	CP	80	GLU	2.4
33	CE	88	ARG	2.4
2	BB	68	LEU	2.4
9	BI	48	VAL	2.4
24	C3	43	THR	2.4
25	C4	63	PRO	2.4
29	CC	12	GLY	2.4
33	CE	129	PRO	2.4
35	CG	80	THR	2.4
36	DH	108	VAL	2.4
54	DI	72	LEU	2.4
37	DJ	91	GLY	2.4
48	CU	29	THR	2.4
3	BC	31	ASP	2.4
6	BF	25	TYR	2.4
42	CO	114	GLU	2.4
46	CS	92	TRP	2.4
37	CJ	135	SER	2.4
1	BA	978	A	2.4
40	CM	87	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
3	AC	7	PRO	2.4
21	BU	19	PHE	2.4
35	CG	171	THR	2.4
31	CA	1217	U	2.4
52	CY	64	ILE	2.4
34	CF	118	SER	2.4
54	DI	105	LYS	2.4
1	AA	1036	A	2.4
13	AM	10	PRO	2.4
19	AS	30	PRO	2.4
31	CA	332	A	2.4
10	AJ	50	THR	2.4
35	CG	177	LYS	2.4
37	DJ	101	ILE	2.4
25	C4	22	PHE	2.4
41	CN	9	PHE	2.4
10	AJ	9	ARG	2.4
13	BM	79	ARG	2.4
35	CG	8	PRO	2.4
1	AA	983	A	2.4
36	CH	36	ALA	2.4
9	AI	87	LEU	2.4
10	AJ	77	VAL	2.4
33	CE	196	VAL	2.4
34	CF	149	VAL	2.4
1	AA	1124	G	2.4
9	BI	57	MET	2.4
14	AN	69	ARG	2.4
27	C0	53	PHE	2.4
31	CA	2116	G	2.4
55	DA	2151	U	2.4
2	BB	12	ALA	2.4
20	BT	46	ALA	2.4
37	DJ	84	ALA	2.4
38	CK	23	LYS	2.4
47	CT	85	ILE	2.4
48	CU	38	ALA	2.4
30	CD	197	THR	2.4
1	BA	101	A	2.3
24	C3	34	ARG	2.3
34	CF	77	PHE	2.3
34	CF	102	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
49	DV	54	GLN	2.3
1	BA	843	U	2.3
13	AM	21	SER	2.3
10	AJ	12	ALA	2.3
19	AS	40	ILE	2.3
36	CH	80	ILE	2.3
37	DJ	15	ALA	2.3
48	CU	45	ALA	2.3
28	CB	27	C	2.3
36	DH	11	ASN	2.3
41	CN	41	LEU	2.3
7	AG	141	VAL	2.3
10	AJ	38	GLY	2.3
10	BJ	96	VAL	2.3
47	CT	9	HIS	2.3
41	CN	92	TRP	2.3
45	CR	57	PHE	2.3
23	C2	50	LYS	2.3
39	CL	3	GLN	2.3
3	AC	146	ALA	2.3
18	BR	21	ILE	2.3
30	CD	100	LEU	2.3
35	CG	174	ALA	2.3
50	CW	63	ILE	2.3
1	BA	1386	G	2.3
3	BC	67	THR	2.3
7	BG	130	ASN	2.3
15	AO	43	PHE	2.3
15	BO	29	VAL	2.3
34	CF	12	VAL	2.3
34	CF	166	GLY	2.3
35	CG	45	HIS	2.3
39	CL	82	ASN	2.3
51	CX	62	LYS	2.3
2	AB	49	MET	2.3
18	BR	22	ASP	2.3
29	CC	79	GLU	2.3
34	CF	163	ASP	2.3
54	DI	29	ASP	2.3
54	DI	52	MET	2.3
7	BG	59	LEU	2.3
25	C4	40	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
31	CA	2147	A	2.3
46	CS	59	ILE	2.3
55	DA	613	A	2.3
3	AC	195	VAL	2.3
3	BC	135	LYS	2.3
31	CA	2783	U	2.3
36	DH	107	GLY	2.3
38	CK	56	VAL	2.3
10	AJ	64	GLN	2.3
44	CQ	112	GLU	2.3
51	CX	83	GLU	2.3
1	BA	1361	G	2.3
28	CB	117	G	2.3
30	CD	187	LEU	2.3
31	CA	408	G	2.3
31	CA	1017	G	2.3
53	CZ	48	ARG	2.3
5	AE	144	LEU	2.3
45	CR	25	TYR	2.3
34	CF	120	LYS	2.3
44	CQ	38	LYS	2.3
53	CZ	34	SER	2.3
1	BA	467	U	2.3
1	BA	1333	A	2.3
13	AM	47	GLU	2.3
48	CU	4	GLU	2.3
50	CW	11	GLU	2.3
6	BF	97	THR	2.3
30	CD	35	THR	2.3
35	CG	34	THR	2.3
50	CW	79	ARG	2.3
27	C0	29	LEU	2.3
36	CH	111	ALA	2.3
52	CY	59	ILE	2.3
2	BB	217	VAL	2.3
5	BE	85	VAL	2.3
31	CA	1063	G	2.3
31	CA	1734	G	2.3
31	CA	2159	G	2.3
33	CE	55	SER	2.3
36	CH	139	PHE	2.3
54	DI	27	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
17	BQ	20	SER	2.3
55	DA	2128	G	2.3
7	BG	10	ARG	2.3
17	AQ	52	GLU	2.3
37	CJ	36	MET	2.3
3	BC	3	GLN	2.3
10	AJ	32	THR	2.3
16	BP	18	GLN	2.3
2	BB	186	ILE	2.3
7	AG	23	LEU	2.3
17	BQ	71	LYS	2.3
33	CE	168	ASP	2.3
33	CE	180	LEU	2.3
11	BK	71	ALA	2.3
15	AO	17	ARG	2.3
47	CT	92	ARG	2.3
31	CA	318	C	2.3
48	CU	64	LYS	2.3
1	AA	842	U	2.3
1	AA	1212	U	2.3
1	BA	121	U	2.3
1	BA	960	U	2.3
31	CA	1742	U	2.3
55	DA	1078	U	2.3
8	BH	75	ILE	2.3
1	AA	1117	A	2.3
31	CA	1111	A	2.3
36	DH	124	THR	2.3
36	CH	121	VAL	2.3
3	BC	17	PRO	2.3
16	BP	41	PRO	2.3
30	CD	205	PRO	2.3
33	CE	125	SER	2.3
36	DH	8	LYS	2.3
11	AK	42	LEU	2.3
47	CT	55	ILE	2.3
8	BH	49	PHE	2.3
1	AA	1347	G	2.3
2	BB	88	ASP	2.3
16	BP	20	VAL	2.3
19	AS	39	THR	2.3
19	AS	78	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
36	DH	147	VAL	2.3
38	CK	21	THR	2.3
40	CM	64	PHE	2.3
44	CQ	109	ARG	2.3
46	CS	53	PHE	2.3
50	CW	49	ASN	2.3
53	CZ	46	VAL	2.3
1	BA	1067	A	2.3
1	BA	1355	G	2.3
31	CA	829	A	2.3
31	CA	2435	A	2.3
7	AG	116	MET	2.3
46	CS	15	SER	2.3
7	AG	18	PHE	2.3
10	BJ	51	VAL	2.3
35	CG	13	ALA	2.3
37	CJ	127	ARG	2.3
31	CA	343	C	2.3
34	CF	116	GLY	2.3
30	CD	131	ASP	2.3
35	CG	48	ASN	2.3
37	DJ	43	ASN	2.3
44	CQ	96	LYS	2.3
45	CR	73	GLY	2.3
44	CQ	11	GLU	2.3
1	AA	1197	A	2.3
1	BA	1138	G	2.3
5	BE	81	LEU	2.3
31	CA	477	A	2.3
31	CA	1277	G	2.3
31	CA	1322	A	2.3
31	CA	1847	A	2.3
9	BI	95	ARG	2.3
12	AL	54	ARG	2.3
16	AP	14	ARG	2.3
31	CA	1873	G	2.3
51	CX	82	ILE	2.3
8	BH	51	VAL	2.3
19	AS	29	LYS	2.3
30	CD	34	VAL	2.3
47	CT	90	LYS	2.3
50	CW	92	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
54	DI	63	ALA	2.3
1	BA	210	C	2.3
28	CB	22	U	2.3
31	CA	335	C	2.3
7	BG	3	ARG	2.3
2	AB	28	LYS	2.3
33	CE	124	PHE	2.3
50	CW	68	LYS	2.3
1	AA	1346	A	2.3
20	BT	58	VAL	2.3
25	C4	65	ALA	2.3
37	CJ	133	ALA	2.3
40	CM	35	HIS	2.3
7	AG	129	GLU	2.2
7	AG	120	LEU	2.2
7	BG	124	LEU	2.2
12	AL	109	ASP	2.2
22	C1	16	ARG	2.2
33	CE	138	LEU	2.2
12	BL	80	ILE	2.2
15	BO	48	LYS	2.2
37	DJ	74	PRO	2.2
3	AC	29	PHE	2.2
36	DH	138	VAL	2.2
37	DJ	139	VAL	2.2
13	AM	37	ALA	2.2
30	CD	74	GLU	2.2
49	CV	98	SER	2.2
1	BA	80	A	2.2
15	AO	47	LYS	2.2
6	BF	6	ILE	2.2
17	BQ	74	THR	2.2
27	C0	41	THR	2.2
31	CA	914	G	2.2
33	CE	48	THR	2.2
7	AG	73	VAL	2.2
7	AG	80	VAL	2.2
45	CR	88	VAL	2.2
48	CU	57	VAL	2.2
55	DA	138	U	2.2
1	BA	1195	C	2.2
10	BJ	66	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
25	C4	27	ALA	2.2
15	AO	53	ARG	2.2
2	AB	114	LEU	2.2
8	AH	32	LEU	2.2
1	AA	1092	A	2.2
2	AB	50	PHE	2.2
2	BB	32	PHE	2.2
16	BP	16	PHE	2.2
3	AC	106	VAL	2.2
26	C5	25	VAL	2.2
43	CP	24	THR	2.2
1	BA	1232	U	2.2
2	AB	53	ALA	2.2
3	BC	110	GLU	2.2
7	AG	145	ALA	2.2
7	BG	9	GLN	2.2
11	AK	43	GLY	2.2
15	AO	40	GLN	2.2
