Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 03:37 AM EDT

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

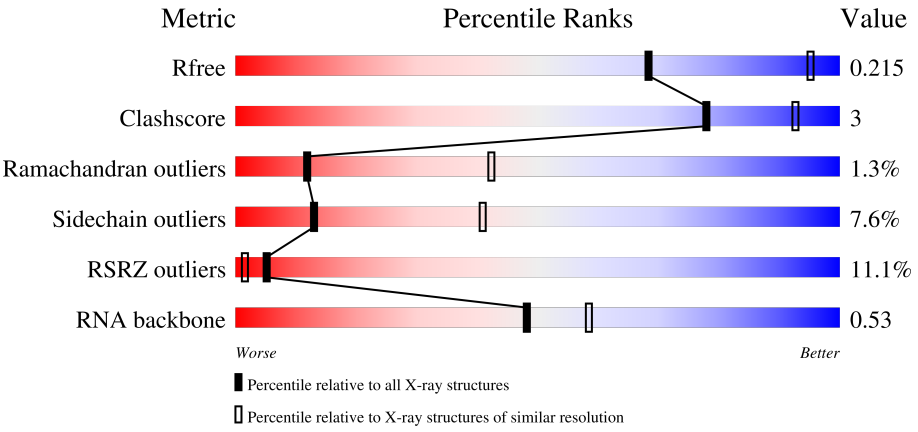
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)
RNA backbone	3102	1034 (3.30-2.78)

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 of 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 <=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	2% 74% 23%
1	BA	1534	10% 74% 23%
2	AB	224	7% 82% 17%
2	BB	224	15% 82% 17%

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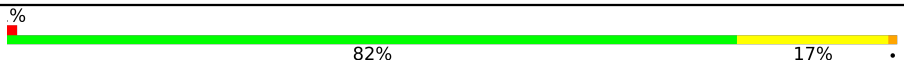
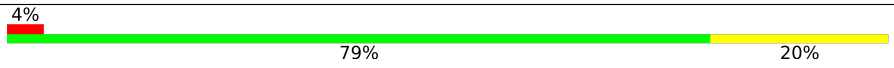
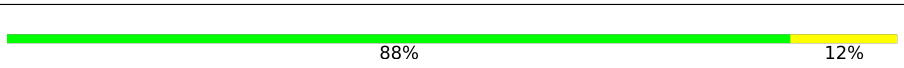
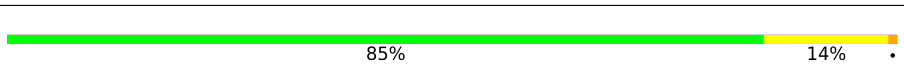
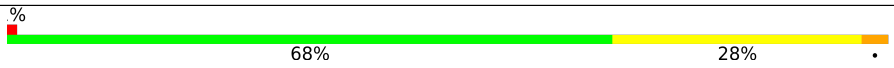
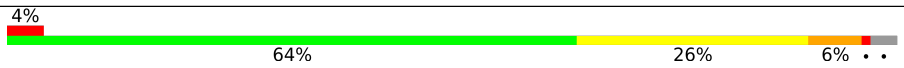
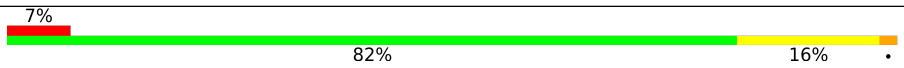
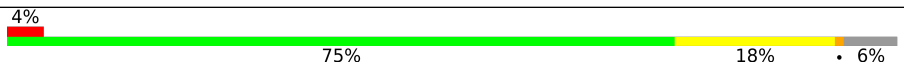
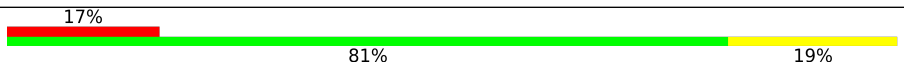
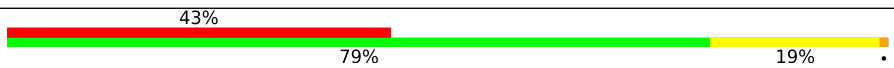
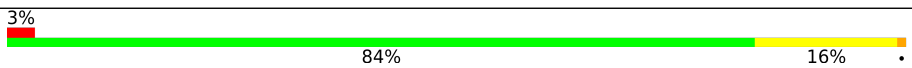
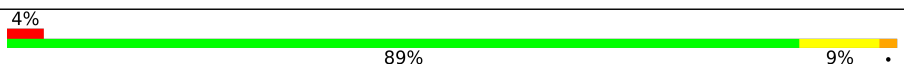
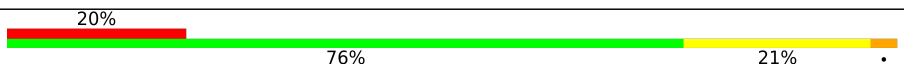
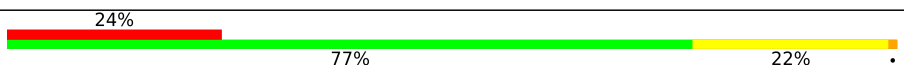
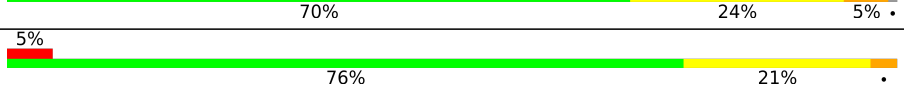
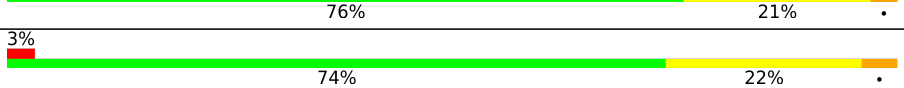
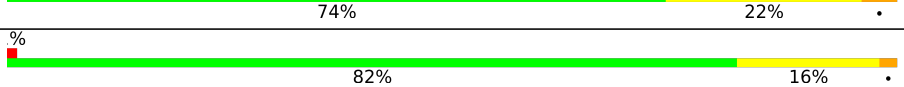
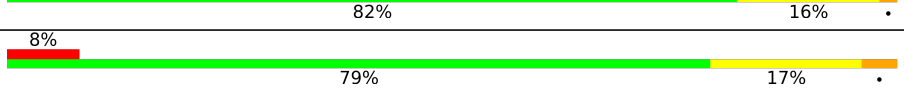
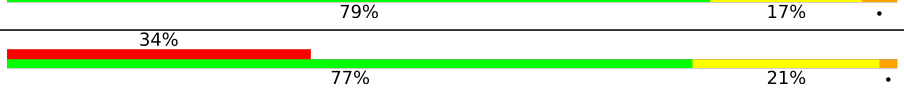
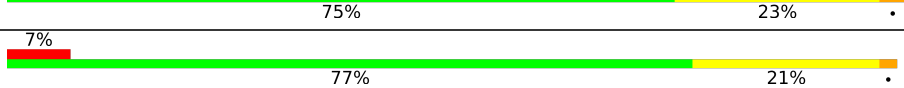
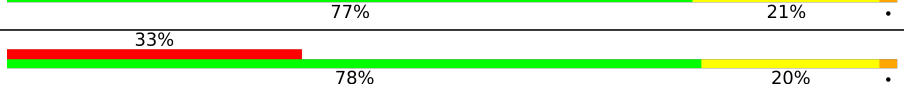
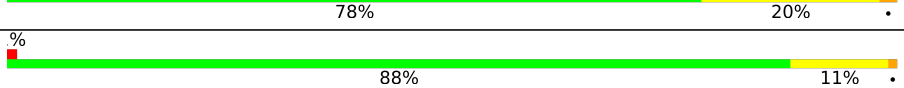
Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	155	
5	BE	155	
6	AF	106	
6	BF	106	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	99	
10	BJ	99	
11	AK	117	
11	BK	117	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	BO	88	11% 86% 10%
16	AP	82	9% 84% 13%
16	BP	82	34% 80% 17%
17	AQ	80	2% 81% 15%
17	BQ	80	26% 68% 25% 6%
18	AR	55	16% 78% 20%
18	BR	55	4% 80% 18%
19	AS	79	22% 68% 28%
19	BS	79	49% 73% 22%
20	AT	86	83% 13% 5%
20	BT	86	43% 84% 12%
21	AU	56	2% 89% 11%
21	BU	56	2% 93% 7%
22	C1	56	29% 75% 23%
22	D1	56	77% 21%
23	C2	51	43% 75% 20%
23	D2	51	78% 20%
24	C3	46	39% 85% 15%
24	D3	46	87% 13%
25	C4	64	9% 91% 9%
25	D4	64	88% 12%
26	C5	38	11% 79% 21%
26	D5	38	84% 13%
27	C0	58	34% 83% 16%
27	D0	58	81% 16%

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Mol	Chain	Length	Quality of chain
28	CB	120	13% 85% 12%
28	DB	120	87% 12%
29	CC	271	3% 82% 15%
29	DC	271	89% 10%
30	CD	209	24% 86% 13%
31	CA	2904	10% 73% 23%
32	DD	209	86% 14%
33	CE	201	20% 85% 12%
33	DE	201	95% 5%
34	CF	177	60% 83% 15%
34	DF	177	76% 22%
35	CG	176	52% 82% 18%
35	DG	176	% 82% 18%
36	CH	149	21% 77% 19%
36	DH	149	19% 82% 17%
37	CJ	134	79% 86% 12%
37	DJ	134	63% 85% 13%
38	CK	142	4% 92% 6%
38	DK	142	93% 6%
39	CL	123	7% 83% 13%
39	DL	123	86% 12%
40	CM	144	34% 78% 20%
40	DM	144	94% 6%
41	CN	136	6% 86% 13%
41	DN	136	82% 17%

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Mol	Chain	Length	Quality of chain
42	CO	125	10% 78% 15%
42	DO	125	% 87% 11%
43	CP	117	56% 84% 15%
43	DP	117	80% 18%
44	CQ	114	21% 88% 11%
44	DQ	114	% 82% 17%
45	CR	117	9% 85% 13%
45	DR	117	% 86% 14%
46	CS	103	35% 84% 16%
46	DS	103	91% 8%
47	CT	110	15% 80% 19%
47	DT	110	83% 17%
48	CU	93	37% 86% 10%
48	DU	93	2% 83% 16%
49	CV	102	57% 81% 18%
49	DV	102	% 89% 10%
50	CW	94	16% 87% 13%
50	DW	94	% 89% 11%
51	CX	76	24% 84% 13%
51	DX	76	% 79% 16% 5%
52	CY	77	4% 82% 17%
52	DY	77	79% 19%
53	CZ	62	45% 90% 10%
53	DZ	62	3% 95% 5%
54	DI	135	27% 71% 24%

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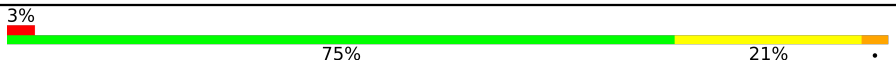
Mol	Chain	Length	Quality of chain
55	DA	2904	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1603	-	-	-	X
56	MG	AA	1606	-	-	-	X
56	MG	AA	1614	-	-	-	X
56	MG	AA	1619	-	-	-	X
56	MG	AA	1622	-	-	-	X
56	MG	AA	1623	-	-	-	X
56	MG	AA	1625	-	-	-	X
56	MG	AA	1626	-	-	-	X
56	MG	AA	1664	-	-	-	X
56	MG	BA	1604	-	-	-	X
56	MG	BA	1638	-	-	-	X
56	MG	CA	3021	-	-	-	X
56	MG	CA	3022	-	-	-	X
56	MG	CA	3047	-	-	-	X
56	MG	CA	3060	-	-	-	X
56	MG	CA	3075	-	-	-	X
56	MG	CA	3105	-	-	-	X
56	MG	CA	3113	-	-	-	X
56	MG	CA	3116	-	-	-	X
56	MG	CA	3122	-	-	-	X
56	MG	CA	3132	-	-	-	X
56	MG	CA	3134	-	-	-	X
56	MG	CA	3139	-	-	-	X
56	MG	CA	3140	-	-	-	X
56	MG	CA	3154	-	-	-	X
56	MG	DA	3158	-	-	-	X
56	MG	DA	3168	-	-	-	X
56	MG	DA	3170	-	-	-	X
56	MG	DA	3171	-	-	-	X
56	MG	DA	3175	-	-	-	X
56	MG	DA	3179	-	-	-	X
56	MG	DA	3181	-	-	-	X
56	MG	DA	3183	-	-	-	X
57	PG4	DR	202	-	-	-	X
58	MPD	DE	301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MPD	DN	201	-	-	-	X
59	PUT	AA	1674	-	-	-	X
59	PUT	AA	1675	-	-	-	X
59	PUT	DA	3198	-	-	-	X
59	PUT	DA	3207	-	-	-	X
59	PUT	DA	3215	-	-	-	X
61	PEG	D1	103	-	-	-	X
61	PEG	D3	102	-	-	-	X
61	PEG	DP	201	-	-	-	X
61	PEG	DQ	201	-	-	-	X
63	PGE	D1	102	-	-	-	X
63	PGE	D3	101	-	-	-	X
63	PGE	DS	201	-	-	-	X
66	ACY	DA	3199	-	X	-	X
68	TRS	DA	3222	-	-	-	X

2 Entry composition (i)

There are 69 unique types of molecules in this entry. The entry contains 295130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0	0
			32933	14695	6044	10660	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32911	14685	6039	10654	1533			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CP	116	Total	C	N	O		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	0	0	0
			947	604	192	151			
45	DR	117	Total	C	N	O	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 857	C 532	N 166	O 156	S 3	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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	AA	71	Total	Mg	0	0
			71	71		
56	BA	43	Total	Mg	0	0
			43	43		
56	CB	3	Total	Mg	0	0
			3	3		
56	CA	156	Total	Mg	0	0
			156	156		
56	DD	1	Total	Mg	0	0
			1	1		
56	DM	1	Total	Mg	0	0
			1	1		
56	DR	1	Total	Mg	0	0
			1	1		

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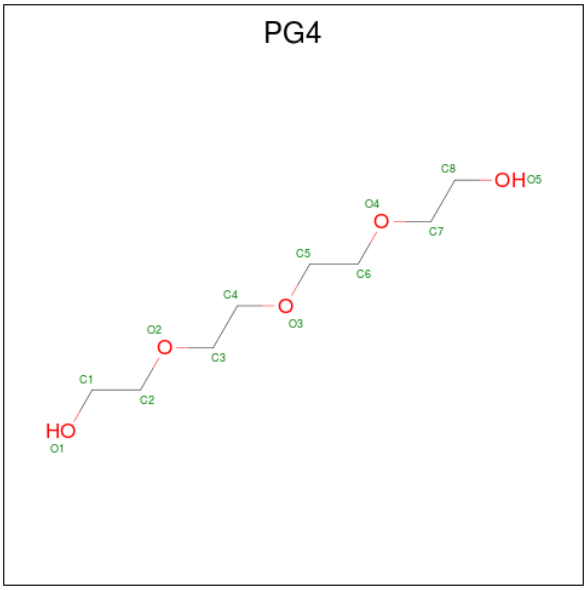
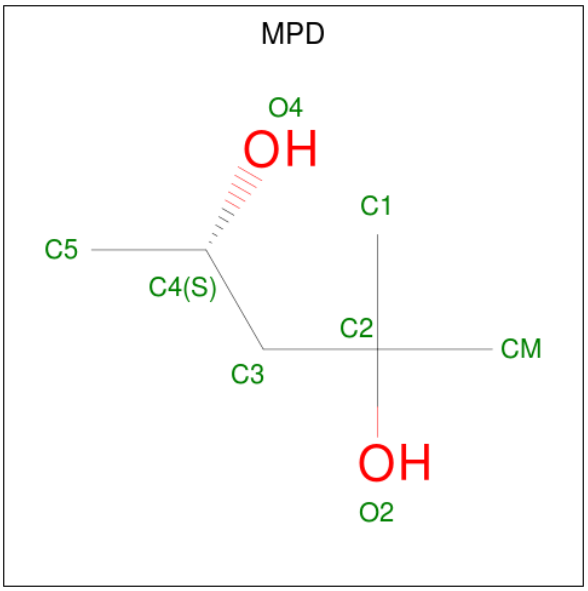
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DB	9	Total Mg 9 9	0	0
56	DA	184	Total Mg 184 184	0	0