31	CA	88	G	2.2
31	CA	1341	G	2.2
31	CA	1421	G	2.2
31	CA	2112	G	2.2
31	CA	2650	U	2.2
47	CT	10	ALA	2.2
55	DA	2107	G	2.2
1	BA	1214	C	2.2
31	CA	854	C	2.2
46	CS	66	HIS	2.2
13	BM	69	LEU	2.2
14	BN	46	LEU	2.2
5	AE	105	ILE	2.2
9	BI	72	ILE	2.2
17	AQ	21	ILE	2.2
33	CE	158	PHE	2.2
14	AN	43	ASN	2.2
21	AU	13	ASP	2.2
1	BA	1213	A	2.2
3	AC	71	ALA	2.2
5	BE	128	TYR	2.2
22	C1	6	ASN	2.2
36	DH	17	ASP	2.2
12	AL	30	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
12	BL	51	LYS	2.2
23	C2	27	LYS	2.2
33	CE	13	THR	2.2
36	CH	124	THR	2.2
40	CM	30	THR	2.2
1	AA	1364	U	2.2
1	BA	114	U	2.2
31	CA	895	U	2.2
31	CA	1015	U	2.2
3	BC	115	LEU	2.2
10	BJ	92	LEU	2.2
36	CH	58	LEU	2.2
1	AA	1149	C	2.2
16	BP	38	PHE	2.2
34	CF	138	PHE	2.2
2	AB	187	VAL	2.2
15	AO	89	ARG	2.2
54	DI	56	ARG	2.2
10	BJ	85	ASP	2.2
17	BQ	69	LYS	2.2
19	BS	64	ASP	2.2
20	AT	59	ASP	2.2
37	CJ	84	ALA	2.2
46	CS	8	GLY	2.2
10	BJ	32	THR	2.2
40	CM	128	THR	2.2
31	CA	1061	U	2.2
31	CA	2344	U	2.2
45	CR	14	HIS	2.2
55	DA	1077	A	2.2
3	AC	173	VAL	2.2
5	AE	141	ILE	2.2
30	CD	98	VAL	2.2
50	CW	71	LYS	2.2
1	AA	976	G	2.2
1	AA	1302	C	2.2
1	BA	1064	G	2.2
9	AI	86	ALA	2.2
31	CA	1037	G	2.2
31	CA	2144	G	2.2
31	CA	2527	C	2.2
34	CF	171	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	AC	115	LEU	2.2
5	BE	144	LEU	2.2
33	CE	164	LEU	2.2
44	CQ	114	LEU	2.2
1	AA	1122	U	2.2
7	BG	114	LYS	2.2
9	AI	85	ARG	2.2
13	AM	103	LYS	2.2
34	DF	175	PHE	2.2
9	AI	55	VAL	2.2
19	AS	38	SER	2.2
13	AM	51	GLY	2.2
8	BH	61	LEU	2.2
13	BM	82	ASP	2.2
37	DJ	64	ASP	2.2
50	CW	66	ASP	2.2
54	DI	100	ALA	2.2
14	BN	94	PRO	2.2
31	CA	2651	C	2.2
36	DH	6	LEU	2.2
13	AM	62	LYS	2.2
36	DH	125	THR	2.2
48	CU	6	ARG	2.2
49	CV	73	PHE	2.2
3	AC	69	HIS	2.2
3	BC	142	MET	2.2
6	AF	37	HIS	2.2
6	AF	62	MET	2.2
29	CC	74	ILE	2.2
29	CC	243	HIS	2.2
46	CS	98	ILE	2.2
28	CB	74	U	2.2
42	CO	7	GLY	2.2
3	AC	42	TYR	2.2
41	CN	56	ALA	2.2
29	CC	13	ARG	2.2
38	CK	49	ASP	2.2
49	CV	43	LYS	2.2
1	AA	217	C	2.2
1	BA	1369	C	2.2
29	CC	239	ASN	2.2
3	AC	75	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
6	BF	29	ILE	2.2
29	CC	104	ILE	2.2
30	CD	1	MET	2.2
37	CJ	112	THR	2.2
35	CG	167	GLU	2.2
36	CH	78	VAL	2.2
49	DV	58	ILE	2.2
1	AA	1215	G	2.2
31	CA	1807	G	2.2
44	CQ	35	GLY	2.2
3	BC	169	ARG	2.2
7	AG	47	LEU	2.2
11	BK	47	ALA	2.2
25	C4	45	ARG	2.2
30	CD	85	ALA	2.2
31	CA	1081	U	2.2
31	CA	1325	U	2.2
34	CF	2	ALA	2.2
47	CT	46	LEU	2.2
50	CW	57	TYR	2.2
54	DI	102	ALA	2.2
31	CA	899	A	2.2
35	DG	116	GLN	2.2
52	CY	31	PRO	2.2
15	BO	26	GLU	2.2
34	CF	21	ASN	2.2
44	CQ	5	ILE	2.2
1	BA	207	C	2.2
31	CA	11	C	2.2
36	CH	89	LYS	2.2
41	CN	40	ARG	2.2
2	BB	114	LEU	2.2
1	BA	1301	U	2.2
7	AG	125	SER	2.2
11	BK	103	ALA	2.2
34	CF	70	ALA	2.2
31	CA	1201	U	2.2
36	CH	131	SER	2.2
3	BC	139	GLN	2.2
43	CP	104	GLN	2.2
55	DA	277	G	2.2
9	BI	19	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	BA	1441	A	2.2
11	BK	43	GLY	2.2
12	AL	108	LYS	2.2
17	BQ	11	ARG	2.2
20	BT	20	HIS	2.2
34	CF	90	THR	2.2
36	CH	35	LYS	2.2
40	CM	124	GLY	2.2
49	DV	57	GLY	2.2
1	AA	1120	C	2.1
31	CA	414	C	2.1
34	CF	45	ALA	2.1
36	CH	69	ALA	2.1
1	AA	992	U	2.1
1	BA	89	U	2.1
31	CA	34	U	2.1
55	DA	1176	U	2.1
3	AC	46	GLU	2.1
9	BI	80	ARG	2.1
14	BN	89	MET	2.1
15	AO	21	ASP	2.1
16	BP	80	LYS	2.1
20	BT	24	ARG	2.1
33	CE	102	ARG	2.1
34	CF	79	ILE	2.1
44	CQ	113	ARG	2.1
48	CU	34	VAL	2.1
1	BA	1117	A	2.1
24	C3	24	THR	2.1
3	AC	189	ALA	2.1
10	BJ	61	ALA	2.1
20	BT	63	ALA	2.1
51	CX	33	ALA	2.1
16	AP	18	GLN	2.1
1	BA	1228	C	2.1
7	BG	11	LYS	2.1
31	CA	1079	C	2.1
31	CA	1518	C	2.1
54	DI	123	ILE	2.1
55	DA	2150	C	2.1
13	AM	58	ASP	2.1
3	BC	29	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
8	AH	55	THR	2.1
50	CW	74	ALA	2.1
54	DI	80	THR	2.1
31	CA	1059	G	2.1
31	CA	1235	G	2.1
45	CR	78	LYS	2.1
46	CS	64	VAL	2.1
11	AK	112	ASP	2.1
13	AM	13	LYS	2.1
14	AN	35	ASN	2.1
30	CD	83	ARG	2.1
35	CG	20	ASN	2.1
48	CU	28	ASN	2.1
43	CP	19	GLN	2.1
1	BA	1193	G	2.1
19	BS	68	GLY	2.1
31	CA	2782	G	2.1
34	CF	61	SER	2.1
1	AA	1118	U	2.1
13	BM	78	LYS	2.1
19	AS	81	ARG	2.1
31	CA	2743	U	2.1
34	CF	8	TYR	2.1
34	CF	115	ARG	2.1
34	CF	174	ASP	2.1
53	CZ	7	ARG	2.1
35	DG	111	HIS	2.1
41	CN	88	ASN	2.1
49	CV	101	GLU	2.1
15	BO	11	ILE	2.1
12	BL	81	LEU	2.1
16	BP	15	PRO	2.1
19	AS	9	PRO	2.1
34	DF	36	LEU	2.1
12	AL	99	ARG	2.1
36	DH	89	LYS	2.1
1	BA	1093	A	2.1
1	AA	1373	G	2.1
13	BM	15	ALA	2.1
15	BO	30	ALA	2.1
25	C4	54	ASP	2.1
1	BA	1123	U	2.1

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Mol	Chain	Res	Type	RSRZ
1	BA	1262	C	2.1
3	BC	167	TRP	2.1
6	AF	96	VAL	2.1
13	BM	91	HIS	2.1
31	CA	440	C	2.1
35	CG	30	ASN	2.1
35	DG	101	ASN	2.1
52	CY	7	VAL	2.1
13	AM	26	GLY	2.1
33	CE	109	LEU	2.1
35	CG	161	GLY	2.1
23	C2	30	LYS	2.1
2	BB	162	PHE	2.1
7	AG	16	PRO	2.1
11	AK	17	SER	2.1
11	AK	50	SER	2.1
43	CP	79	ALA	2.1
47	CT	58	ALA	2.1
1	AA	1150	A	2.1
1	BA	4	U	2.1
9	AI	28	ILE	2.1
31	CA	1522	A	2.1
47	CT	4	ILE	2.1
2	AB	117	LEU	2.1
7	AG	102	ARG	2.1
9	BI	69	GLY	2.1
10	AJ	4	GLN	2.1
55	DA	895	U	2.1
12	AL	71	GLY	2.1
39	CL	55	GLY	2.1
50	CW	38	LEU	2.1
55	DA	2168	G	2.1
34	DF	84	PRO	2.1
11	AK	77	TYR	2.1
12	BL	117	TYR	2.1
47	CT	81	SER	2.1
7	AG	27	VAL	2.1
17	AQ	48	ASP	2.1
27	C0	44	ILE	2.1
35	CG	175	LYS	2.1
11	AK	100	LEU	2.1
24	C3	5	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
40	CM	67	THR	2.1
16	AP	48	GLU	2.1
18	AR	51	TYR	2.1
31	CA	2000	C	2.1
31	CA	2178	C	2.1
35	CG	156	PRO	2.1
22	C1	2	ALA	2.1
3	BC	149	ILE	2.1
14	AN	65	ARG	2.1
45	CR	6	ARG	2.1
45	CR	110	VAL	2.1
52	CY	35	SER	2.1
3	BC	18	TRP	2.1
12	BL	69	GLY	2.1
25	C4	21	GLY	2.1
42	CO	72	ASP	2.1
37	DJ	117	MET	2.1
1	AA	85	U	2.1
3	BC	37	PHE	2.1
15	BO	79	THR	2.1
36	DH	104	THR	2.1
42	CO	70	THR	2.1
1	AA	1004	A	2.1
1	AA	1170	A	2.1
31	CA	849	A	2.1
33	CE	21	ARG	2.1
35	CG	160	LYS	2.1
28	CB	4	C	2.1
31	CA	475	C	2.1
34	CF	13	VAL	2.1
34	DF	70	ALA	2.1
37	DJ	62	TYR	2.1
37	DJ	98	VAL	2.1
38	CK	20	ALA	2.1
1	AA	1273	C	2.1
14	AN	58	SER	2.1
1	AA	540	G	2.1
18	BR	68	LEU	2.1
5	AE	111	MET	2.1
12	AL	104	CYS	2.1
36	CH	135	HIS	2.1
47	CT	34	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
20	AT	54	MET	2.1
1	AA	218	U	2.1
16	BP	56	ARG	2.1
19	BS	3	ARG	2.1
30	CD	167	ASN	2.1
33	CE	197	GLU	2.1
40	CM	143	GLU	2.1
49	CV	92	LYS	2.1
8	AH	129	VAL	2.1
36	DH	84	ALA	2.1
43	CP	77	ALA	2.1
1	BA	1042	A	2.1
1	BA	1227	A	2.1
34	CF	111	ILE	2.1
13	AM	6	GLY	2.1
30	CD	87	GLY	2.1
40	CM	45	GLY	2.1
1	AA	1245	C	2.1
19	AS	56	GLN	2.0
4	AD	160	GLU	2.0
5	BE	112	ARG	2.0
35	CG	55	ARG	2.0
1	BA	1194	U	2.0
6	BF	89	VAL	2.0
39	CL	52	VAL	2.0
49	CV	64	ALA	2.0
2	AB	67	ILE	2.0
5	BE	105	ILE	2.0
45	CR	94	ILE	2.0
22	C1	35	GLY	2.0
41	CN	107	GLY	2.0
1	BA	1368	A	2.0
7	AG	9	GLN	2.0
30	CD	94	GLN	2.0
31	CA	213	A	2.0
31	CA	631	A	2.0
31	CA	2793	C	2.0
15	BO	75	VAL	2.0
21	BU	6	VAL	2.0
36	DH	56	ALA	2.0
46	CS	33	VAL	2.0
3	AC	174	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
7	AG	42	ILE	2.0
10	AJ	33	GLY	2.0
12	AL	73	ASN	2.0
27	C0	27	LEU	2.0
1	AA	107	G	2.0
31	CA	1108	U	2.0
31	CA	2526	G	2.0
33	CE	42	GLY	2.0
34	CF	72	LYS	2.0
36	CH	71	LYS	2.0
33	CE	44	ARG	2.0
44	CQ	103	ARG	2.0
8	AH	107	SER	2.0
18	BR	54	GLN	2.0
30	CD	36	GLN	2.0
3	BC	56	VAL	2.0
11	AK	16	VAL	2.0
16	BP	19	VAL	2.0
17	AQ	76	VAL	2.0
31	CA	902	C	2.0
31	CA	1531	C	2.0
49	CV	2	ALA	2.0
7	AG	88	PRO	2.0
37	DJ	75	PRO	2.0
42	CO	21	PHE	2.0
1	BA	992	U	2.0
2	BB	6	MET	2.0
31	CA	1729	U	2.0
50	CW	48	MET	2.0
1	AA	202	G	2.0
1	AA	1015	G	2.0
1	BA	941	G	2.0
1	BA	1385	G	2.0
14	AN	4	GLN	2.0
31	CA	1408	G	2.0
43	CP	98	GLN	2.0
2	BB	147	SER	2.0
7	BG	33	ASP	2.0
36	CH	128	HIS	2.0
49	CV	100	SER	2.0
3	BC	175	LEU	2.0
10	BJ	59	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
16	AP	4	ILE	2.0
19	AS	28	LYS	2.0
33	CE	98	LYS	2.0
45	CR	45	TYR	2.0
49	CV	14	LEU	2.0
31	CA	222	A	2.0
8	AH	93	PRO	2.0
31	CA	1868	C	2.0
39	CL	112	PHE	2.0
16	AP	29	ASN	2.0
48	DU	1	MET	2.0
1	AA	1224	U	2.0
1	BA	632	U	2.0
30	CD	204	LYS	2.0
31	CA	894	U	2.0
2	AB	196	VAL	2.0
3	AC	190	HIS	2.0
9	AI	61	LEU	2.0
12	BL	109	ASP	2.0
13	AM	82	ASP	2.0
46	CS	48	LYS	2.0
2	AB	60	ILE	2.0
40	CM	95	LEU	2.0
45	CR	113	ALA	2.0
1	BA	455	G	2.0
1	BA	587	G	2.0
1	BA	951	G	2.0
1	BA	1127	G	2.0
31	CA	407	G	2.0
31	CA	1016	G	2.0
49	CV	55	PRO	2.0
1	BA	532	A	2.0
45	CR	89	GLU	2.0
49	CV	60	GLU	2.0
1	AA	1037	C	2.0
1	BA	1226	C	2.0
16	AP	13	LYS	2.0
13	AM	3	ARG	2.0
15	BO	63	ARG	2.0
17	BQ	29	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	2MG	BA	966	24/25	0.43	0.57	258,264,268,268	0
1	5MC	BA	967	21/22	0.55	0.61	258,263,266,266	0
1	2MG	BA	1207	24/25	0.70	0.39	256,257,258,259	0
1	5MC	AA	967	21/22	0.75	0.28	214,216,219,220	0
1	2MG	AA	966	24/25	0.78	0.24	211,213,215,216	0
1	2MG	AA	1207	24/25	0.80	0.19	234,239,241,243	0
31	3TD	CA	1915	21/22	0.87	0.19	162,165,170,171	0
31	OMU	CA	2552	21/22	0.87	0.44	106,111,115,116	0
31	PSU	CA	746	20/21	0.90	0.19	135,137,142,142	0
1	PSU	BA	516	20/21	0.90	0.14	111,121,128,129	0
31	PSU	CA	1917	20/21	0.91	0.17	132,140,149,149	0
31	PSU	CA	955	20/21	0.91	0.17	126,130,135,136	0
31	PSU	CA	1911	20/21	0.92	0.14	152,158,159,161	0
31	OMC	CA	2498	21/22	0.92	0.29	116,124,130,132	0
31	5MU	CA	747	21/22	0.92	0.17	131,134,136,137	0
31	OMG	CA	2251	24/25	0.92	0.26	111,114,115,116	0
41	4D4	CN	81	12/13	0.92	0.42	118,121,132,133	0
31	PSU	CA	2504	20/21	0.93	0.21	106,114,117,120	0
1	MA6	BA	1518	24/25	0.93	0.24	91,97,102,103	0
1	2MG	BA	1516	24/25	0.93	0.19	105,110,116,117	0
31	2MA	CA	2503	23/24	0.94	0.23	117,126,137,138	0
31	6MZ	CA	1618	23/24	0.94	0.29	160,164,168,172	0
1	MA6	BA	1519	24/25	0.94	0.24	100,102,107,110	0
31	6MZ	CA	2030	23/24	0.94	0.19	117,125,134,134	0
31	7MG	CA	2069	24/25	0.94	0.20	104,111,124,124	0
31	2MG	CA	1835	24/25	0.94	0.21	100,103,106,110	0
1	4OC	BA	1402	22/23	0.94	0.19	111,116,127,128	0
12	D2T	BL	89	10/11	0.94	0.39	106,110,113,114	0
1	PSU	AA	516	20/21	0.94	0.15	135,138,139,141	0
31	1MG	CA	745	24/25	0.94	0.17	123,126,132,134	0
31	2MG	CA	2445	24/25	0.94	0.28	103,109,112,114	0
1	UR3	BA	1498	21/22	0.95	0.14	118,122,126,127	0
1	5MC	BA	1407	21/22	0.95	0.14	111,121,124,125	0
12	D2T	AL	89	10/11	0.95	0.29	109,114,125,128	0
55	PSU	DA	1911	20/21	0.95	0.14	107,118,120,121	0
1	7MG	BA	527	24/25	0.95	0.18	100,108,118,120	0
31	PSU	CA	2580	20/21	0.95	0.18	118,125,130,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	5MU	CA	1939	21/22	0.95	0.17	95,99,105,107	0
31	PSU	CA	2457	20/21	0.96	0.19	118,122,126,127	0
1	4OC	AA	1402	22/23	0.96	0.17	94,99,103,104	0
55	3TD	DA	1915	21/22	0.96	0.12	133,140,146,147	0
1	5MC	AA	1407	21/22	0.96	0.16	80,88,90,91	0
31	PSU	CA	2605	20/21	0.96	0.17	97,101,106,106	0
1	2MG	AA	1516	24/25	0.96	0.17	74,82,84,86	0
55	2MG	DA	1835	24/25	0.96	0.21	59,65,71,72	0
1	7MG	AA	527	24/25	0.96	0.16	102,109,115,118	0
31	5MC	CA	1962	21/22	0.96	0.20	103,106,110,112	0
1	MA6	AA	1518	24/25	0.97	0.16	67,77,81,85	0
1	MA6	AA	1519	24/25	0.97	0.20	72,76,80,81	0
55	PSU	DA	1917	20/21	0.97	0.13	109,113,119,119	0
1	UR3	AA	1498	21/22	0.97	0.18	86,92,97,100	0