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



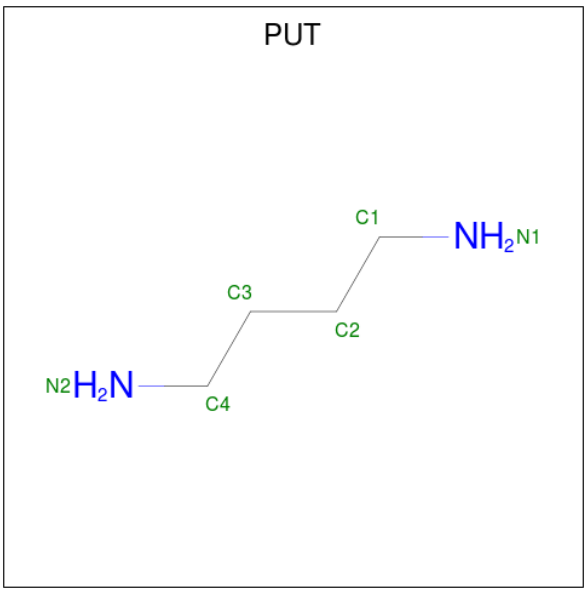
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	1	Total C O 13 8 5	0	0
57	BA	1	Total C O 13 8 5	0	0
57	DQ	1	Total C O 13 8 5	0	0
57	DR	1	Total C O 13 8 5	0	0
57	DS	1	Total C O 13 8 5	0	0
57	DA	1	Total C O 13 8 5	0	0
57	DA	1	Total C O 13 8 5	0	0

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



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

- Molecule 59 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



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

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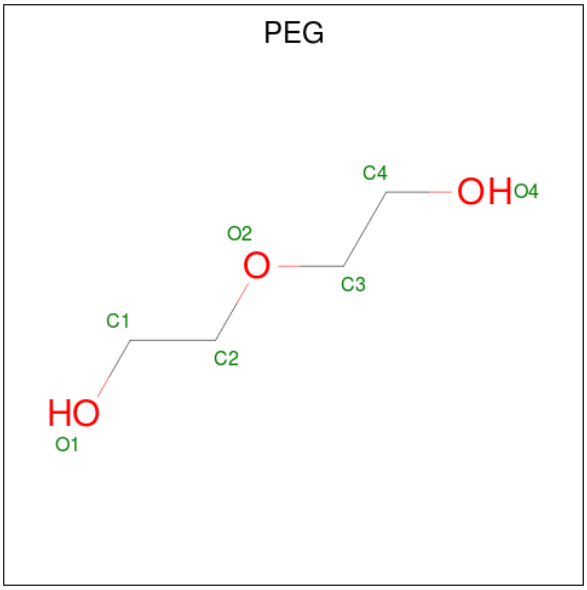
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0

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

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

- Molecule 61 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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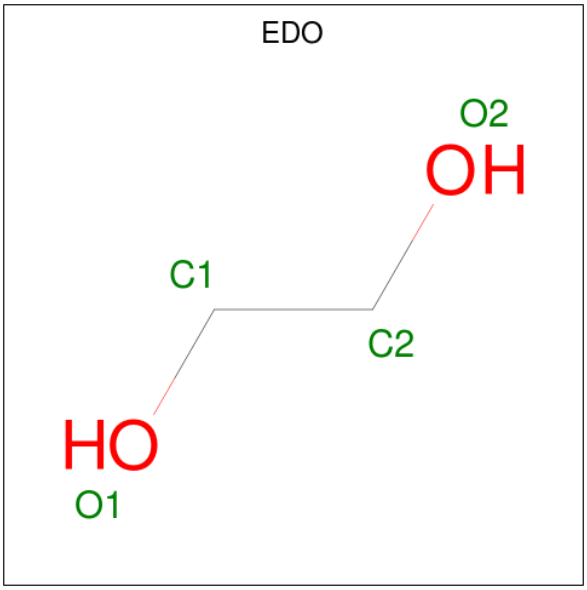
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	DL	1	Total C O 7 4 3	0	0
61	DP	1	Total C O 7 4 3	0	0
61	DQ	1	Total C O 7 4 3	0	0
61	DA	1	Total C O 7 4 3	0	0
61	DA	1	Total C O 7 4 3	0	0
61	DA	1	Total C O 7 4 3	0	0
61	DA	1	Total C O 7 4 3	0	0
61	DA	1	Total C O 7 4 3	0	0

- Molecule 62 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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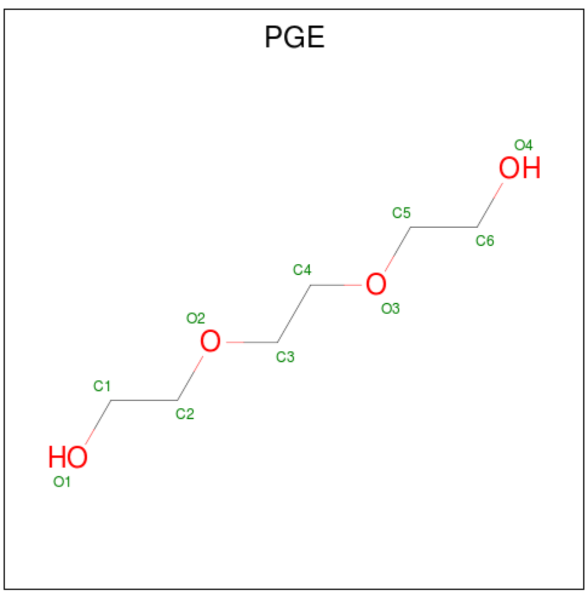
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0

- Molecule 63 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

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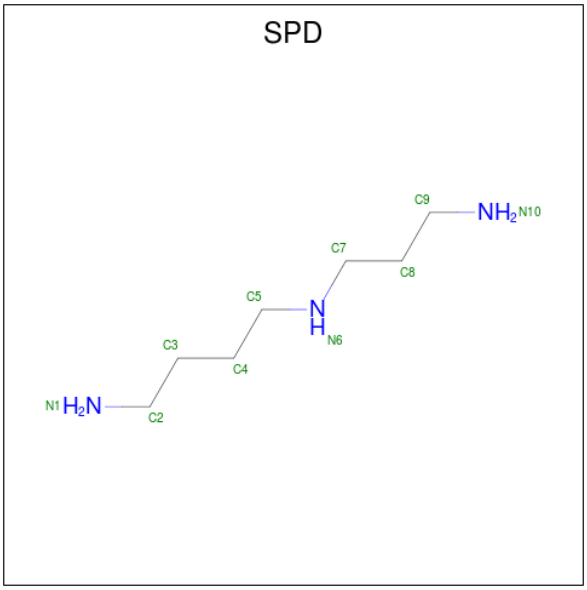
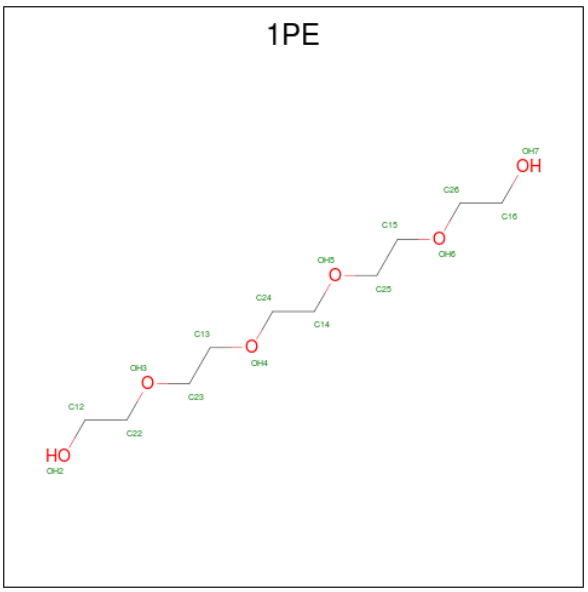
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	DD	1	Total C O 10 6 4	0	0
63	DS	1	Total C O 10 6 4	0	0
63	DU	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0

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



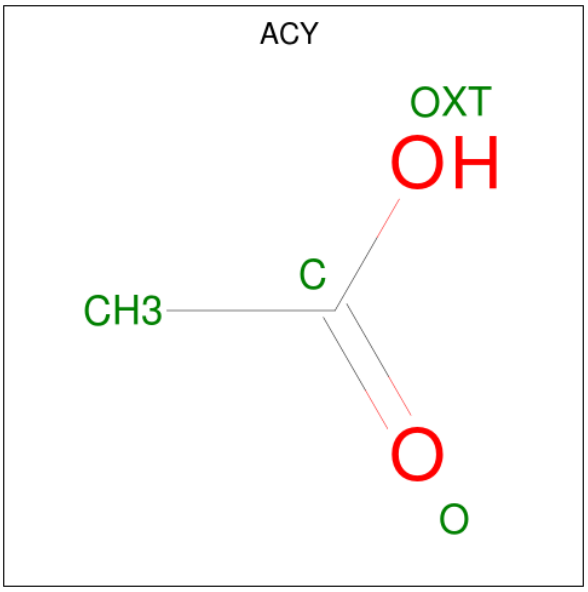
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0

- 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 16 10 6	0	0
65	DA	1	Total C O 16 10 6	0	0

- 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 4 2 2	0	0

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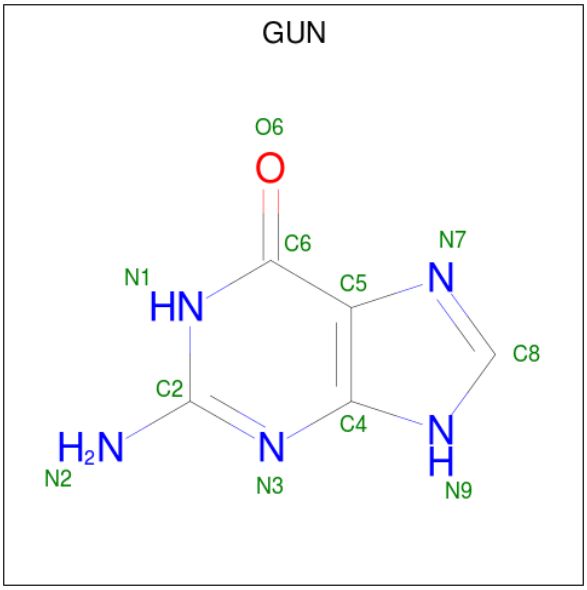
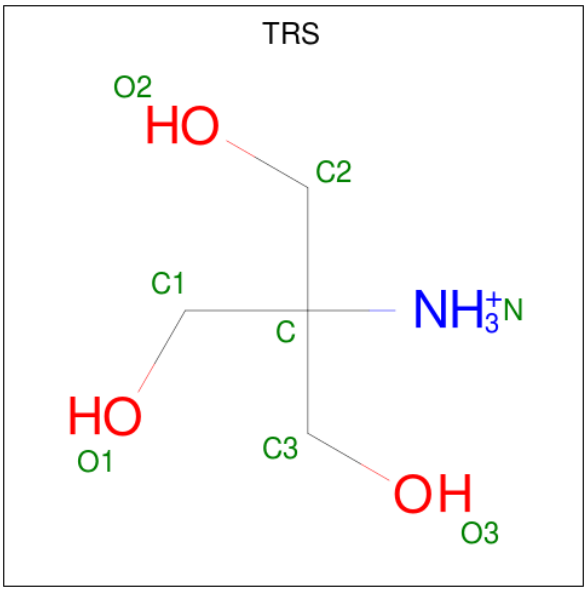
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
66	DA	1	Total C O 4 2 2	0	0
66	DA	1	Total C O 4 2 2	0	0

- 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 11 5 5 1	0	0

- 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 8 4 1 3	0	0

- Molecule 69 is water.

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	D3	28	Total O 28 28	0	0
69	D4	33	Total O 33 33	0	0
69	D5	11	Total O 11 11	0	0
69	D0	26	Total O 26 26	0	0
69	CB	13	Total O 13 13	0	0
69	CC	8	Total O 8 8	0	0
69	CD	7	Total O 7 7	0	0
69	CA	693	Total O 693 693	0	0
69	DC	102	Total O 102 102	0	0
69	DD	95	Total O 95 95	0	0
69	CE	4	Total O 4 4	0	0
69	CL	1	Total O 1 1	0	0
69	CM	4	Total O 4 4	0	0
69	CO	2	Total O 2 2	0	0
69	CQ	1	Total O 1 1	0	0
69	CU	3	Total O 3 3	0	0
69	CV	1	Total O 1 1	0	0
69	CW	1	Total O 1 1	0	0
69	CY	1	Total O 1 1	0	0
69	DE	63	Total O 63 63	0	0
69	DF	16	Total O 16 16	0	0