41	4D4	DN	81[B]	12/13	0.98	0.23	37,45,50,50	9
55	5MC	DA	1962	21/22	0.98	0.19	46,61,65,66	0
41	4D4	DN	81[A]	12/13	0.98	0.23	49,59,65,66	9
55	PSU	DA	2605	20/21	0.98	0.17	51,59,64,65	0
55	PSU	DA	2504	20/21	0.98	0.19	50,51,54,56	0
55	2MG	DA	2445	24/25	0.99	0.20	39,45,50,62	0
55	OMC	DA	2498	21/22	0.99	0.21	37,39,46,47	0
55	6MZ	DA	1618	23/24	0.99	0.20	34,42,47,49	0
55	1MG	DA	745	24/25	0.99	0.19	31,37,42,44	0
32	MEQ	DD	150[B]	10/11	0.99	0.28	35,38,44,45	10
55	5MU	DA	747	21/22	0.99	0.19	41,43,52,58	0
55	PSU	DA	2457	20/21	0.99	0.18	44,46,52,53	0
55	6MZ	DA	2030	23/24	0.99	0.20	27,33,38,40	0
55	5MU	DA	1939	21/22	0.99	0.20	53,58,65,69	0
55	PSU	DA	2604	20/21	0.99	0.17	58,63,70,72	0
55	PSU	DA	2580	20/21	0.99	0.20	30,35,41,43	0
55	7MG	DA	2069	24/25	0.99	0.18	41,48,53,53	0
55	OMU	DA	2552	21/22	0.99	0.21	45,48,52,57	0
32	MEQ	DD	150[A]	10/11	0.99	0.28	31,32,37,37	10
55	OMG	DA	2251	24/25	0.99	0.18	29,48,54,62	0
55	PSU	DA	955	20/21	0.99	0.19	32,35,39,41	0
55	2MA	DA	2503	23/24	0.99	0.21	44,51,58,62	0
55	H2U	DA	2449	20/21	0.99	0.23	33,39,46,46	0
55	PSU	DA	746	20/21	1.00	0.18	38,44,46,47	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	CA	3132	1/1	0.17	0.62	157,157,157,157	0
56	MG	CA	3139	1/1	0.17	0.83	140,140,140,140	0
56	MG	BA	1624	1/1	0.17	2.21	293,293,293,293	0
56	MG	AA	1628	1/1	0.23	0.26	137,137,137,137	0
56	MG	AA	1622	1/1	0.24	0.84	106,106,106,106	0
56	MG	AA	1627	1/1	0.27	1.21	115,115,115,115	0
56	MG	DA	3130	1/1	0.27	0.89	109,109,109,109	0
56	MG	BA	1637	1/1	0.28	0.54	121,121,121,121	0
59	PUT	AA	1675	6/6	0.36	0.61	172,174,174,175	0
56	MG	CA	3154	1/1	0.38	0.71	110,110,110,110	0
56	MG	CA	3124	1/1	0.40	0.28	159,159,159,159	0
56	MG	CA	3061	1/1	0.42	0.20	270,270,270,270	0
56	MG	CA	3104	1/1	0.46	0.46	249,249,249,249	0
56	MG	CA	3007	1/1	0.47	0.66	257,257,257,257	0
61	PEG	DQ	201	7/7	0.51	0.82	162,166,170,170	0
56	MG	DA	3168	1/1	0.51	0.54	119,119,119,119	0
56	MG	AA	1603	1/1	0.52	0.67	111,111,111,111	0
56	MG	AA	1616	1/1	0.52	0.69	105,105,105,105	0
59	PUT	AA	1672	6/6	0.53	0.30	149,150,150,150	0
56	MG	CA	3075	1/1	0.54	1.12	231,231,231,231	0
56	MG	AA	1618	1/1	0.54	0.11	172,172,172,172	0
56	MG	DA	3156	1/1	0.55	0.69	83,83,83,83	0
56	MG	DA	3152	1/1	0.56	0.27	115,115,115,115	0
56	MG	CA	3126	1/1	0.57	0.35	115,115,115,115	0
56	MG	DA	3137	1/1	0.59	0.34	61,61,61,61	0
56	MG	CA	3145	1/1	0.60	0.98	78,78,78,78	0
56	MG	DA	3163	1/1	0.60	0.52	87,87,87,87	0
56	MG	CA	3105	1/1	0.61	0.18	252,252,252,252	0
56	MG	CA	3135	1/1	0.61	0.48	78,78,78,78	0
57	PG4	DR	201	13/13	0.61	0.34	156,168,173,173	0
56	MG	AA	1660	1/1	0.62	0.53	283,283,283,283	0
56	MG	BA	1623	1/1	0.62	0.86	277,277,277,277	0
56	MG	AA	1623	1/1	0.63	0.77	87,87,87,87	0
56	MG	AA	1621	1/1	0.64	0.50	97,97,97,97	0
61	PEG	AL	201	7/7	0.64	0.30	132,133,135,136	0
61	PEG	D3	102	7/7	0.66	1.33	136,138,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1615	1/1	0.68	0.67	129,129,129,129	0
58	MPD	DE	301	8/8	0.69	1.05	172,174,179,179	0
56	MG	CA	3056	1/1	0.69	0.48	77,77,77,77	0
61	PEG	DP	201	7/7	0.69	0.69	149,153,164,165	0
68	TRS	DA	3220	8/8	0.69	0.80	184,187,190,191	0
56	MG	DA	3147	1/1	0.69	0.29	108,108,108,108	0
56	MG	CA	3140	1/1	0.69	0.54	108,108,108,108	0
59	PUT	DA	3195	6/6	0.69	0.44	100,104,108,108	0
56	MG	AA	1626	1/1	0.70	0.95	120,120,120,120	0
64	SPD	DA	3206	10/10	0.71	0.23	142,143,144,144	0
62	EDO	DA	3002	4/4	0.71	0.61	176,176,176,177	0
56	MG	DA	3182	1/1	0.71	0.43	55,55,55,55	0
56	MG	BA	1626	1/1	0.72	0.91	255,255,255,255	0
61	PEG	DA	3200	7/7	0.72	0.35	124,124,125,125	0
56	MG	CA	3026	1/1	0.73	1.05	245,245,245,245	0
62	EDO	DA	3198	4/4	0.73	0.43	109,110,112,112	0
58	MPD	DT	202	8/8	0.75	0.37	138,139,144,145	0
56	MG	CA	3116	1/1	0.75	0.41	92,92,92,92	0
56	MG	CA	3113	1/1	0.76	0.44	76,76,76,76	0
56	MG	DA	3162	1/1	0.76	0.30	79,79,79,79	0
56	MG	AA	1665	1/1	0.76	0.71	274,274,274,274	0
56	MG	CA	3092	1/1	0.76	0.08	163,163,163,163	0
62	EDO	DB	210	4/4	0.76	0.39	125,126,126,127	0
56	MG	AA	1604	1/1	0.77	0.66	79,79,79,79	0
61	PEG	DA	3218	7/7	0.77	0.28	179,180,181,181	0
56	MG	BA	1625	1/1	0.77	0.77	288,288,288,288	0
56	MG	AA	1625	1/1	0.77	0.58	83,83,83,83	0
59	PUT	AA	1673	6/6	0.77	0.67	142,145,148,150	0
56	MG	CA	3022	1/1	0.78	0.71	259,259,259,259	0
56	MG	CA	3077	1/1	0.78	0.44	244,244,244,244	0
56	MG	CA	3055	1/1	0.78	0.11	193,193,193,193	0
59	PUT	AA	1674	6/6	0.79	0.77	109,113,116,117	0
56	MG	AA	1659	1/1	0.79	0.33	273,273,273,273	0
56	MG	AA	1605	1/1	0.79	0.52	87,87,87,87	0
56	MG	CA	3123	1/1	0.80	0.69	142,142,142,142	0
56	MG	CA	3122	1/1	0.80	0.53	89,89,89,89	0
56	MG	DA	3170	1/1	0.80	0.18	59,59,59,59	0
56	MG	DA	3123	1/1	0.80	0.36	84,84,84,84	0
62	EDO	DA	3003	4/4	0.80	0.28	135,137,140,141	0
56	MG	CA	3130	1/1	0.80	0.13	84,84,84,84	0
56	MG	BA	1635	1/1	0.80	0.16	209,209,209,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1602	1/1	0.80	0.44	78,78,78,78	0
56	MG	CA	3009	1/1	0.80	0.15	259,259,259,259	0
56	MG	DA	3134	1/1	0.81	0.60	98,98,98,98	0
56	MG	BA	1638	1/1	0.81	0.44	65,65,65,65	0
56	MG	CA	3006	1/1	0.81	0.10	221,221,221,221	0
57	PG4	AA	1670	13/13	0.81	0.26	111,116,118,119	0
63	PGE	DA	3225	10/10	0.81	0.39	100,120,131,131	0
61	PEG	DA	3201	7/7	0.81	0.47	146,150,151,152	0
56	MG	CA	3080	1/1	0.81	0.11	108,108,108,108	0
56	MG	DA	3155	1/1	0.81	0.41	86,86,86,86	0
59	PUT	DA	3221	6/6	0.82	0.46	112,120,122,122	0
63	PGE	D3	101	10/10	0.82	0.54	121,123,125,126	0
56	MG	AA	1663	1/1	0.82	0.24	230,230,230,230	0
56	MG	DA	3148	1/1	0.82	0.22	67,67,67,67	0
59	PUT	DA	3213	6/6	0.82	0.27	156,156,157,157	0
56	MG	AA	1610	1/1	0.82	0.28	99,99,99,99	0
56	MG	CA	3093	1/1	0.82	0.16	143,143,143,143	0
56	MG	CA	3034	1/1	0.82	0.14	228,228,228,228	0
56	MG	CA	3151	1/1	0.82	0.54	102,102,102,102	0
56	MG	AA	1620	1/1	0.82	0.80	116,116,116,116	0
56	MG	BA	1606	1/1	0.83	0.17	270,270,270,270	0
56	MG	AA	1624	1/1	0.83	0.30	82,82,82,82	0
63	PGE	D1	102	10/10	0.83	0.36	142,145,152,153	0
62	EDO	DA	3194	4/4	0.83	0.31	89,90,90,90	0
58	MPD	DK	201	8/8	0.83	0.27	125,126,127,127	0
56	MG	DA	3178	1/1	0.83	0.33	93,93,93,93	0
56	MG	DA	3176	1/1	0.84	0.31	81,81,81,81	0
56	MG	CA	3071	1/1	0.84	0.35	228,228,228,228	0
61	PEG	DA	3199	7/7	0.84	0.46	99,106,112,113	0
56	MG	AA	1642	1/1	0.84	0.77	275,275,275,275	0
56	MG	DA	3154	1/1	0.84	0.35	60,60,60,60	0
56	MG	CA	3125	1/1	0.84	0.28	136,136,136,136	0
57	PG4	DQ	202	13/13	0.84	0.26	84,89,100,101	0
61	PEG	DA	3227	7/7	0.84	0.34	109,114,120,120	0
56	MG	DA	3157	1/1	0.84	0.26	74,74,74,74	0
56	MG	AA	1601	1/1	0.84	0.75	62,62,62,62	0
56	MG	CA	3119	1/1	0.84	0.37	100,100,100,100	0
59	PUT	DA	3212	6/6	0.85	0.22	114,115,117,117	0
58	MPD	DA	3204	8/8	0.85	0.61	116,119,125,127	0
56	MG	BA	1630	1/1	0.85	0.07	197,197,197,197	0
56	MG	CA	3110	1/1	0.85	0.35	129,129,129,129	0
56	MG	BA	1604	1/1	0.85	0.49	257,257,257,257	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	1641	1/1	0.85	0.37	140,140,140,140	0
56	MG	CA	3094	1/1	0.86	0.11	132,132,132,132	0
63	PGE	DU	201	10/10	0.86	0.45	135,141,147,147	0
56	MG	CA	3146	1/1	0.86	0.10	174,174,174,174	0
63	PGE	DA	3214	10/10	0.86	0.60	67,87,91,92	0
56	MG	DA	3158	1/1	0.86	0.49	107,107,107,107	0
59	PUT	DA	3219	6/6	0.86	0.29	100,102,103,103	0
56	MG	AA	1609	1/1	0.86	0.55	107,107,107,107	0
56	MG	BA	1634	1/1	0.86	0.10	216,216,216,216	0
56	MG	CA	3019	1/1	0.86	0.21	87,87,87,87	0
56	MG	CA	3067	1/1	0.86	0.21	274,274,274,274	0
58	MPD	AA	1676	8/8	0.86	0.63	145,146,148,148	0
56	MG	CA	3142	1/1	0.86	0.17	102,102,102,102	0
56	MG	DA	3160	1/1	0.86	0.36	64,64,64,64	0
56	MG	CA	3128	1/1	0.86	0.35	116,116,116,116	0
56	MG	DA	3171	1/1	0.86	0.82	111,111,111,111	0
56	MG	CA	3131	1/1	0.87	0.34	123,123,123,123	0
61	PEG	DA	3226	7/7	0.87	0.32	125,126,131,131	0
56	MG	CA	3156	1/1	0.87	0.16	263,263,263,263	0
58	MPD	DT	201	8/8	0.87	0.31	110,115,125,126	0
63	PGE	DS	201	10/10	0.87	0.34	96,99,101,101	0
56	MG	CB	201	1/1	0.87	0.06	235,235,235,235	0
56	MG	CA	3060	1/1	0.87	0.42	238,238,238,238	0
56	MG	AA	1677	1/1	0.87	0.08	101,101,101,101	0
56	MG	CA	3133	1/1	0.87	0.32	110,110,110,110	0
56	MG	CA	3118	1/1	0.87	0.52	87,87,87,87	0
56	MG	CA	3001	1/1	0.87	0.30	291,291,291,291	0
62	EDO	DA	3215	4/4	0.88	0.32	64,67,70,73	0
56	MG	CA	3021	1/1	0.88	1.30	253,253,253,253	0
61	PEG	DL	201	7/7	0.88	0.31	102,103,109,110	0
56	MG	CA	3072	1/1	0.88	1.07	258,258,258,258	0
56	MG	CA	3111	1/1	0.88	0.29	103,103,103,103	0
57	PG4	DA	3193	13/13	0.88	0.96	109,113,119,120	0
56	MG	BA	1636	1/1	0.88	0.47	77,77,77,77	0
56	MG	DA	3128	1/1	0.88	1.11	57,57,57,57	0
58	MPD	DA	3190	8/8	0.89	0.31	100,102,103,106	0
58	MPD	DA	3207	8/8	0.89	0.44	121,125,128,129	0
57	PG4	BA	1642	13/13	0.89	0.45	113,117,132,132	0
57	PG4	DA	3216	13/13	0.89	0.28	111,122,132,134	0
56	MG	CA	3141	1/1	0.89	0.22	78,78,78,78	0
56	MG	AA	1606	1/1	0.89	0.14	124,124,124,124	0
56	MG	CA	3054	1/1	0.89	0.12	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3014	1/1	0.89	0.19	273,273,273,273	0
56	MG	BA	1612	1/1	0.89	0.22	262,262,262,262	0
56	MG	AA	1656	1/1	0.89	0.11	274,274,274,274	0
56	MG	CA	3030	1/1	0.89	0.09	82,82,82,82	0
56	MG	CA	3048	1/1	0.89	0.16	147,147,147,147	0
56	MG	DA	3129	1/1	0.89	0.22	51,51,51,51	0
56	MG	DA	3133	1/1	0.89	0.26	52,52,52,52	0
56	MG	DA	3180	1/1	0.89	0.80	77,77,77,77	0
63	PGE	DD	301	10/10	0.89	0.31	120,122,129,130	0
56	MG	AA	1654	1/1	0.89	0.14	178,178,178,178	0
56	MG	CA	3107	1/1	0.90	0.34	81,81,81,81	0
56	MG	AA	1661	1/1	0.90	0.68	223,223,223,223	0
56	MG	BA	1619	1/1	0.90	0.48	228,228,228,228	0
63	PGE	DA	3217	10/10	0.90	0.34	87,89,93,94	0
56	MG	DA	3172	1/1	0.90	0.38	85,85,85,85	0
56	MG	DA	3124	1/1	0.90	0.52	90,90,90,90	0
57	PG4	DS	202	13/13	0.90	0.31	72,73,85,86	0
56	MG	CA	3147	1/1	0.90	0.25	36,36,36,36	1
56	MG	DA	3098	1/1	0.90	0.21	246,246,246,246	0
56	MG	CA	3148	1/1	0.90	0.42	43,43,43,43	1
56	MG	DA	3161	1/1	0.90	0.22	73,73,73,73	0
56	MG	DA	3165	1/1	0.90	0.27	63,63,63,63	0
56	MG	CA	3008	1/1	0.90	0.09	202,202,202,202	0
58	MPD	DN	201	8/8	0.91	0.35	109,117,119,121	0
62	EDO	D1	101	4/4	0.91	0.23	70,71,73,75	0
56	MG	DA	3153	1/1	0.91	0.28	102,102,102,102	0
56	MG	BA	1603	1/1	0.91	0.21	278,278,278,278	0
56	MG	BA	1629	1/1	0.91	1.35	217,217,217,217	0
56	MG	CA	3047	1/1	0.91	0.26	100,100,100,100	0
56	MG	CA	3052	1/1	0.91	0.07	124,124,124,124	0
56	MG	CA	3137	1/1	0.91	0.31	164,164,164,164	0
56	MG	AA	1613	1/1	0.91	0.62	80,80,80,80	0
56	MG	AA	1647	1/1	0.91	0.30	145,145,145,145	0
56	MG	DA	3125	1/1	0.91	0.22	51,51,51,51	0
56	MG	CA	3138	1/1	0.91	0.12	98,98,98,98	0
62	EDO	DA	3209	4/4	0.91	0.62	94,96,98,99	0
56	MG	CA	3057	1/1	0.91	0.14	111,111,111,111	0
58	MPD	AA	1671	8/8	0.91	0.70	143,144,147,148	0
56	MG	DA	3001	1/1	0.91	0.45	47,47,47,47	0
67	GUN	DA	3211	11/11	0.91	0.26	116,122,123,124	0
56	MG	AA	1658	1/1	0.91	0.34	212,212,212,212	0
64	SPD	DA	3224	10/10	0.91	0.30	58,71,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3070	1/1	0.91	0.31	234,234,234,234	0
56	MG	AA	1614	1/1	0.92	0.13	83,83,83,83	0
56	MG	CA	3053	1/1	0.92	0.11	86,86,86,86	0
56	MG	CA	3121	1/1	0.92	0.23	83,83,83,83	0
59	PUT	DA	3222	6/6	0.92	0.31	77,81,83,83	0
56	MG	CA	3064	1/1	0.92	0.29	271,271,271,271	0
59	PUT	DA	3184	6/6	0.92	0.43	65,70,74,74	0
56	MG	CA	3028	1/1	0.92	0.80	284,284,284,284	0
59	PUT	DA	3205	6/6	0.92	0.30	106,108,108,109	0
56	MG	CA	3038	1/1	0.92	0.17	252,252,252,252	0
56	MG	CA	3039	1/1	0.92	0.58	190,190,190,190	0
56	MG	DA	3131	1/1	0.92	0.24	83,83,83,83	0
56	MG	CA	3083	1/1	0.92	0.35	254,254,254,254	0
56	MG	CA	3117	1/1	0.92	0.13	59,59,59,59	0
56	MG	AA	1612	1/1	0.92	0.36	77,77,77,77	0
56	MG	DA	3138	1/1	0.92	0.34	29,29,29,29	1
56	MG	CA	3149	1/1	0.92	0.44	76,76,76,76	0
56	MG	CA	3090	1/1	0.92	0.16	187,187,187,187	0
56	MG	CA	3120	1/1	0.92	0.13	130,130,130,130	0
56	MG	DB	206	1/1	0.92	0.31	73,73,73,73	0
56	MG	CA	3032	1/1	0.92	0.35	197,197,197,197	0
65	1PE	DA	3203	16/16	0.92	0.30	98,105,109,109	0
56	MG	CB	203	1/1	0.92	0.15	237,237,237,237	0
56	MG	CA	3002	1/1	0.92	0.15	224,224,224,224	0
62	EDO	D0	101	4/4	0.92	0.26	79,80,85,89	0
58	MPD	DA	3210	8/8	0.92	0.30	110,118,123,125	0
56	MG	CA	3096	1/1	0.92	0.08	89,89,89,89	0
56	MG	BA	1639	1/1	0.92	0.27	117,117,117,117	0
56	MG	CA	3152	1/1	0.92	0.16	160,160,160,160	0
56	MG	CA	3059	1/1	0.92	0.10	118,118,118,118	0
56	MG	CA	3099	1/1	0.93	0.12	174,174,174,174	0
56	MG	CA	3018	1/1	0.93	0.10	147,147,147,147	0
56	MG	DA	3126	1/1	0.93	0.31	77,77,77,77	0
56	MG	CA	3010	1/1	0.93	0.10	259,259,259,259	0
56	MG	DA	3143	1/1	0.93	0.31	63,63,63,63	0
56	MG	CA	3068	1/1	0.93	0.26	174,174,174,174	0
56	MG	AA	1638	1/1	0.93	0.14	142,142,142,142	0
56	MG	CA	3155	1/1	0.93	0.26	181,181,181,181	0
56	MG	CA	3036	1/1	0.93	0.15	227,227,227,227	0
56	MG	BA	1627	1/1	0.93	0.68	203,203,203,203	0
58	MPD	DE	302	8/8	0.93	0.41	101,102,103,104	0
56	MG	DA	3062	1/1	0.93	0.28	269,269,269,269	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3087	1/1	0.93	0.17	232,232,232,232	0
56	MG	CA	3134	1/1	0.93	0.12	167,167,167,167	0
56	MG	DA	3144	1/1	0.93	0.63	79,79,79,79	0
62	EDO	DA	3197	4/4	0.93	0.29	75,76,77,77	0
64	SPD	DA	3183	10/10	0.93	0.45	80,95,97,98	0
59	PUT	DA	3188	6/6	0.93	0.20	89,93,93,94	0
56	MG	CA	3109	1/1	0.93	0.34	67,67,67,67	0
56	MG	CA	3129	1/1	0.93	0.13	135,135,135,135	0
56	MG	DA	3146	1/1	0.93	0.28	76,76,76,76	0
60	ZN	C5	101	1/1	0.93	0.07	175,175,175,175	0
56	MG	DA	3121	1/1	0.94	0.53	111,111,111,111	0
56	MG	CA	3136	1/1	0.94	0.24	107,107,107,107	0
56	MG	AA	1617	1/1	0.94	0.21	88,88,88,88	0
56	MG	CA	3040	1/1	0.94	0.13	122,122,122,122	0
56	MG	BA	1610	1/1	0.94	0.07	107,107,107,107	0
56	MG	CA	3106	1/1	0.94	0.13	74,74,74,74	0
56	MG	AA	1662	1/1	0.94	0.20	164,164,164,164	0
56	MG	DA	3179	1/1	0.94	1.13	85,85,85,85	0
56	MG	AA	1641	1/1	0.94	0.06	122,122,122,122	0
56	MG	CA	3062	1/1	0.94	0.11	168,168,168,168	0
56	MG	DA	3132	1/1	0.94	0.21	56,56,56,56	0
56	MG	CA	3066	1/1	0.94	0.11	91,91,91,91	0
56	MG	CA	3003	1/1	0.94	1.80	272,272,272,272	0
56	MG	AA	1611	1/1	0.94	0.15	133,133,133,133	0
56	MG	CA	3084	1/1	0.94	0.21	172,172,172,172	0
56	MG	CA	3031	1/1	0.94	0.19	128,128,128,128	0
56	MG	CA	3085	1/1	0.94	0.08	116,116,116,116	0
56	MG	AA	1608	1/1	0.94	0.36	128,128,128,128	0
64	SPD	DA	3187	10/10	0.94	0.26	78,82,85,85	0
65	1PE	DA	3185	16/16	0.94	0.21	74,89,123,123	0
56	MG	BA	1633	1/1	0.94	0.55	237,237,237,237	0
56	MG	DB	207	1/1	0.94	0.77	92,92,92,92	0
56	MG	BA	1620	1/1	0.94	0.12	172,172,172,172	0
56	MG	DB	204	1/1	0.94	0.16	85,85,85,85	0
56	MG	DA	3145	1/1	0.95	0.20	45,45,45,45	0
56	MG	AA	1634	1/1	0.95	0.33	179,179,179,179	0
56	MG	DA	3079	1/1	0.95	0.32	179,179,179,179	0
56	MG	CA	3004	1/1	0.95	0.11	192,192,192,192	0
56	MG	BA	1616	1/1	0.95	0.12	151,151,151,151	0
63	PGE	DA	3186	10/10	0.95	0.20	58,65,71,71	0
59	PUT	DA	3189	6/6	0.95	0.25	49,55,59,62	0
59	PUT	DM	201	6/6	0.95	0.21	63,66,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1653	1/1	0.95	0.06	108,108,108,108	0
56	MG	DA	3118	1/1	0.95	0.10	31,31,31,31	0
66	ACY	DA	3191	4/4	0.95	0.25	79,80,81,81	0
56	MG	CA	3114	1/1	0.95	0.31	67,67,67,67	0
56	MG	DA	3141	1/1	0.95	0.41	80,80,80,80	0
60	ZN	AB	301	1/1	0.95	0.04	165,165,165,165	0
56	MG	CA	3029	1/1	0.95	0.17	143,143,143,143	0
56	MG	CA	3046	1/1	0.95	0.13	99,99,99,99	0
56	MG	DA	3080	1/1	0.95	0.10	195,195,195,195	0
56	MG	DA	3164	1/1	0.95	0.26	78,78,78,78	0
58	MPD	DA	3192	8/8	0.95	0.57	84,90,92,94	0
56	MG	CA	3101	1/1	0.95	0.12	239,239,239,239	0
56	MG	AA	1619	1/1	0.95	0.54	122,122,122,122	0
56	MG	DB	205	1/1	0.95	0.66	148,148,148,148	0
56	MG	CA	3058	1/1	0.95	0.14	124,124,124,124	0
56	MG	AA	1637	1/1	0.95	0.15	106,106,106,106	0
56	MG	DA	3033	1/1	0.95	0.13	46,46,46,46	0
56	MG	CA	3023	1/1	0.95	0.39	255,255,255,255	0
56	MG	AA	1607	1/1	0.95	0.47	90,90,90,90	0
56	MG	AA	1657	1/1	0.95	0.46	134,134,134,134	0
56	MG	CA	3108	1/1	0.96	0.23	89,89,89,89	0
56	MG	CA	3020	1/1	0.96	0.15	116,116,116,116	0
56	MG	CA	3153	1/1	0.96	0.20	77,77,77,77	0
56	MG	DA	3007	1/1	0.96	0.09	127,127,127,127	0
56	MG	CA	3150	1/1	0.96	0.77	79,79,79,79	0
56	MG	AA	1664	1/1	0.96	0.71	265,265,265,265	0
56	MG	AA	1630	1/1	0.96	0.20	205,205,205,205	0
56	MG	AA	1648	1/1	0.96	0.05	84,84,84,84	0
56	MG	DA	3177	1/1	0.96	0.36	52,52,52,52	0
56	MG	AA	1668	1/1	0.96	0.13	110,110,110,110	0
56	MG	DA	3142	1/1	0.96	0.26	80,80,80,80	0
56	MG	AA	1635	1/1	0.96	0.14	220,220,220,220	0
56	MG	CA	3112	1/1	0.96	0.36	103,103,103,103	0
56	MG	DA	3008	1/1	0.96	0.12	280,280,280,280	0
56	MG	DB	209	1/1	0.96	0.15	83,83,83,83	0
56	MG	CA	3097	1/1	0.96	0.14	112,112,112,112	0
56	MG	DA	3174	1/1	0.96	0.23	87,87,87,87	0
56	MG	CA	3065	1/1	0.96	0.15	115,115,115,115	0
56	MG	DA	3095	1/1	0.96	0.14	65,65,65,65	0
56	MG	AA	1640	1/1	0.96	0.10	131,131,131,131	0
56	MG	DB	201	1/1	0.96	0.11	121,121,121,121	0
62	EDO	DB	211	4/4	0.96	0.22	131,131,132,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3143	1/1	0.96	0.14	72,72,72,72	0
56	MG	DA	3175	1/1	0.96	0.60	115,115,115,115	0
56	MG	CA	3082	1/1	0.96	0.26	168,168,168,168	0
56	MG	BA	1607	1/1	0.96	0.24	280,280,280,280	0
56	MG	CA	3050	1/1	0.96	0.18	166,166,166,166	0
56	MG	BA	1617	1/1	0.96	0.12	165,165,165,165	0
66	ACY	DA	3196	4/4	0.96	0.24	61,69,69,72	0
56	MG	CA	3051	1/1	0.96	0.39	248,248,248,248	0
56	MG	BA	1622	1/1	0.96	0.10	240,240,240,240	0
56	MG	DA	3120	1/1	0.96	0.55	66,66,66,66	0
56	MG	CA	3103	1/1	0.96	0.15	176,176,176,176	0
56	MG	BA	1609	1/1	0.96	0.14	156,156,156,156	0
56	MG	DA	3044	1/1	0.97	0.08	124,124,124,124	0
56	MG	DA	3149	1/1	0.97	0.24	96,96,96,96	0
56	MG	CA	3073	1/1	0.97	0.23	139,139,139,139	0
56	MG	CA	3005	1/1	0.97	0.37	233,233,233,233	0
56	MG	CA	3127	1/1	0.97	0.14	73,73,73,73	0
56	MG	BA	1631	1/1	0.97	0.11	132,132,132,132	0
56	MG	DA	3097	1/1	0.97	0.11	75,75,75,75	0
56	MG	DA	3012	1/1	0.97	0.14	141,141,141,141	0
56	MG	CA	3033	1/1	0.97	0.09	150,150,150,150	0
56	MG	BA	1618	1/1	0.97	0.22	172,172,172,172	0
56	MG	DA	3166	1/1	0.97	0.34	74,74,74,74	0
56	MG	CA	3016	1/1	0.97	0.90	218,218,218,218	0
56	MG	AA	1655	1/1	0.97	0.08	152,152,152,152	0
56	MG	DD	302	1/1	0.97	0.22	62,62,62,62	0
56	MG	BA	1628	1/1	0.97	0.15	120,120,120,120	0
56	MG	CA	3095	1/1	0.97	0.12	174,174,174,174	0
56	MG	AA	1649	1/1	0.97	0.06	111,111,111,111	0
59	PUT	DA	3223	6/6	0.97	0.19	75,81,84,84	0
56	MG	BA	1602	1/1	0.97	0.11	102,102,102,102	0
56	MG	DA	3122	1/1	0.97	0.28	48,48,48,48	0
56	MG	DR	202	1/1	0.97	0.30	269,269,269,269	0
66	ACY	DA	3202	4/4	0.97	0.19	93,96,96,97	0
56	MG	BA	1601	1/1	0.97	0.22	135,135,135,135	0
56	MG	CA	3012	1/1	0.97	0.14	115,115,115,115	0
56	MG	DA	3139	1/1	0.97	0.13	42,42,42,42	0
56	MG	CA	3115	1/1	0.97	0.30	111,111,111,111	0
56	MG	CA	3027	1/1	0.97	0.21	88,88,88,88	0
56	MG	CA	3063	1/1	0.97	0.13	155,155,155,155	0
56	MG	CA	3017	1/1	0.97	0.12	192,192,192,192	0
56	MG	CA	3081	1/1	0.97	0.16	254,254,254,254	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1650	1/1	0.97	0.13	115,115,115,115	0
56	MG	DA	3167	1/1	0.97	0.43	97,97,97,97	0
56	MG	CA	3079	1/1	0.97	0.28	131,131,131,131	0
62	EDO	DA	3208	4/4	0.97	0.21	111,113,113,113	0
56	MG	DA	3135	1/1	0.97	0.17	146,146,146,146	0
56	MG	AA	1645	1/1	0.97	0.13	70,70,70,70	0
56	MG	DA	3173	1/1	0.97	0.87	100,100,100,100	0
56	MG	DA	3117	1/1	0.97	0.12	70,70,70,70	0
56	MG	CA	3091	1/1	0.97	0.09	81,81,81,81	0
56	MG	AA	1632	1/1	0.97	0.10	162,162,162,162	0
56	MG	DA	3099	1/1	0.97	0.19	45,45,45,45	0
56	MG	DA	3181	1/1	0.97	0.29	66,66,66,66	0
56	MG	CA	3078	1/1	0.98	0.30	198,198,198,198	0
56	MG	CA	3025	1/1	0.98	0.13	133,133,133,133	0
56	MG	CA	3074	1/1	0.98	0.10	145,145,145,145	0
56	MG	CA	3037	1/1	0.98	0.27	234,234,234,234	0
56	MG	CA	3069	1/1	0.98	0.14	107,107,107,107	0
56	MG	DA	3054	1/1	0.98	0.17	167,167,167,167	0
56	MG	CA	3049	1/1	0.98	0.12	53,53,53,53	0
56	MG	DA	3048	1/1	0.98	0.12	59,59,59,59	0
56	MG	AA	1652	1/1	0.98	0.26	42,42,42,42	0
56	MG	DA	3108	1/1	0.98	0.08	36,36,36,36	0
56	MG	DA	3030	1/1	0.98	0.20	88,88,88,88	0
56	MG	DA	3004	1/1	0.98	0.14	149,149,149,149	0
56	MG	CA	3044	1/1	0.98	0.17	113,113,113,113	0
56	MG	DA	3085	1/1	0.98	0.14	100,100,100,100	0
56	MG	BA	1605	1/1	0.98	0.08	136,136,136,136	0
56	MG	DA	3127	1/1	0.98	0.45	69,69,69,69	0
56	MG	CA	3024	1/1	0.98	0.06	85,85,85,85	0
56	MG	BA	1611	1/1	0.98	0.13	84,84,84,84	0
56	MG	CA	3015	1/1	0.98	0.22	84,84,84,84	0
56	MG	AA	1667	1/1	0.98	0.14	76,76,76,76	0
56	MG	DA	3231	1/1	0.98	0.26	70,70,70,70	0
56	MG	DA	3094	1/1	0.98	0.19	29,29,29,29	0
56	MG	DA	3031	1/1	0.98	0.16	51,51,51,51	0
56	MG	CA	3042	1/1	0.98	0.06	96,96,96,96	0
56	MG	DA	3067	1/1	0.98	0.11	75,75,75,75	0
56	MG	DA	3071	1/1	0.98	0.08	56,56,56,56	0
56	MG	BA	1608	1/1	0.98	0.19	144,144,144,144	0
56	MG	DA	3111	1/1	0.98	0.47	283,283,283,283	0
56	MG	BA	1614	1/1	0.98	0.14	217,217,217,217	0
56	MG	CA	3100	1/1	0.98	0.25	243,243,243,243	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3011	1/1	0.98	0.17	95,95,95,95	0
56	MG	DA	3115	1/1	0.98	0.20	52,52,52,52	0
56	MG	CA	3144	1/1	0.98	0.06	66,66,66,66	0
56	MG	DA	3151	1/1	0.98	0.26	48,48,48,48	0
56	MG	AA	1643	1/1	0.98	0.14	70,70,70,70	0
56	MG	DA	3053	1/1	0.98	0.10	54,54,54,54	0
56	MG	AA	1639	1/1	0.98	0.50	225,225,225,225	0
56	MG	DA	3043	1/1	0.98	0.14	40,40,40,40	0
56	MG	AA	1631	1/1	0.98	0.09	75,75,75,75	0
56	MG	AA	1636	1/1	0.98	0.39	209,209,209,209	0
56	MG	DA	3150	1/1	0.98	0.08	72,72,72,72	0
56	MG	CA	3045	1/1	0.98	0.08	167,167,167,167	0
56	MG	DA	3088	1/1	0.98	0.09	75,75,75,75	0
58	MPD	DS	203	8/8	0.98	0.22	62,64,65,67	0
56	MG	BA	1615	1/1	0.98	0.16	103,103,103,103	0
56	MG	DA	3159	1/1	0.98	0.14	131,131,131,131	0
56	MG	DA	3169	1/1	0.98	0.11	41,41,41,41	0
56	MG	CA	3086	1/1	0.98	0.21	106,106,106,106	0
56	MG	CA	3043	1/1	0.99	0.06	90,90,90,90	0
56	MG	DA	3026	1/1	0.99	0.18	228,228,228,228	0
56	MG	DA	3103	1/1	0.99	0.15	59,59,59,59	0
56	MG	DA	3089	1/1	0.99	0.15	24,24,24,24	0
56	MG	DA	3228	1/1	0.99	0.14	18,18,18,18	0
56	MG	DA	3102	1/1	0.99	0.13	32,32,32,32	0
56	MG	DA	3060	1/1	0.99	0.14	23,23,23,23	0
56	MG	DA	3074	1/1	0.99	0.12	54,54,54,54	0
56	MG	DA	3038	1/1	0.99	0.11	35,35,35,35	0
56	MG	DA	3051	1/1	0.99	0.13	37,37,37,37	0
56	MG	DA	3029	1/1	0.99	0.21	44,44,44,44	0
56	MG	DB	208	1/1	0.99	0.17	57,57,57,57	0
56	MG	DA	3010	1/1	0.99	0.11	48,48,48,48	0
56	MG	DA	3025	1/1	0.99	0.11	57,57,57,57	0
56	MG	DA	3016	1/1	0.99	0.16	74,74,74,74	0
56	MG	DA	3136	1/1	0.99	0.18	72,72,72,72	0
56	MG	DA	3086	1/1	0.99	0.09	82,82,82,82	0
56	MG	DA	3059	1/1	0.99	0.07	25,25,25,25	0
56	MG	AA	1644	1/1	0.99	0.14	180,180,180,180	0
56	MG	DA	3023	1/1	0.99	0.23	57,57,57,57	0
56	MG	CA	3098	1/1	0.99	0.07	98,98,98,98	0
56	MG	DA	3006	1/1	0.99	0.11	266,266,266,266	0
56	MG	DA	3112	1/1	0.99	0.18	46,46,46,46	0
56	MG	DA	3070	1/1	0.99	0.12	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	1632	1/1	0.99	0.12	74,74,74,74	0
56	MG	DA	3077	1/1	0.99	0.12	71,71,71,71	0
56	MG	BA	1640	1/1	0.99	0.08	103,103,103,103	0
56	MG	AA	1669	1/1	0.99	0.25	239,239,239,239	0
56	MG	DA	3015	1/1	0.99	0.16	78,78,78,78	0
56	MG	DA	3107	1/1	0.99	0.15	50,50,50,50	0
56	MG	CB	202	1/1	0.99	0.08	116,116,116,116	0
56	MG	CA	3041	1/1	0.99	0.08	50,50,50,50	0
56	MG	DA	3066	1/1	0.99	0.12	43,43,43,43	0
56	MG	AA	1651	1/1	0.99	0.12	75,75,75,75	0
56	MG	DA	3082	1/1	0.99	0.11	109,109,109,109	0
56	MG	AA	1646	1/1	0.99	0.12	80,80,80,80	0
56	MG	DA	3014	1/1	0.99	0.17	31,31,31,31	0
56	MG	DA	3028	1/1	0.99	0.10	116,116,116,116	0
56	MG	DA	3040	1/1	0.99	0.09	55,55,55,55	0
56	MG	DA	3114	1/1	0.99	0.08	52,52,52,52	0
56	MG	DA	3140	1/1	0.99	0.18	51,51,51,51	0
56	MG	DM	202	1/1	0.99	0.04	90,90,90,90	0
56	MG	DA	3020	1/1	0.99	0.06	69,69,69,69	0
56	MG	CA	3089	1/1	0.99	0.21	64,64,64,64	0
56	MG	DA	3035	1/1	0.99	0.14	24,24,24,24	0
56	MG	CA	3102	1/1	0.99	0.11	99,99,99,99	0
56	MG	DA	3078	1/1	0.99	0.06	47,47,47,47	0
56	MG	DB	202	1/1	0.99	0.10	56,56,56,56	0
56	MG	DA	3068	1/1	0.99	0.20	43,43,43,43	0
56	MG	DA	3017	1/1	0.99	0.12	34,34,34,34	0
56	MG	DA	3081	1/1	0.99	0.07	46,46,46,46	0
56	MG	AA	1633	1/1	0.99	0.12	116,116,116,116	0
56	MG	DA	3047	1/1	0.99	0.13	42,42,42,42	0
56	MG	DA	3083	1/1	0.99	0.07	57,57,57,57	0
56	MG	DA	3105	1/1	0.99	0.17	33,33,33,33	0
56	MG	DA	3092	1/1	0.99	0.12	50,50,50,50	0
56	MG	DA	3106	1/1	0.99	0.16	45,45,45,45	0
56	MG	CA	3088	1/1	0.99	0.13	86,86,86,86	0
56	MG	DA	3009	1/1	0.99	0.12	39,39,39,39	0
56	MG	DA	3027	1/1	0.99	0.20	49,49,49,49	0
56	MG	CA	3035	1/1	0.99	0.20	100,100,100,100	0
56	MG	BA	1621	1/1	0.99	0.17	45,45,45,45	0
56	MG	DA	3229	1/1	0.99	0.08	107,107,107,107	0
56	MG	CA	3013	1/1	0.99	0.11	71,71,71,71	0
56	MG	DA	3096	1/1	0.99	0.13	28,28,28,28	0
56	MG	DA	3022	1/1	0.99	0.13	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3113	1/1	0.99	0.16	113,113,113,113	0
56	MG	DB	203	1/1	0.99	0.10	88,88,88,88	0
56	MG	AA	1629	1/1	0.99	0.10	110,110,110,110	0
56	MG	DA	3063	1/1	0.99	0.15	111,111,111,111	0
56	MG	DA	3018	1/1	0.99	0.10	95,95,95,95	0
56	MG	DA	3055	1/1	0.99	0.26	52,52,52,52	0
56	MG	DA	3050	1/1	0.99	0.13	41,41,41,41	0
56	MG	DA	3052	1/1	0.99	0.29	251,251,251,251	0
56	MG	DA	3076	1/1	0.99	0.19	46,46,46,46	0
56	MG	DA	3090	1/1	0.99	0.17	26,26,26,26	0
56	MG	DA	3045	1/1	0.99	0.10	73,73,73,73	0
56	MG	DA	3042	1/1	0.99	0.11	87,87,87,87	0
56	MG	DA	3093	1/1	0.99	0.17	23,23,23,23	0
56	MG	DA	3061	1/1	0.99	0.14	44,44,44,44	0
56	MG	DA	3032	1/1	0.99	0.19	33,33,33,33	0
56	MG	DA	3109	1/1	0.99	0.16	38,38,38,38	0
56	MG	DA	3056	1/1	0.99	0.22	55,55,55,55	0
56	MG	DA	3013	1/1	0.99	0.20	13,13,13,13	0
56	MG	DA	3005	1/1	0.99	0.13	67,67,67,67	0
56	MG	DA	3116	1/1	0.99	0.10	72,72,72,72	0
56	MG	DA	3101	1/1	0.99	0.15	90,90,90,90	0
56	MG	CA	3076	1/1	0.99	0.31	218,218,218,218	0
56	MG	BA	1613	1/1	0.99	0.26	149,149,149,149	0
56	MG	AA	1666	1/1	0.99	0.07	100,100,100,100	0
56	MG	DA	3034	1/1	1.00	0.16	44,44,44,44	0
56	MG	DA	3041	1/1	1.00	0.23	22,22,22,22	0
56	MG	DA	3065	1/1	1.00	0.13	41,41,41,41	0
60	ZN	D5	101	1/1	1.00	0.10	84,84,84,84	0
56	MG	DA	3039	1/1	1.00	0.11	34,34,34,34	0
56	MG	DA	3037	1/1	1.00	0.16	13,13,13,13	0
56	MG	DA	3046	1/1	1.00	0.18	27,27,27,27	0
56	MG	DA	3049	1/1	1.00	0.13	52,52,52,52	0
56	MG	DA	3084	1/1	1.00	0.18	55,55,55,55	0
56	MG	DA	3104	1/1	1.00	0.22	43,43,43,43	0
56	MG	DA	3036	1/1	1.00	0.18	32,32,32,32	0
56	MG	DA	3019	1/1	1.00	0.26	16,16,16,16	0
56	MG	DA	3024	1/1	1.00	0.17	44,44,44,44	0
56	MG	DA	3058	1/1	1.00	0.09	66,66,66,66	0
56	MG	DA	3087	1/1	1.00	0.19	32,32,32,32	0
56	MG	DA	3073	1/1	1.00	0.16	40,40,40,40	0
56	MG	DA	3110	1/1	1.00	0.16	31,31,31,31	0
56	MG	DA	3057	1/1	1.00	0.14	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3091	1/1	1.00	0.13	29,29,29,29	0
56	MG	DA	3011	1/1	1.00	0.10	23,23,23,23	0
56	MG	DA	3021	1/1	1.00	0.14	31,31,31,31	0
56	MG	DA	3069	1/1	1.00	0.10	64,64,64,64	0
56	MG	DA	3072	1/1	1.00	0.20	86,86,86,86	0
56	MG	DA	3100	1/1	1.00	0.20	34,34,34,34	0
56	MG	DA	3075	1/1	1.00	0.18	25,25,25,25	0
56	MG	DA	3064	1/1	1.00	0.14	75,75,75,75	0
56	MG	DA	3230	1/1	1.00	0.13	76,76,76,76	0
56	MG	DA	3119	1/1	1.00	0.30	41,41,41,41	0

6.5 Other polymers

There are no such residues in this entry.