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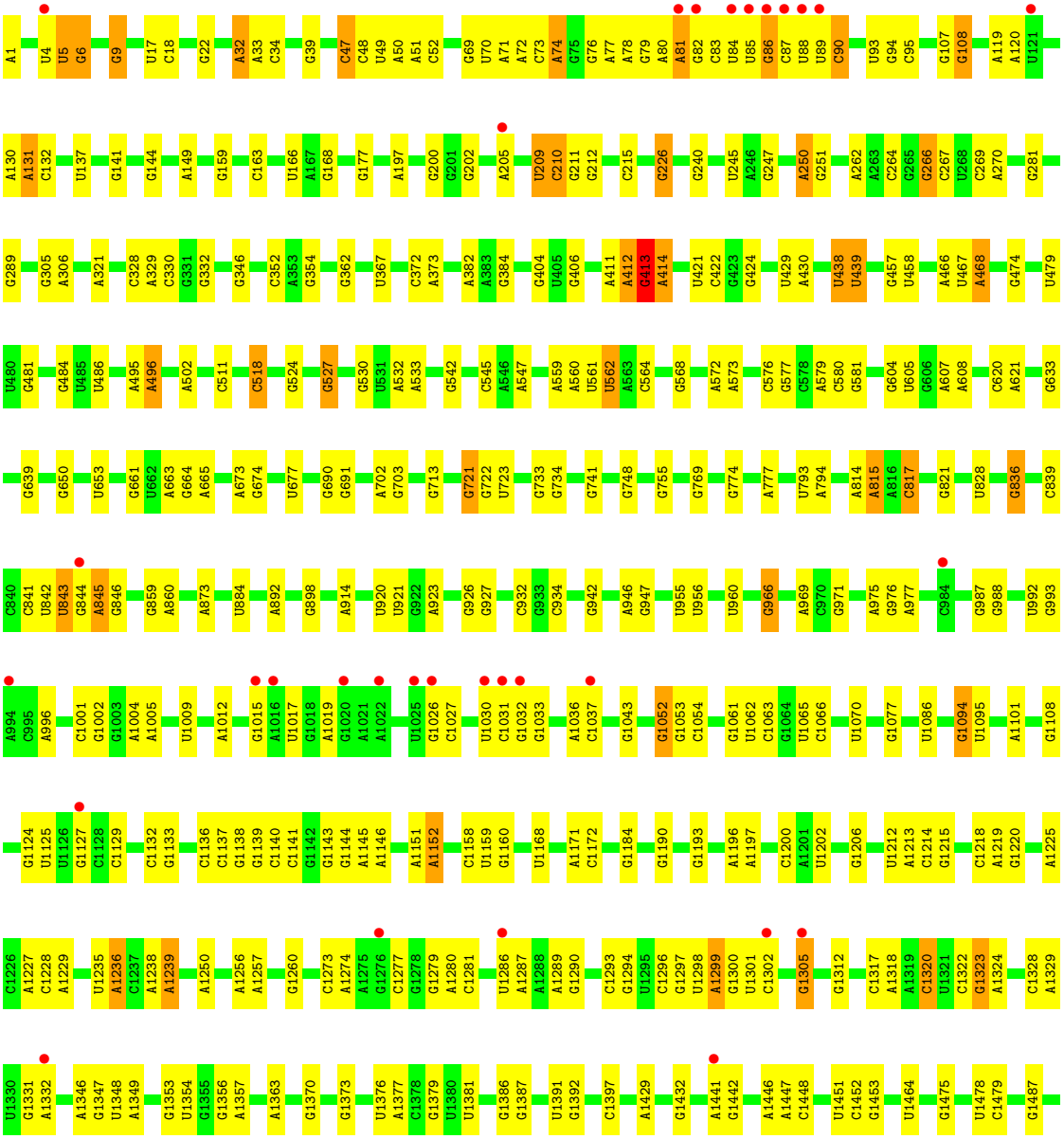
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	DG	7	Total O 7 7	0	0
69	DH	2	Total O 2 2	0	0
69	DK	60	Total O 60 60	0	0
69	DL	51	Total O 51 51	0	0
69	DM	68	Total O 68 68	0	0
69	DN	73	Total O 73 73	0	0
69	DO	49	Total O 49 49	0	0
69	DP	38	Total O 38 38	0	0
69	DQ	29	Total O 29 29	0	0
69	DR	61	Total O 61 61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

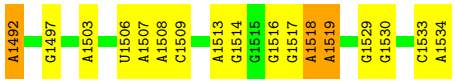
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

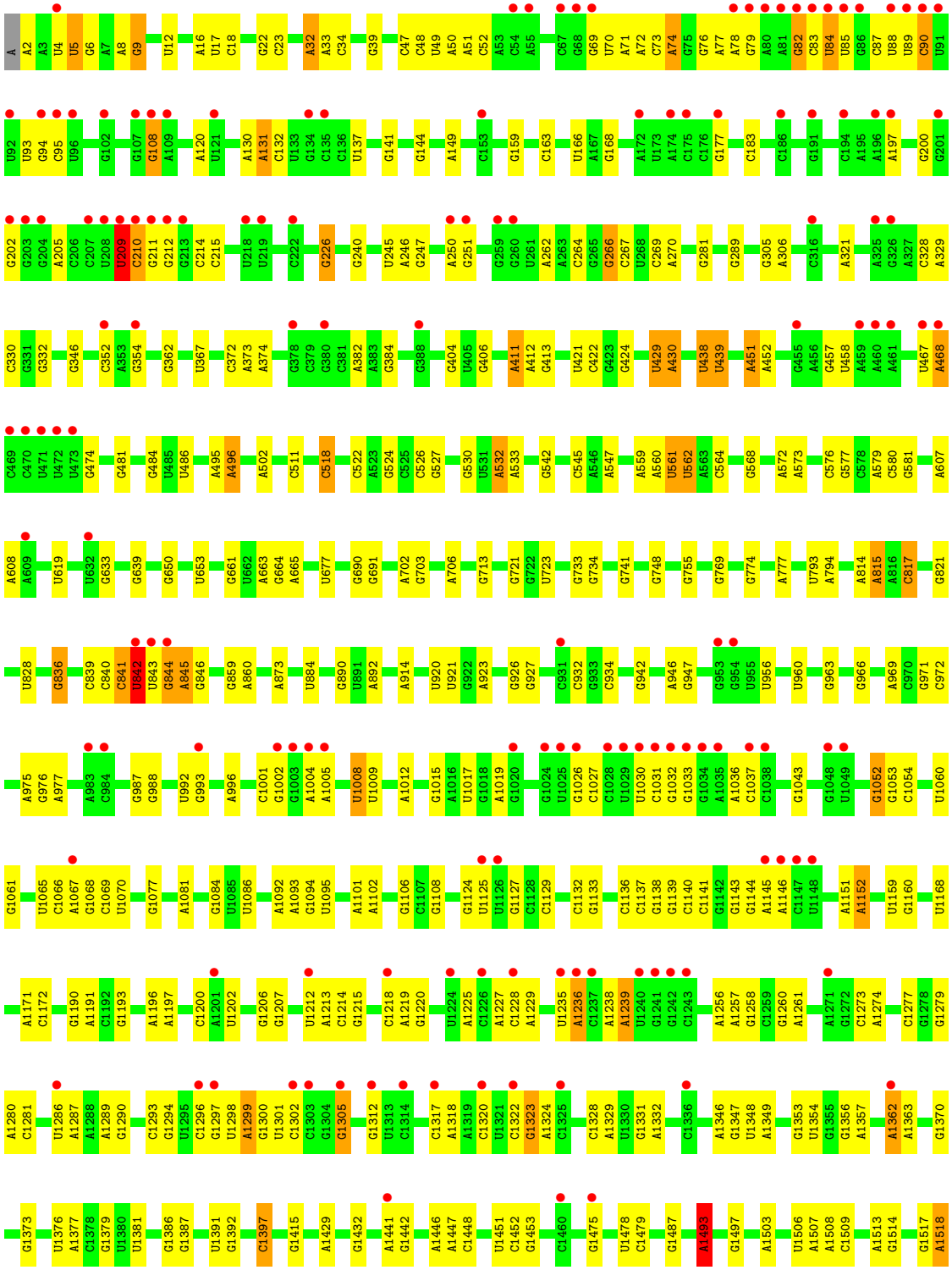
Chain AA: 





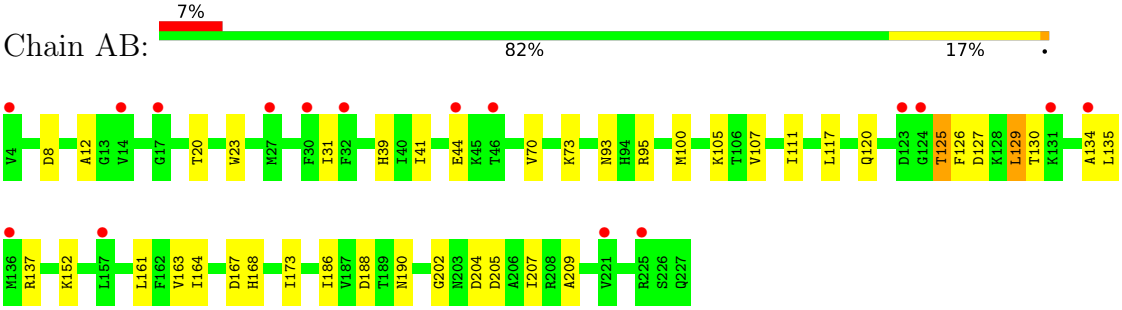
• Molecule 1: 16S rRNA

Chain BA:



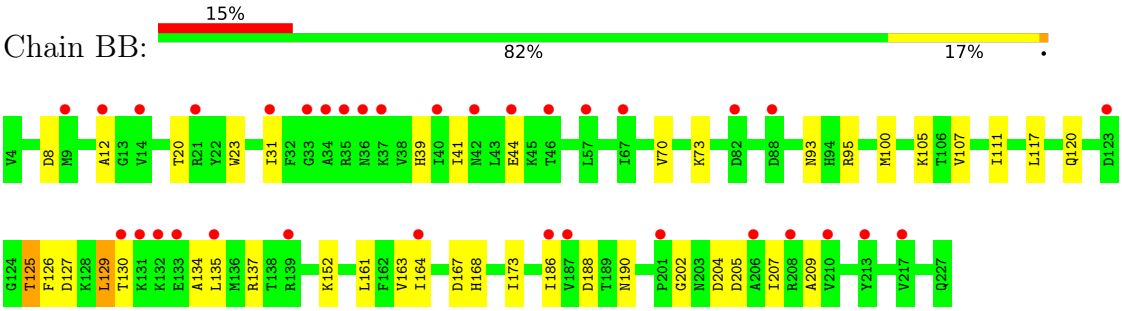
• Molecule 2: 30S ribosomal protein S2

Chain AB:



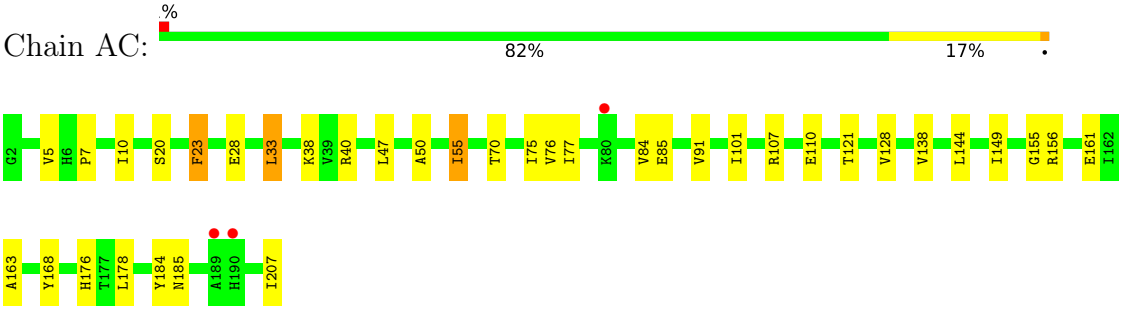
• Molecule 2: 30S ribosomal protein S2

Chain BB:



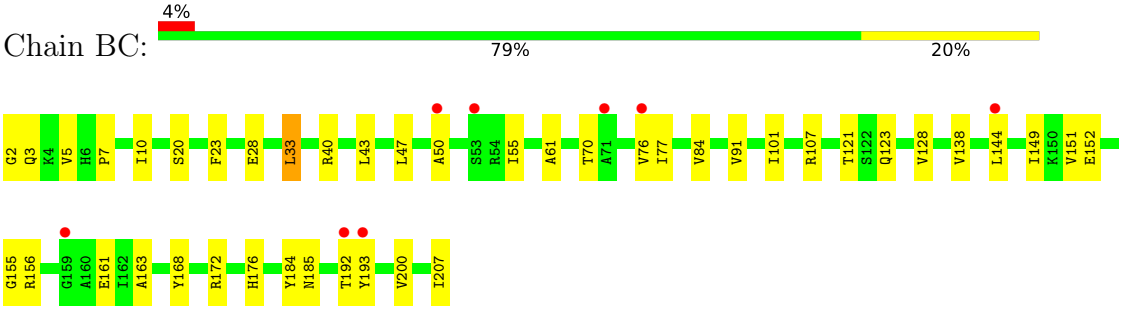
• Molecule 3: 30S ribosomal protein S3

Chain AC:



• Molecule 3: 30S ribosomal protein S3

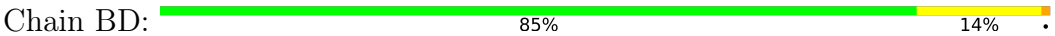
Chain BC:



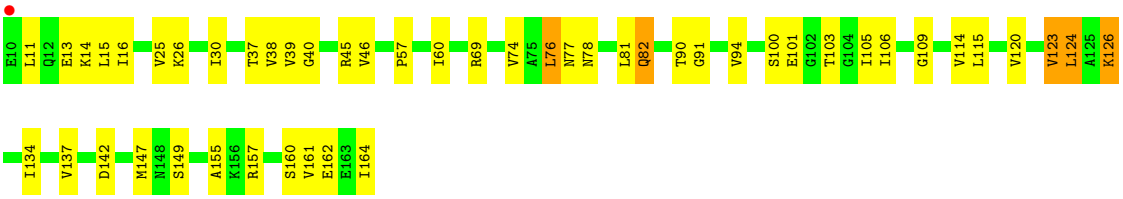
• Molecule 4: 30S ribosomal protein S4

Chain AD:

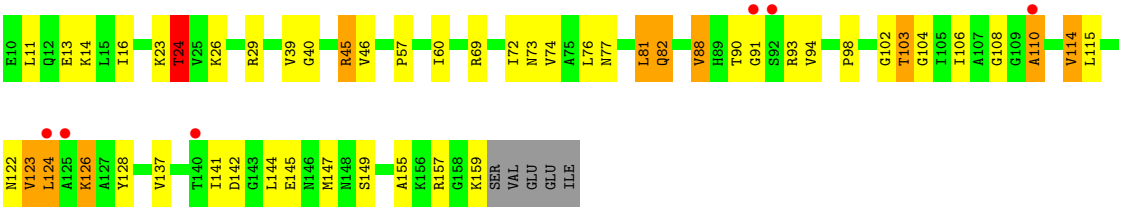
• Molecule 4: 30S ribosomal protein S4



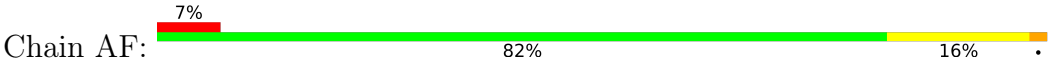
• Molecule 5: 30S ribosomal protein S5

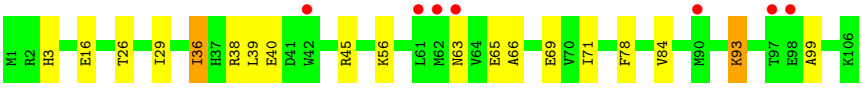


• Molecule 5: 30S ribosomal protein S5

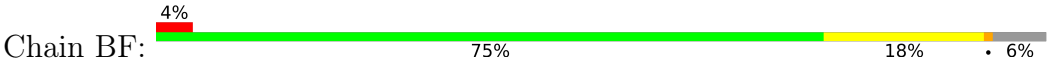


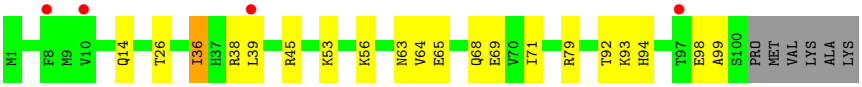
• Molecule 6: 30S ribosomal protein S6



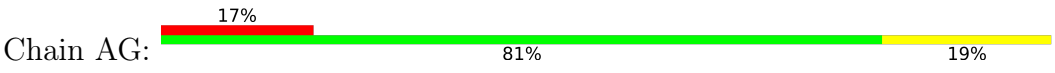


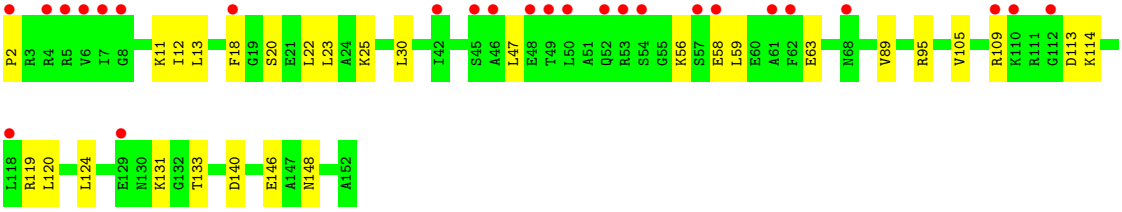
• Molecule 6: 30S ribosomal protein S6



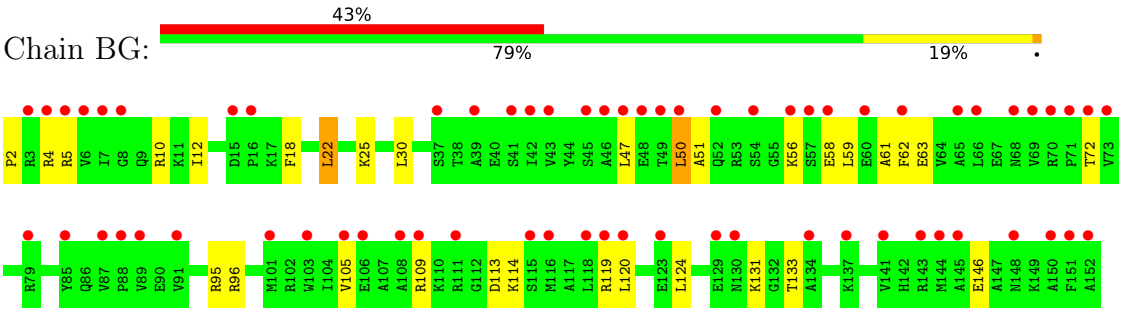


• Molecule 7: 30S ribosomal protein S7

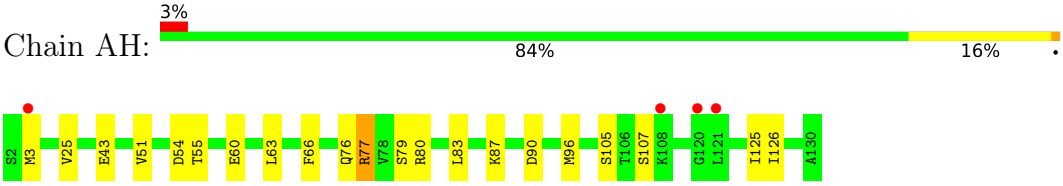




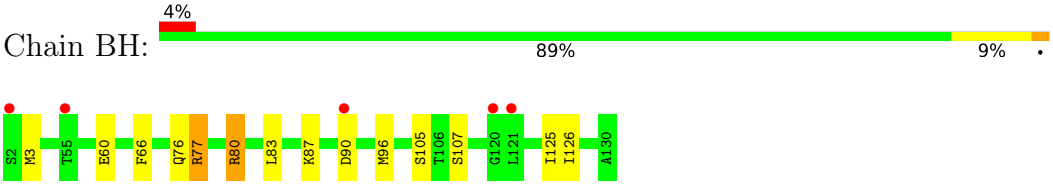
• Molecule 7: 30S ribosomal protein S7



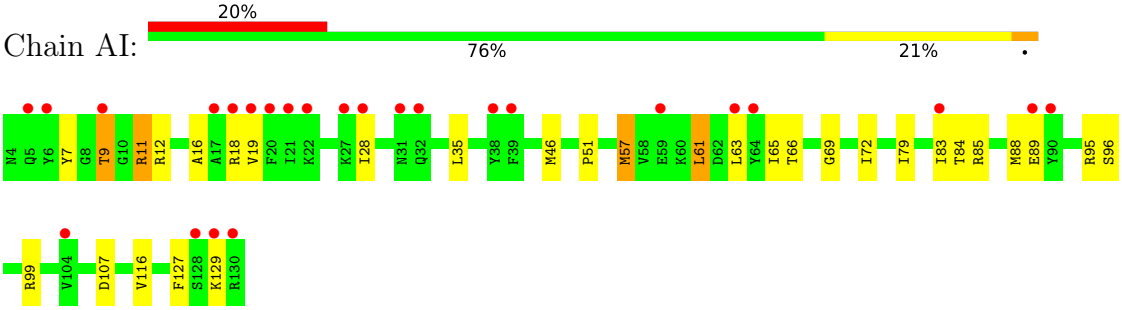
• Molecule 8: 30S ribosomal protein S8



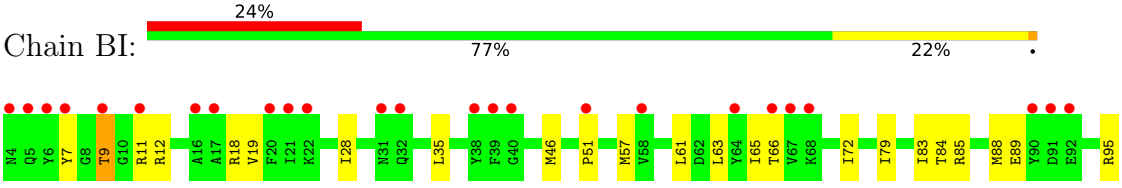
• Molecule 8: 30S ribosomal protein S8

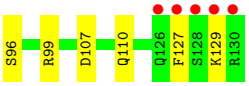


• Molecule 9: 30S ribosomal protein S9



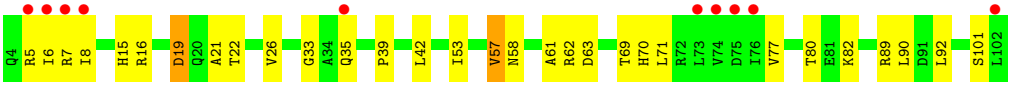
• Molecule 9: 30S ribosomal protein S9





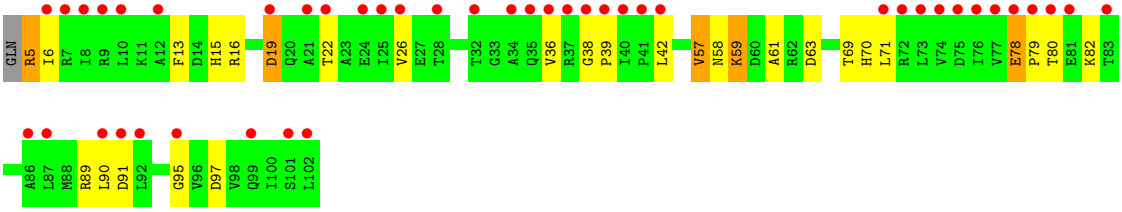
• Molecule 10: 30S ribosomal protein S10

Chain AJ:



• Molecule 10: 30S ribosomal protein S10

Chain BJ:

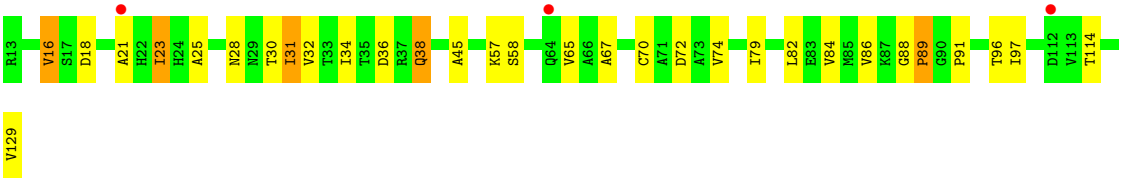


• Molecule 11: 30S ribosomal protein S11

Chain AK:

• Molecule 11: 30S ribosomal protein S11

Chain BK:

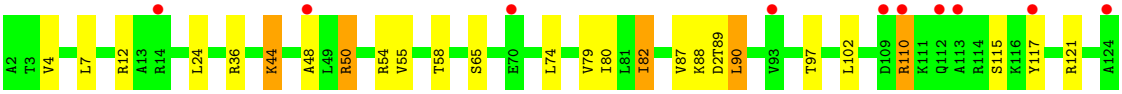


• Molecule 12: 30S ribosomal protein S12

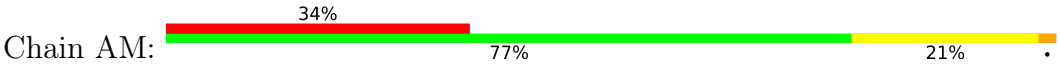
Chain AL:

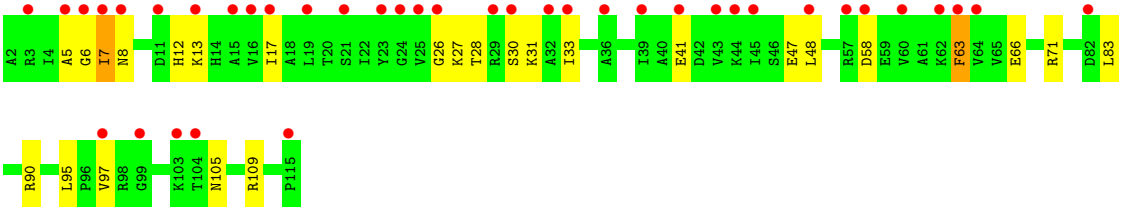
• Molecule 12: 30S ribosomal protein S12

Chain BL:

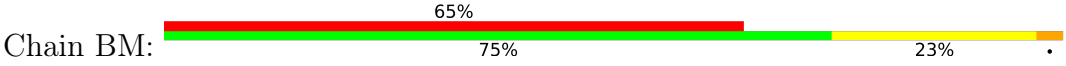


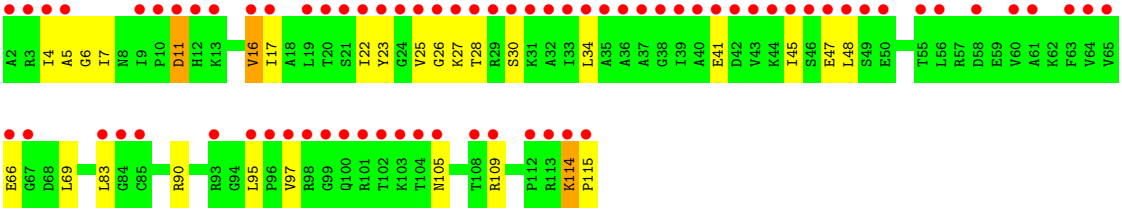
• Molecule 13: 30S ribosomal protein S13



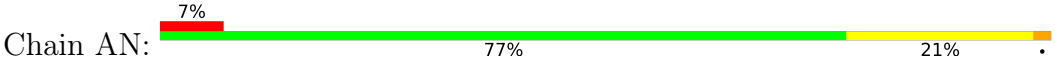


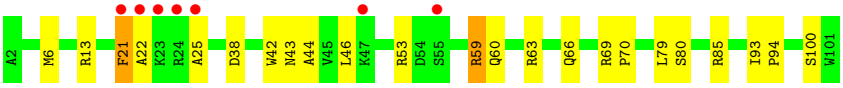
• Molecule 13: 30S ribosomal protein S13



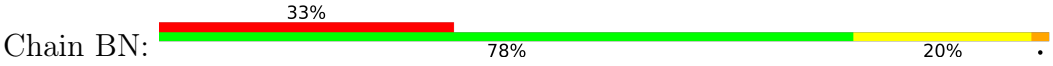


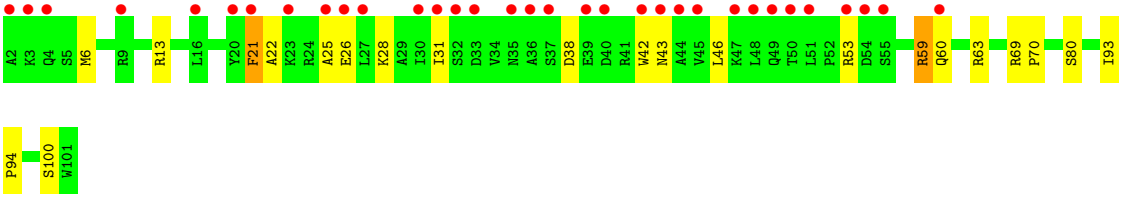
• Molecule 14: 30S ribosomal protein S14



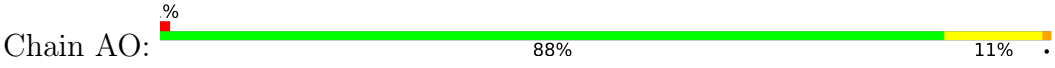


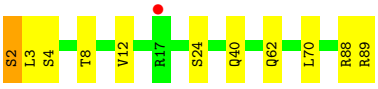
• Molecule 14: 30S ribosomal protein S14





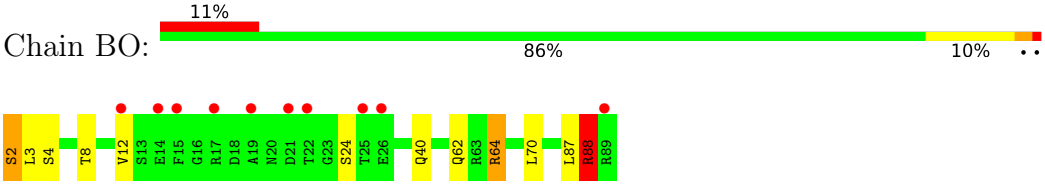
• Molecule 15: 30S ribosomal protein S15





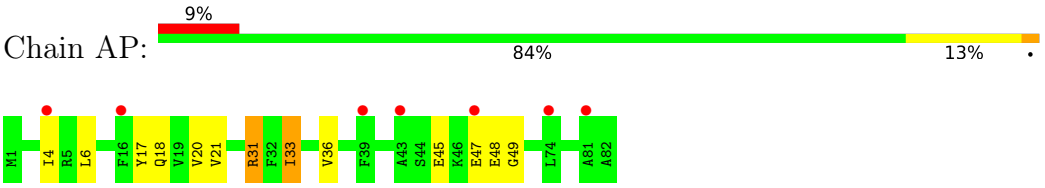
• Molecule 15: 30S ribosomal protein S15

Chain BO:



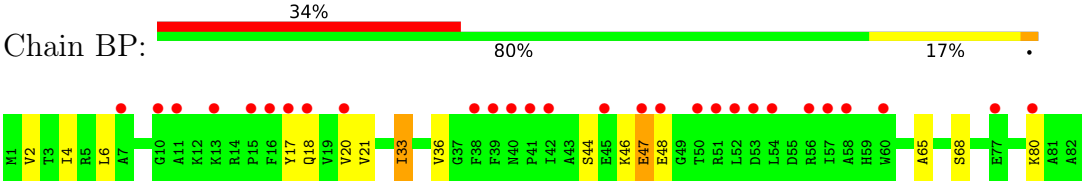
• Molecule 16: 30S ribosomal protein S16

Chain AP:



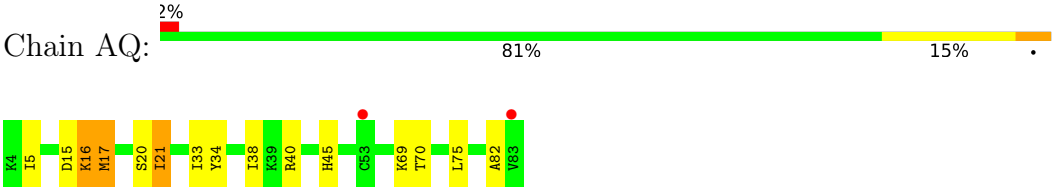
• Molecule 16: 30S ribosomal protein S16

Chain BP:



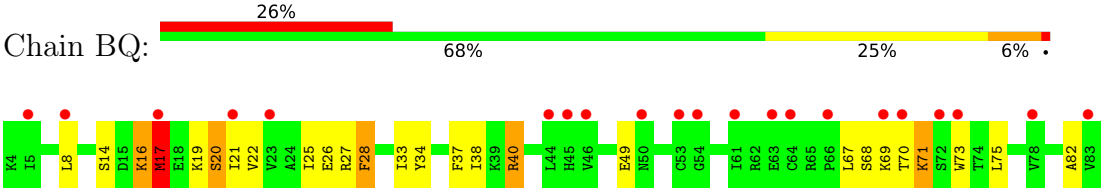
• Molecule 17: 30S ribosomal protein S17

Chain AQ:



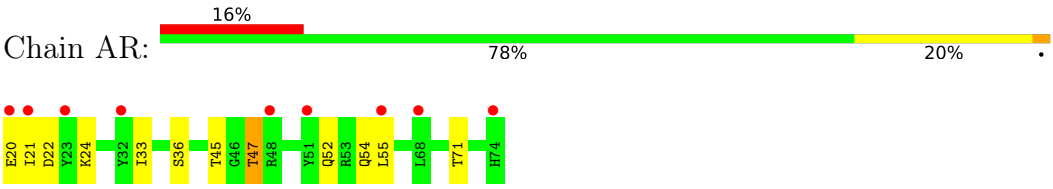
• Molecule 17: 30S ribosomal protein S17

Chain BQ:



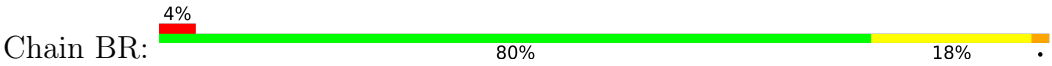
• Molecule 18: 30S ribosomal protein S18

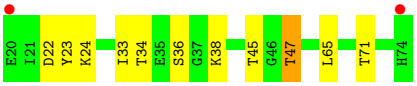
Chain AR:



• Molecule 18: 30S ribosomal protein S18

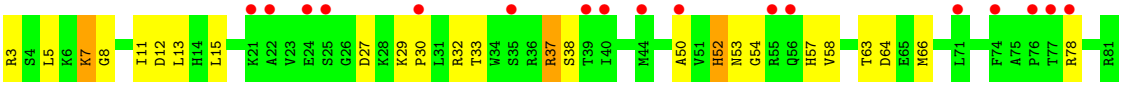
Chain BR:





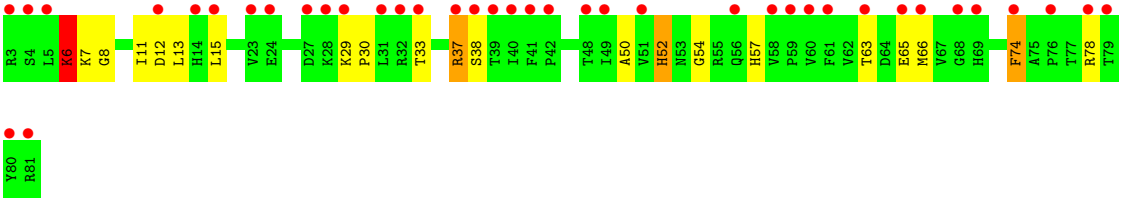
• Molecule 19: 30S ribosomal protein S19

Chain AS:



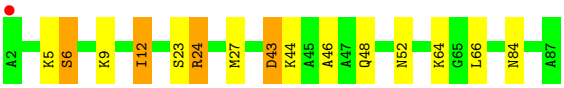
• Molecule 19: 30S ribosomal protein S19

Chain BS:



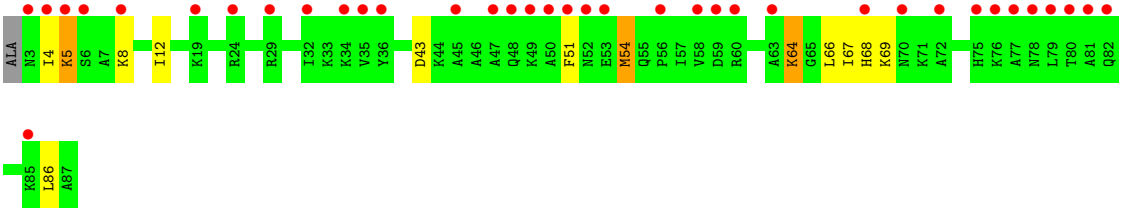
• Molecule 20: 30S ribosomal protein S20

Chain AT:



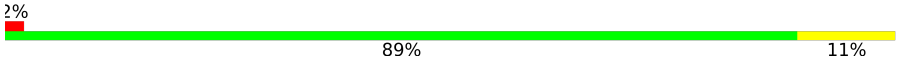
• Molecule 20: 30S ribosomal protein S20

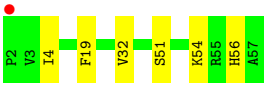
Chain BT:



• Molecule 21: 30S ribosomal protein S21

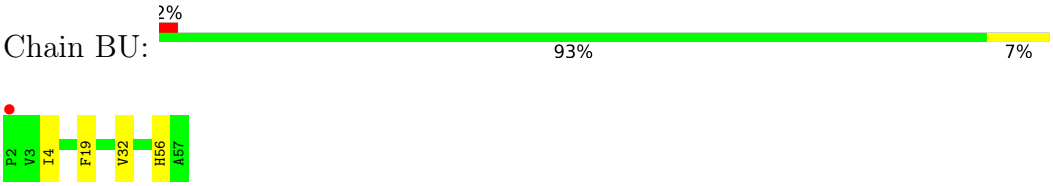
Chain AU:





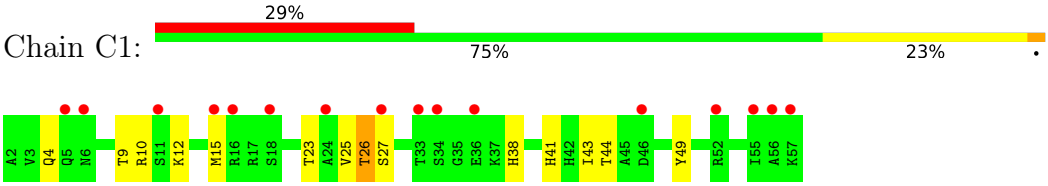
• Molecule 21: 30S ribosomal protein S21

Chain BU:



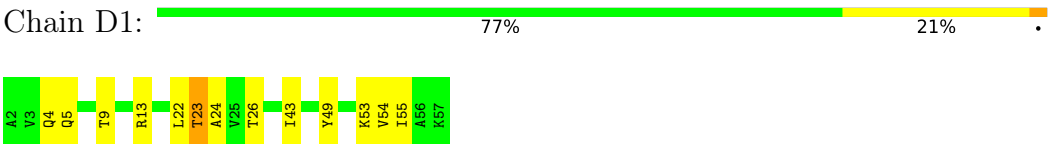
• Molecule 22: 50S ribosomal protein L32

Chain C1:



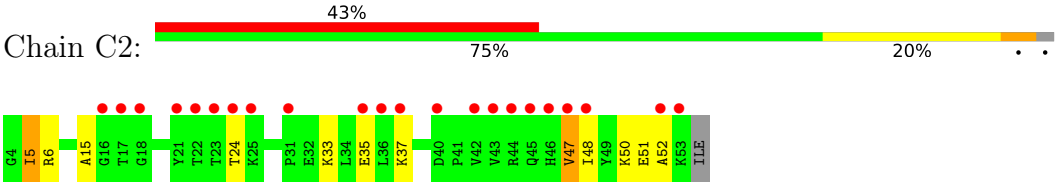
• Molecule 22: 50S ribosomal protein L32

Chain D1:



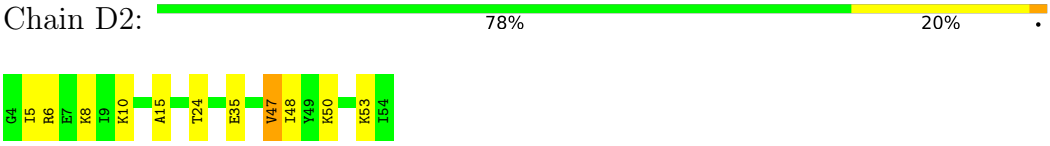
• Molecule 23: 50S ribosomal protein L33

Chain C2:



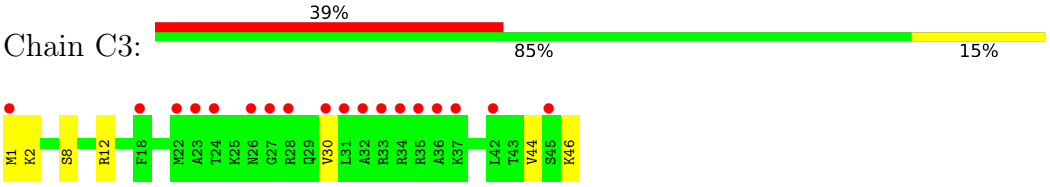
• Molecule 23: 50S ribosomal protein L33

Chain D2:



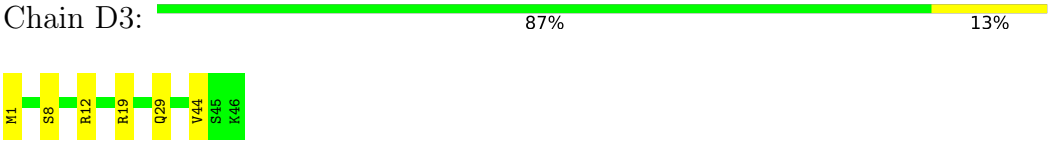
• Molecule 24: 50S ribosomal protein L34

Chain C3:



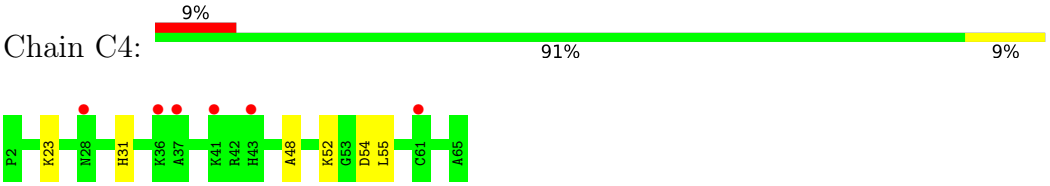
• Molecule 24: 50S ribosomal protein L34

Chain D3:



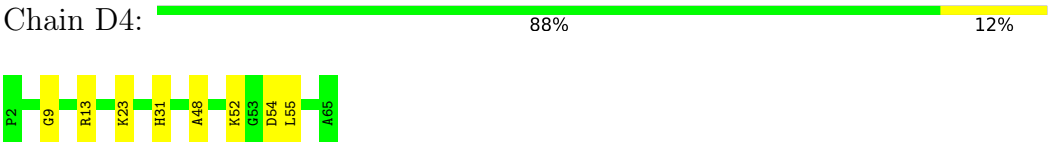
• Molecule 25: 50S ribosomal protein L35

Chain C4:



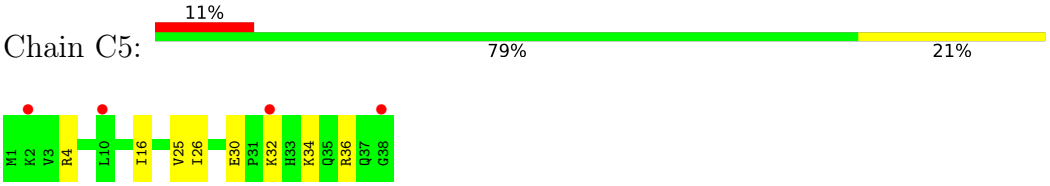
• Molecule 25: 50S ribosomal protein L35

Chain D4:



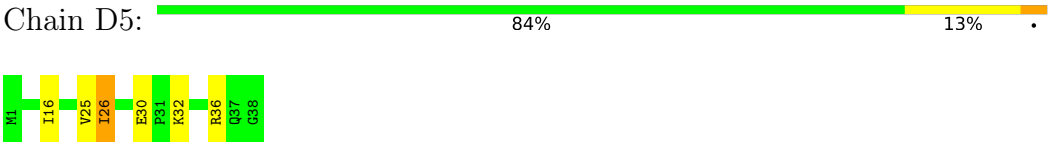
• Molecule 26: 50S ribosomal protein L36

Chain C5:



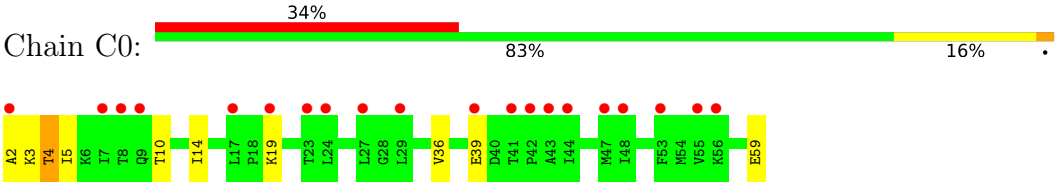
• Molecule 26: 50S ribosomal protein L36

Chain D5:



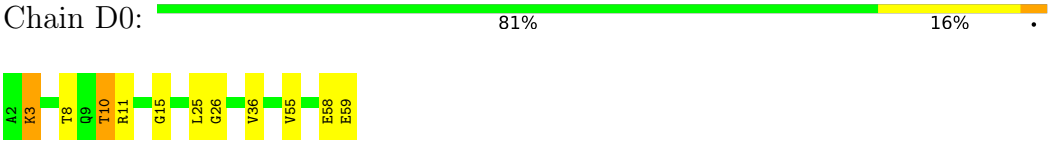
• Molecule 27: 50S ribosomal protein L30

Chain C0:



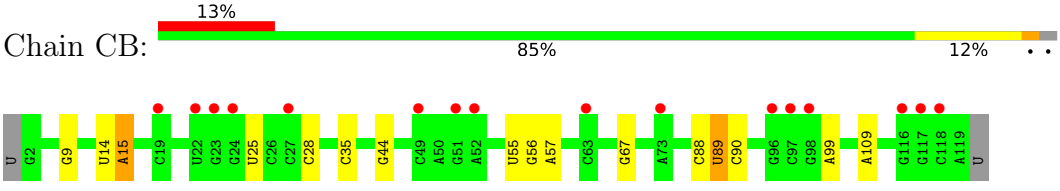
• Molecule 27: 50S ribosomal protein L30

Chain D0:



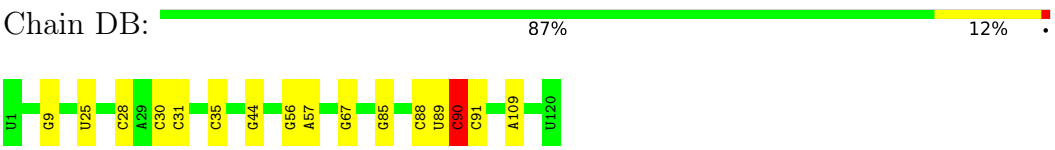
• Molecule 28: 5S rRNA

Chain CB:



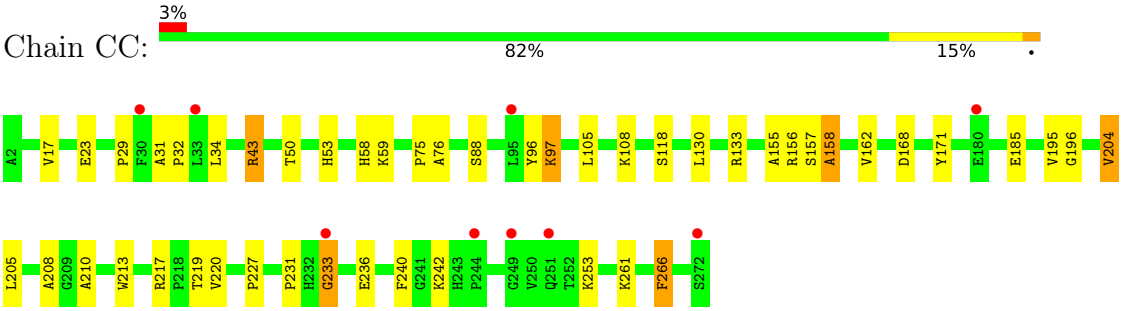
• Molecule 28: 5S rRNA

Chain DB:



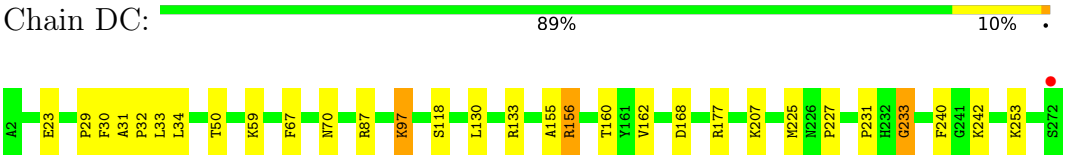
• Molecule 29: 50S ribosomal protein L2

Chain CC:



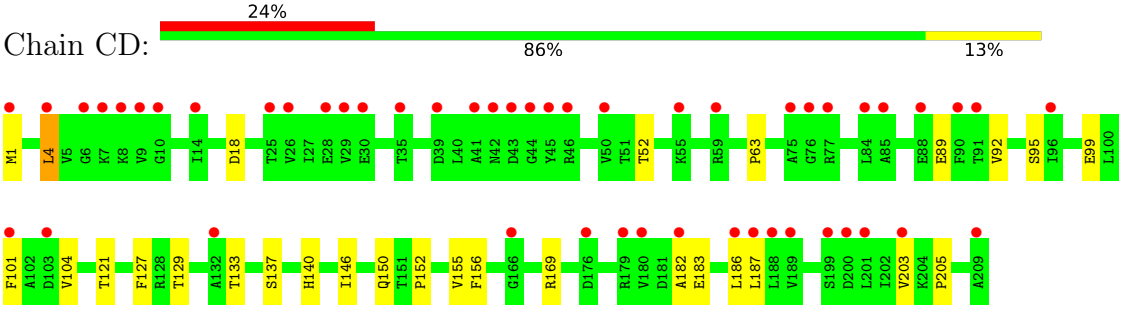
• Molecule 29: 50S ribosomal protein L2

Chain DC:



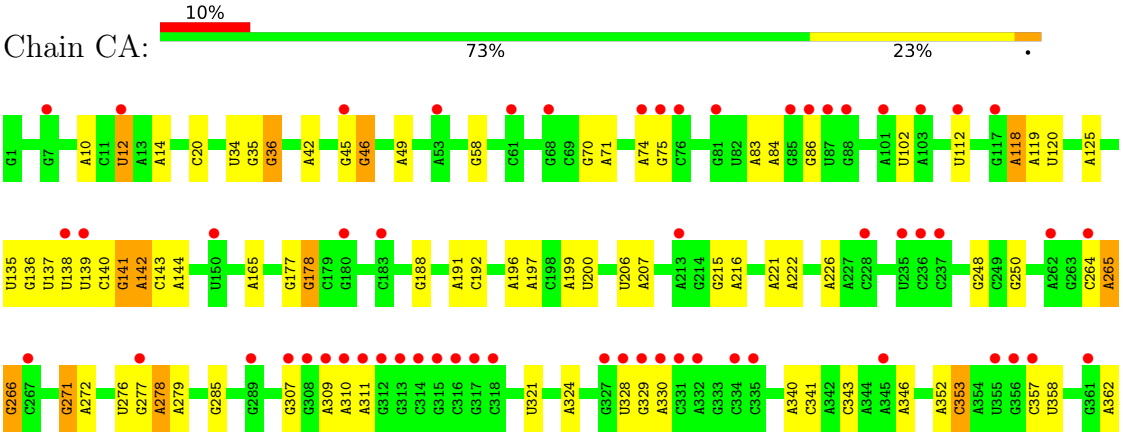
• Molecule 30: 50S ribosomal protein L3

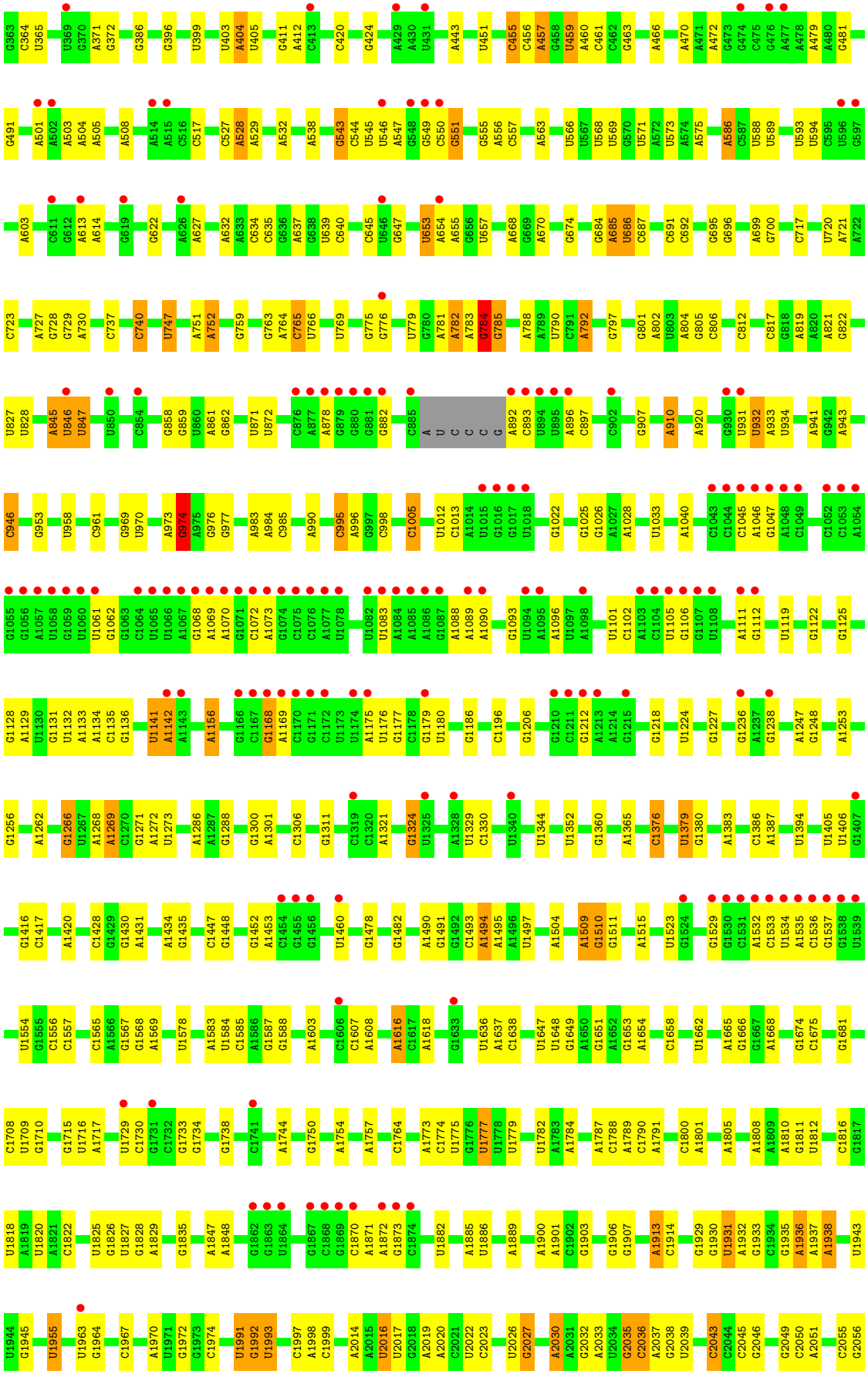
Chain CD:



• Molecule 31: 23S rRNA

Chain CA:

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G491 A501 A502 A503 A504 A505 A508 A514 A515 C516 C517 C527 A528 A529 A532 A538 G543 C544 U545 U546 A547 G548 G549 C550 G551 G555 A556 C557 A563 U566 U567 U568 U569 G570 U571 A572 U573 A574 A575 A586 C587 U588 U589 U593 U594 C595 U596 G597
A603 C611 G612 A613 A614 G619 G622 A626 A627 A632 A633 C634 C635 G636 A637 G638 U639 C640 C645 U646 G647 U653 A654 A655 G656 U657 A668 G669 A670 G674 G684 A685 U686 C687 C691 C692 G695 G696 A699 G700 C717 U720 A721 A722
C723 A727 G728 G729 A730 C737 C740 U747 A751 A752 G759 G763 A764 C765 U766 U769 G775 G776 U779 G780 A781 A782 A783 G784 G785 A788 A789 U790 C791 A792 G797 G801 A802 U803 A804 G805 C806 C812 C817 G818 A819 A820 A821 G822
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G1055 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1093 U1094 A1095 A1096 U1097 A1098 U1101 C1102 A1103 C1104 U1105 C1106 G1107 U1108 A1111 G1112 U1119 G1122 G1125
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C1708 U1709 G1710 G1715 U1716 A1717 U1729 C1730 G1731 C1732 G1733 G1734 G1738 C1741 A1744 G1750 A1754 A1757 C1764 A1773 C1774 U1775 G1776 U1777 U1778 U1779 U1782 A1783 A1784 A1787 C1788 A1789 C1790 A1791 C1800 A1801 A1805 A1808 A1809 A1810 G1811 U1812 C1816 G1817
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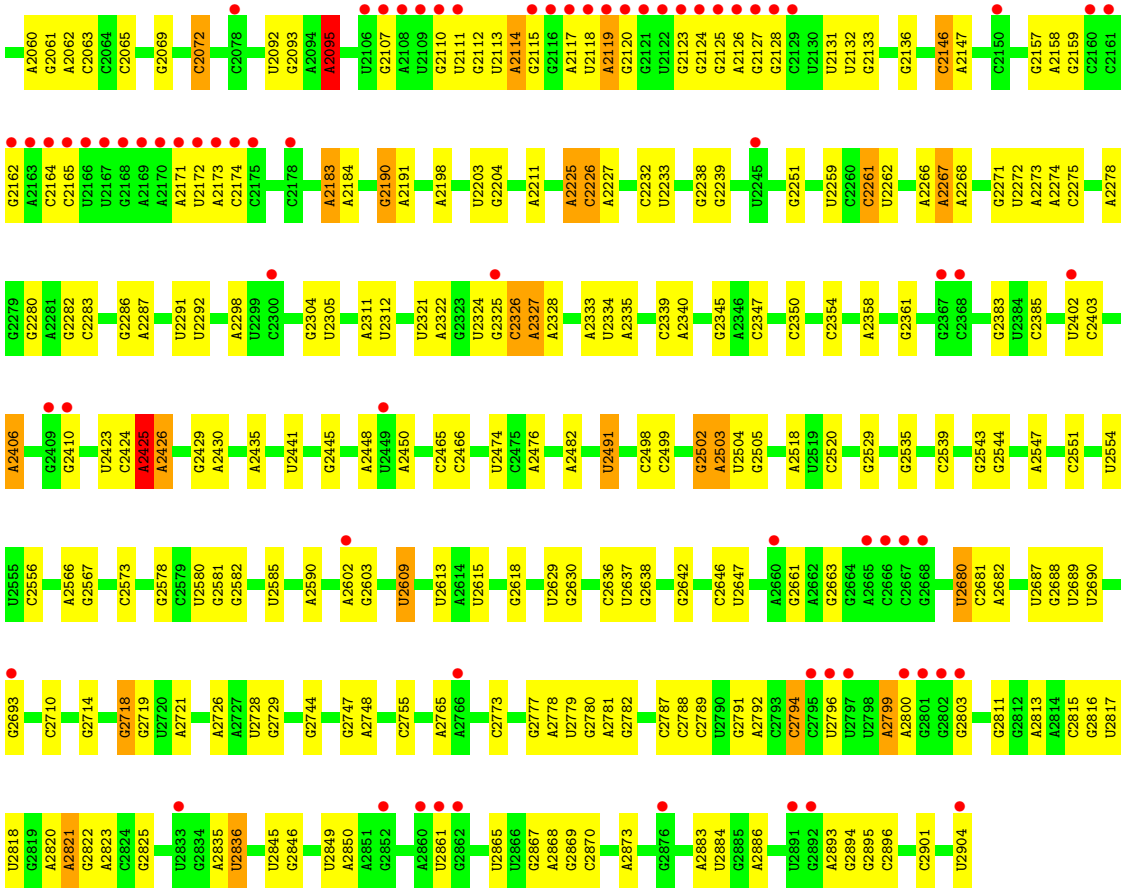
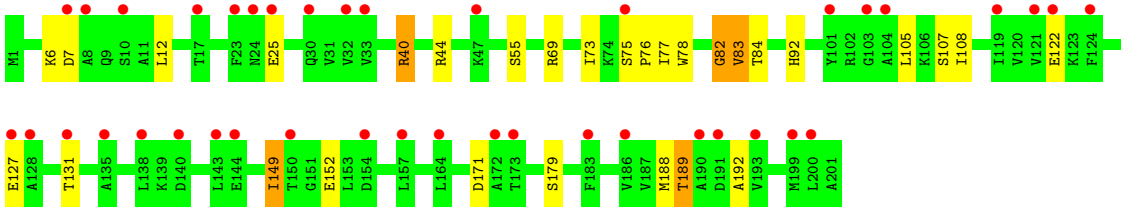


• Molecule 32: 50S ribosomal protein L3

Chain DD:

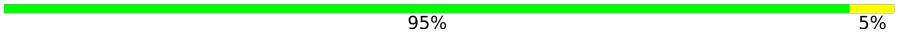
• Molecule 33: 50S ribosomal protein L4

Chain CE:



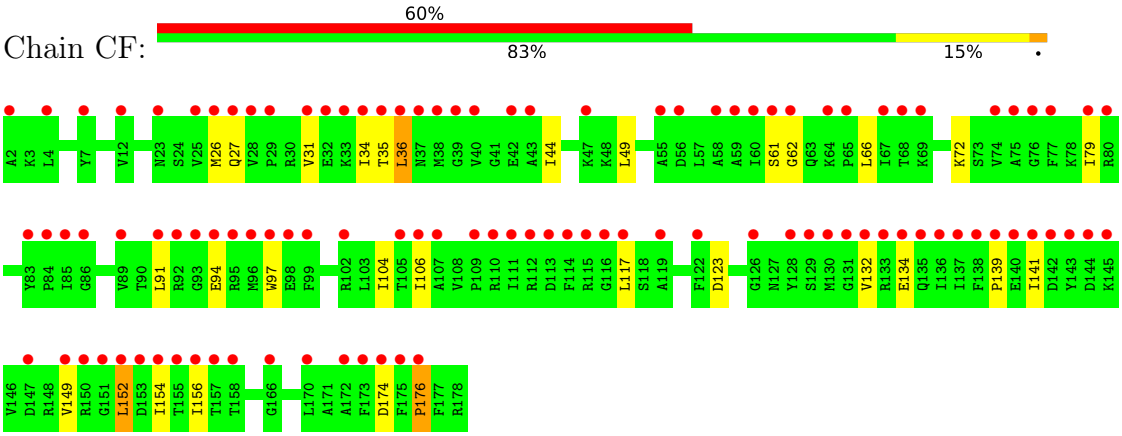
• Molecule 33: 50S ribosomal protein L4

Chain DE:



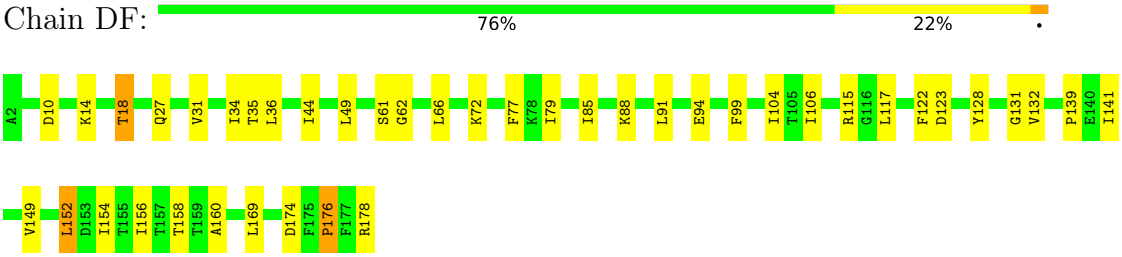
• Molecule 34: 50S ribosomal protein L5

Chain CF:



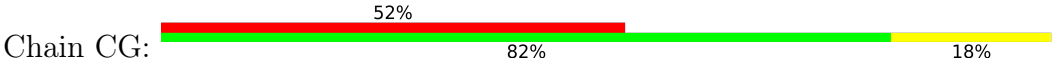
• Molecule 34: 50S ribosomal protein L5

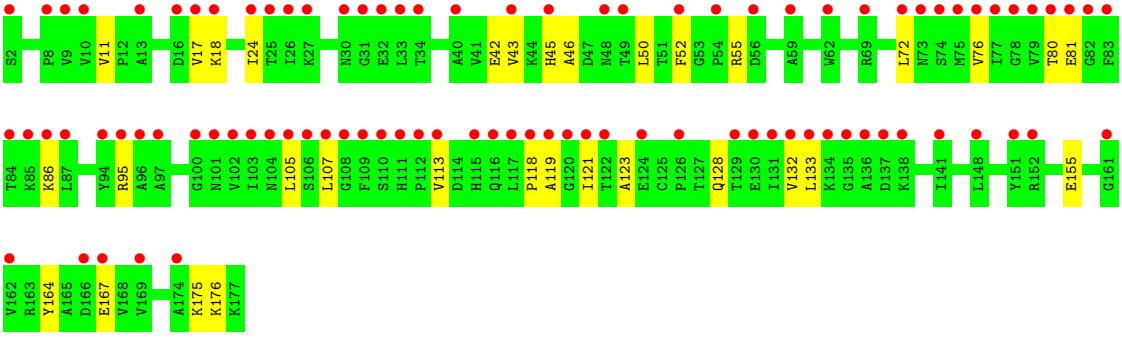
Chain DF:



• Molecule 35: 50S ribosomal protein L6

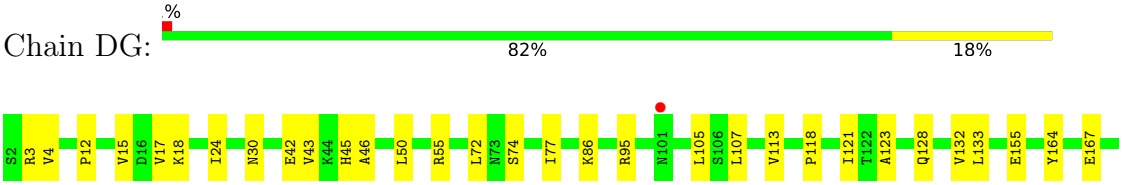
Chain CG:





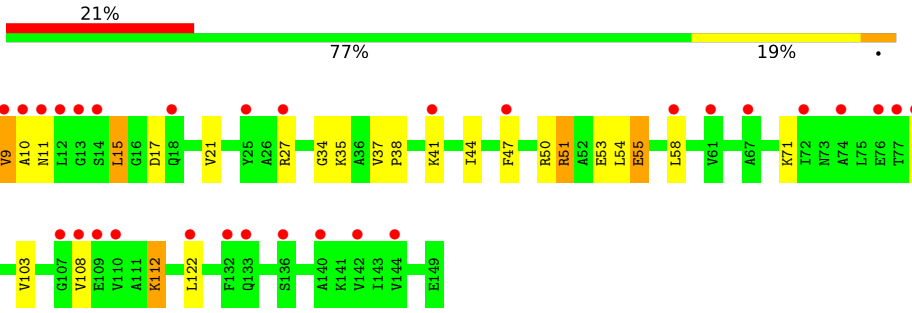
• Molecule 35: 50S ribosomal protein L6

Chain DG:



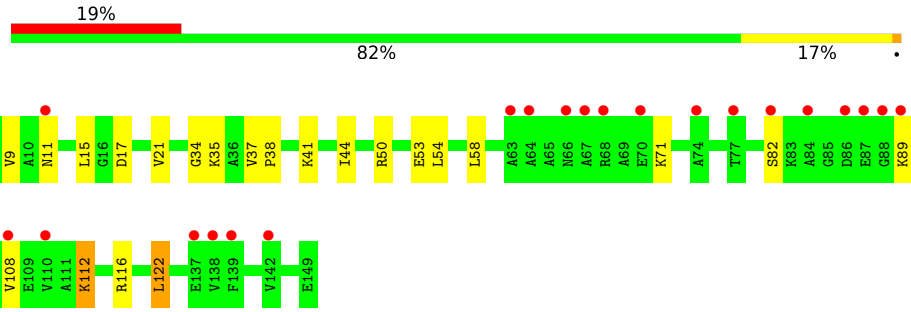
• Molecule 36: 50S ribosomal protein L9

Chain CH:



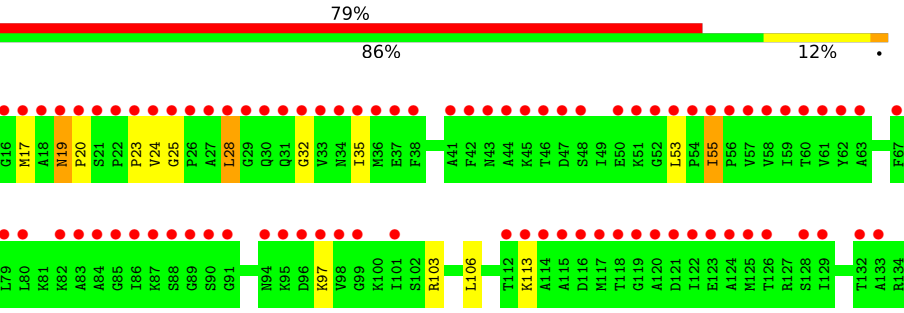
• Molecule 36: 50S ribosomal protein L9

Chain DH:



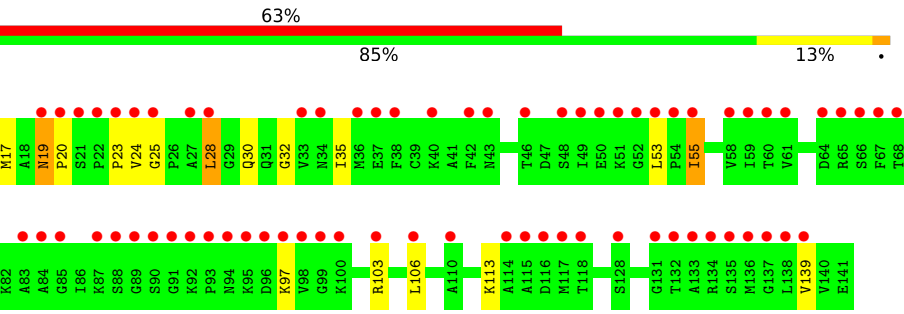
• Molecule 37: 50S ribosomal protein L11

Chain CJ:



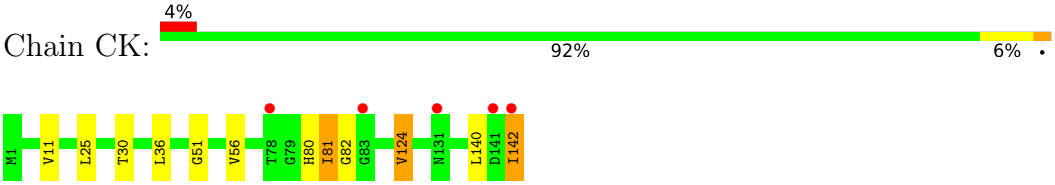
• Molecule 37: 50S ribosomal protein L11

Chain DJ:



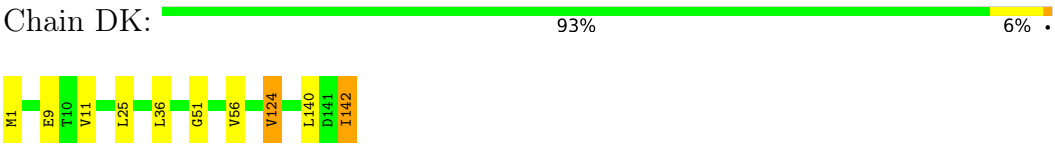
• Molecule 38: 50S ribosomal protein L13

Chain CK:



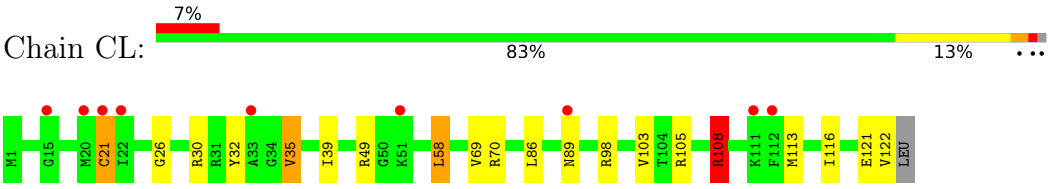
• Molecule 38: 50S ribosomal protein L13

Chain DK:



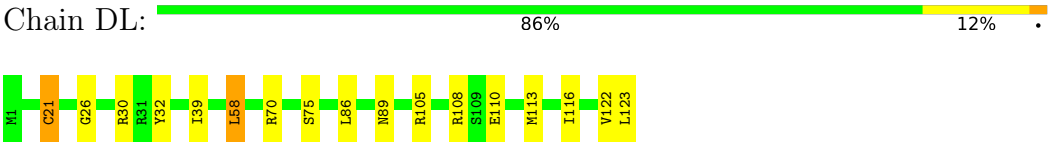
• Molecule 39: 50S ribosomal protein L14

Chain CL:



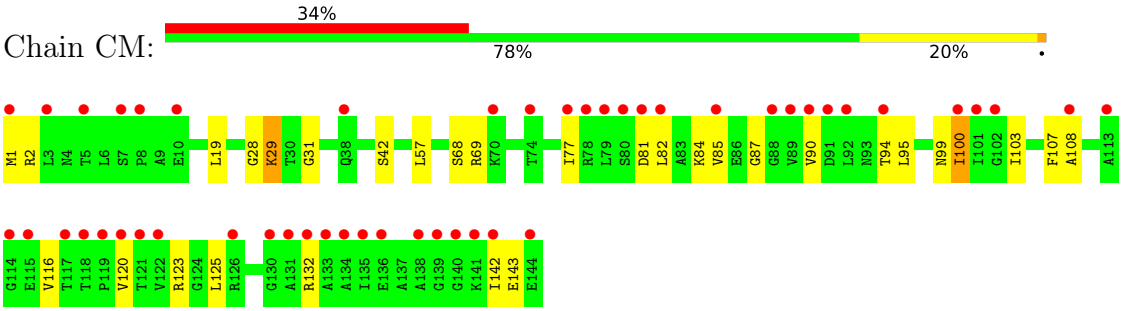
• Molecule 39: 50S ribosomal protein L14

Chain DL:



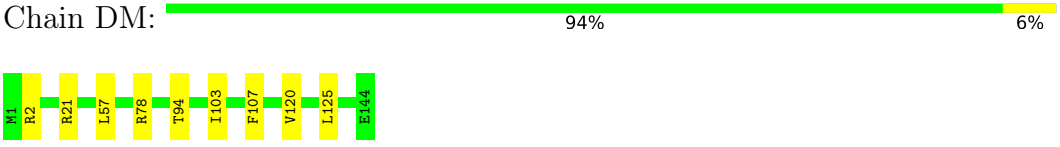
• Molecule 40: 50S ribosomal protein L15

Chain CM:



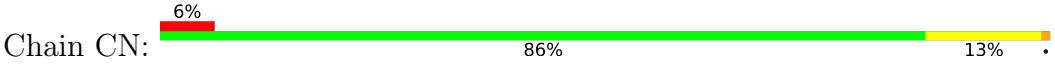
• Molecule 40: 50S ribosomal protein L15

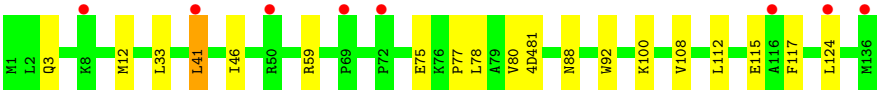
Chain DM:



• Molecule 41: 50S ribosomal protein L16

Chain CN:



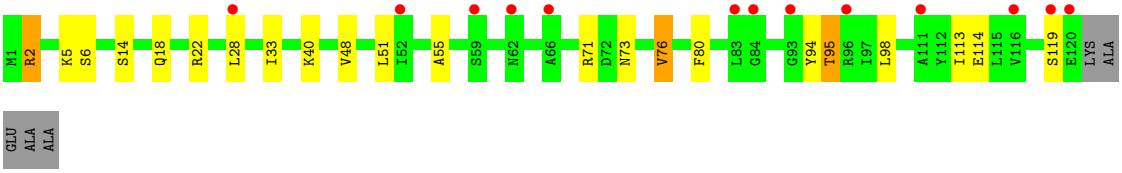


• Molecule 41: 50S ribosomal protein L16

Chain DN:

• Molecule 42: 50S ribosomal protein L17

Chain CO:

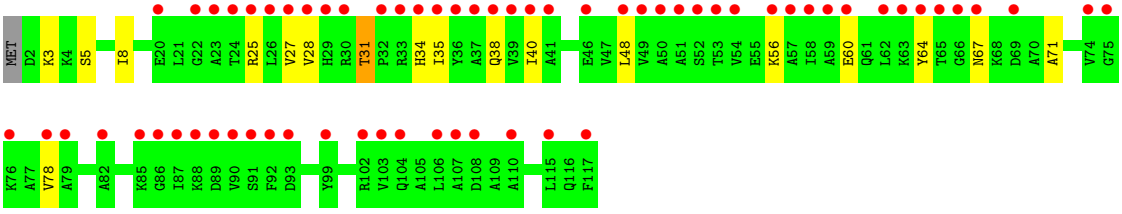


• Molecule 42: 50S ribosomal protein L17

Chain DO:

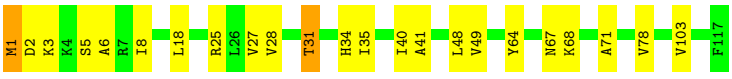
• Molecule 43: 50S ribosomal protein L18

Chain CP:



• Molecule 43: 50S ribosomal protein L18

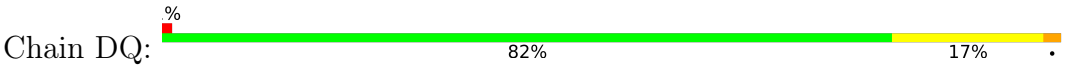
Chain DP:

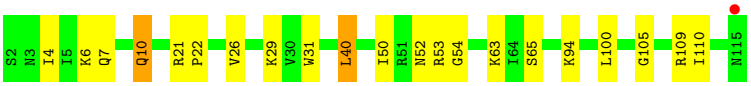


• Molecule 44: 50S ribosomal protein L19

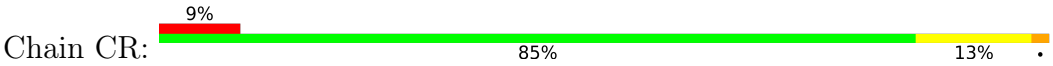
Chain CQ:

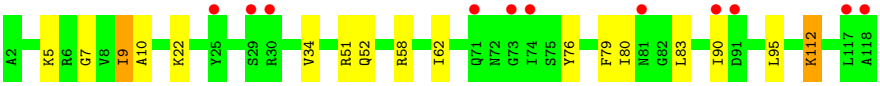
• Molecule 44: 50S ribosomal protein L19



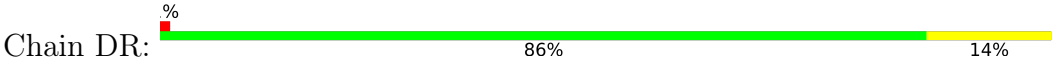


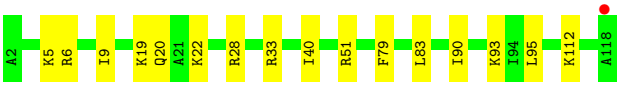
• Molecule 45: 50S ribosomal protein L20



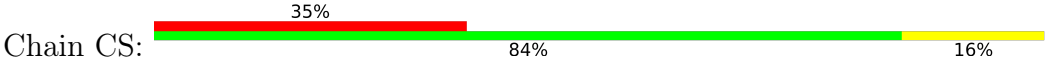


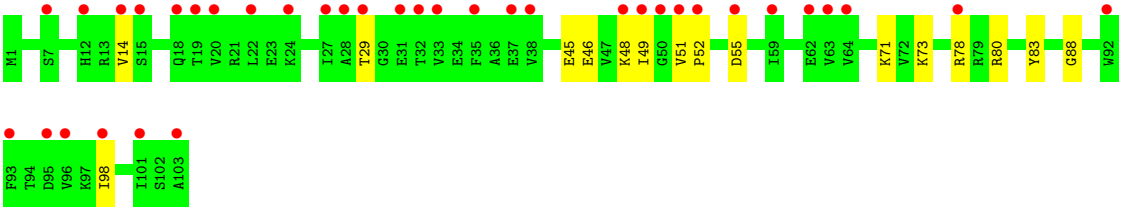
• Molecule 45: 50S ribosomal protein L20



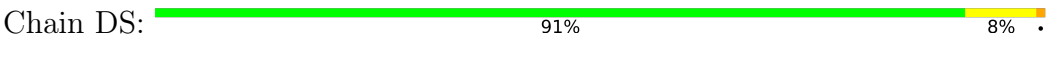


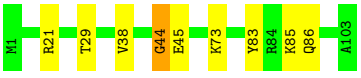
• Molecule 46: 50S ribosomal protein L21



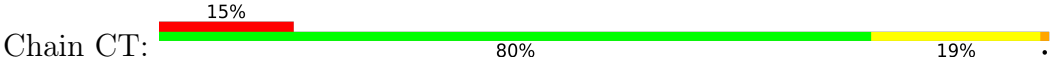


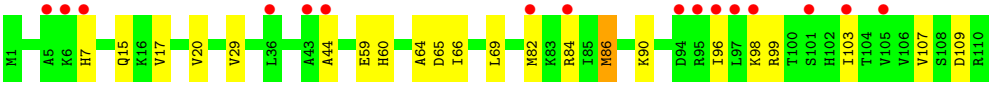
• Molecule 46: 50S ribosomal protein L21





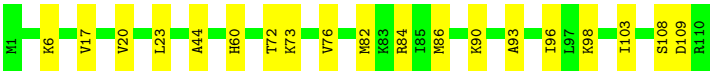
• Molecule 47: 50S ribosomal protein L22





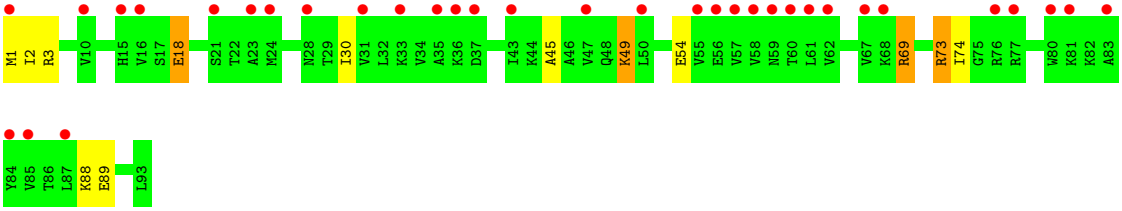
• Molecule 47: 50S ribosomal protein L22

Chain DT:



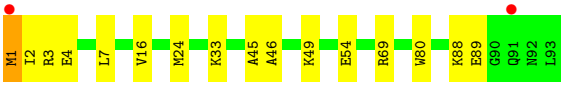
• Molecule 48: 50S ribosomal protein L23

Chain CU:



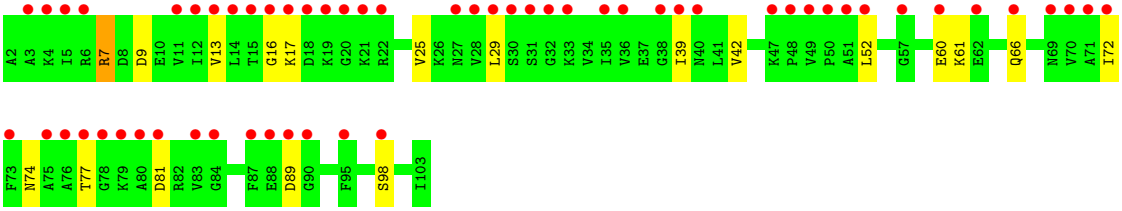
• Molecule 48: 50S ribosomal protein L23

Chain DU:



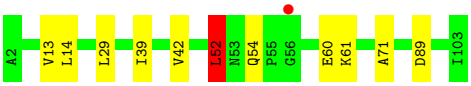
• Molecule 49: 50S ribosomal protein L24

Chain CV:



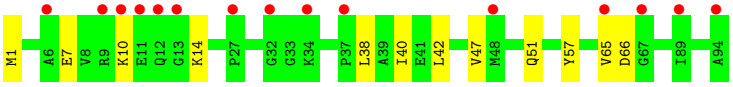
• Molecule 49: 50S ribosomal protein L24

Chain DV:

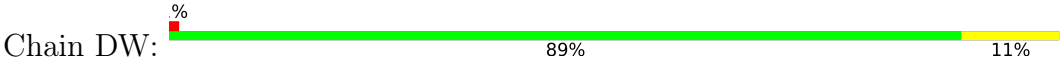


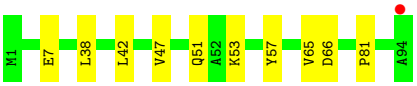
• Molecule 50: 50S ribosomal protein L25

Chain CW:

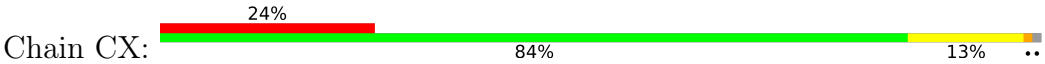


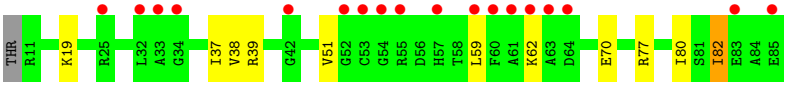
• Molecule 50: 50S ribosomal protein L25



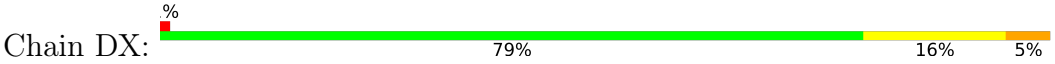


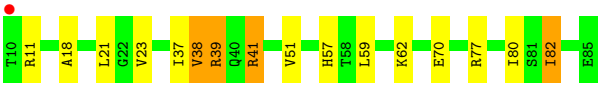
• Molecule 51: 50S ribosomal protein L27



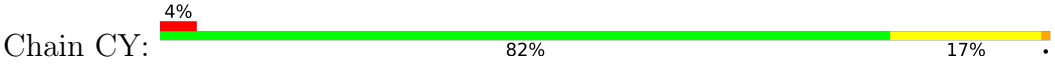


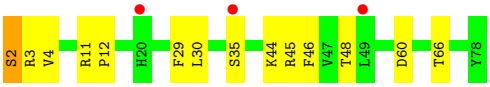
• Molecule 51: 50S ribosomal protein L27



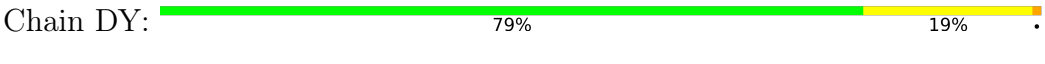


• Molecule 52: 50S ribosomal protein L28

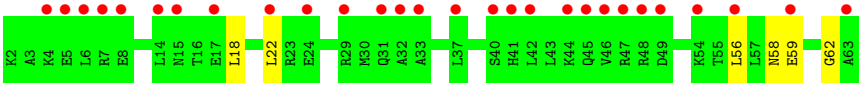




• Molecule 52: 50S ribosomal protein L28

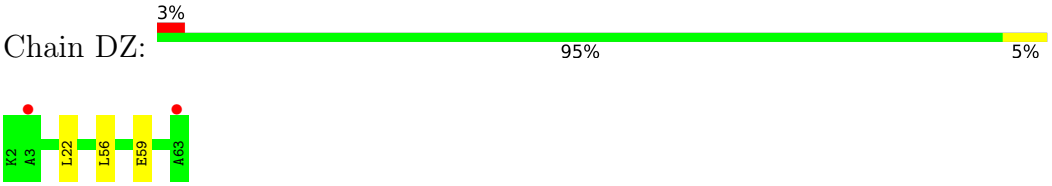


• Molecule 53: 50S ribosomal protein L29



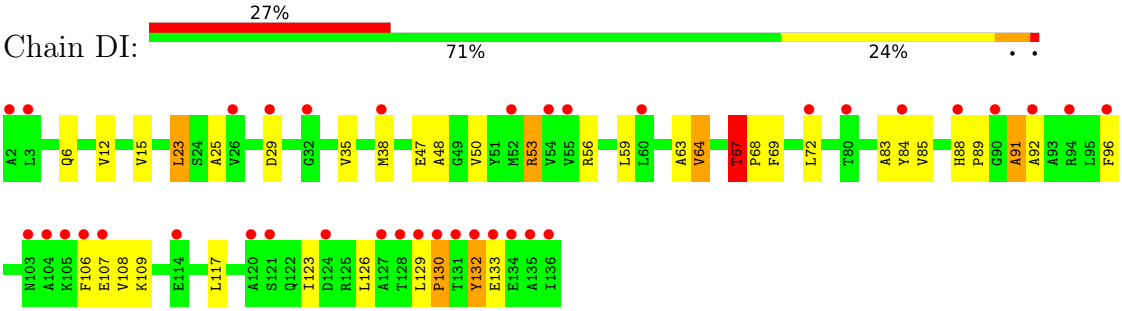
• Molecule 53: 50S ribosomal protein L29

Chain DZ:



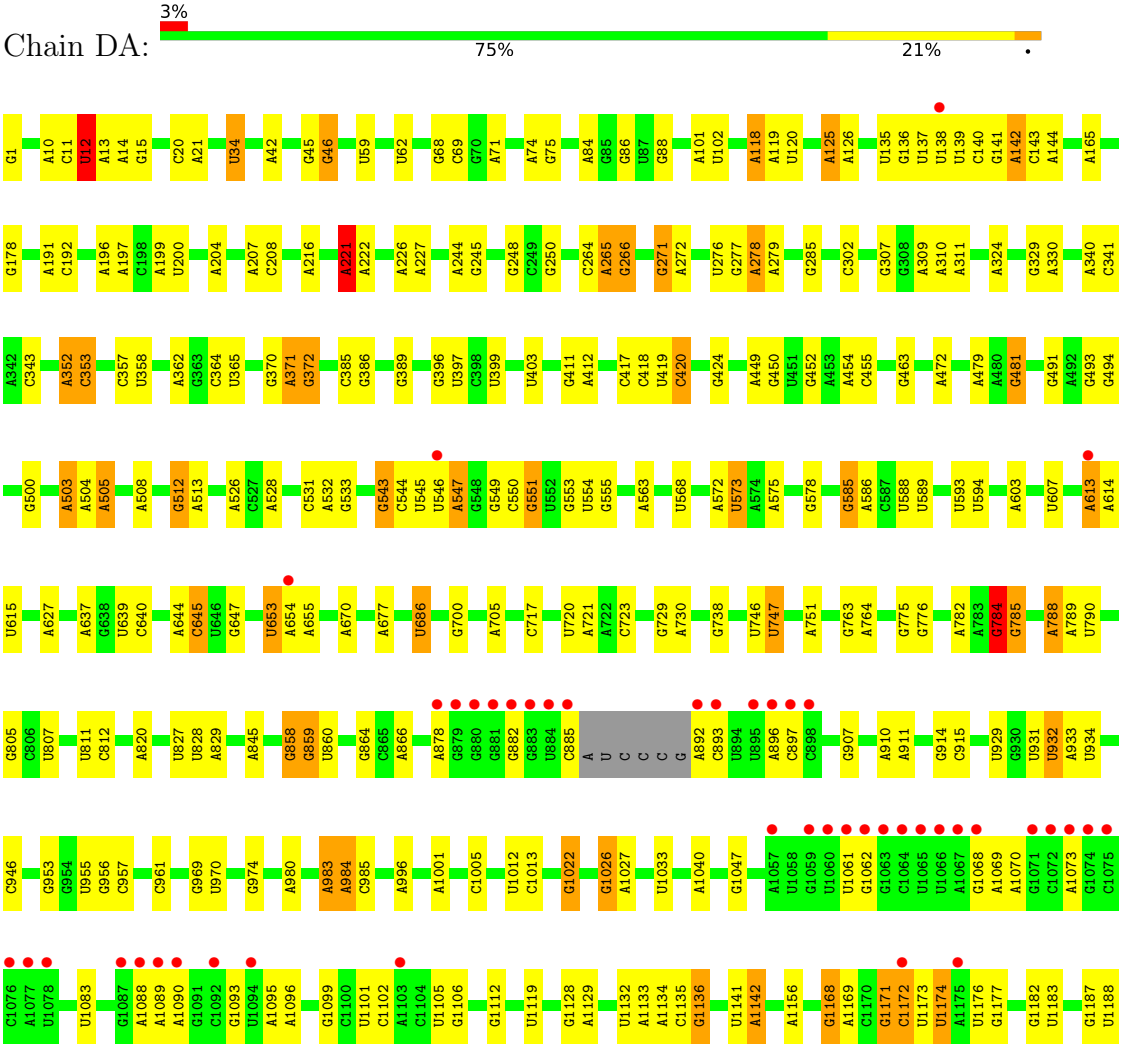
• Molecule 54: 50S ribosomal protein L10

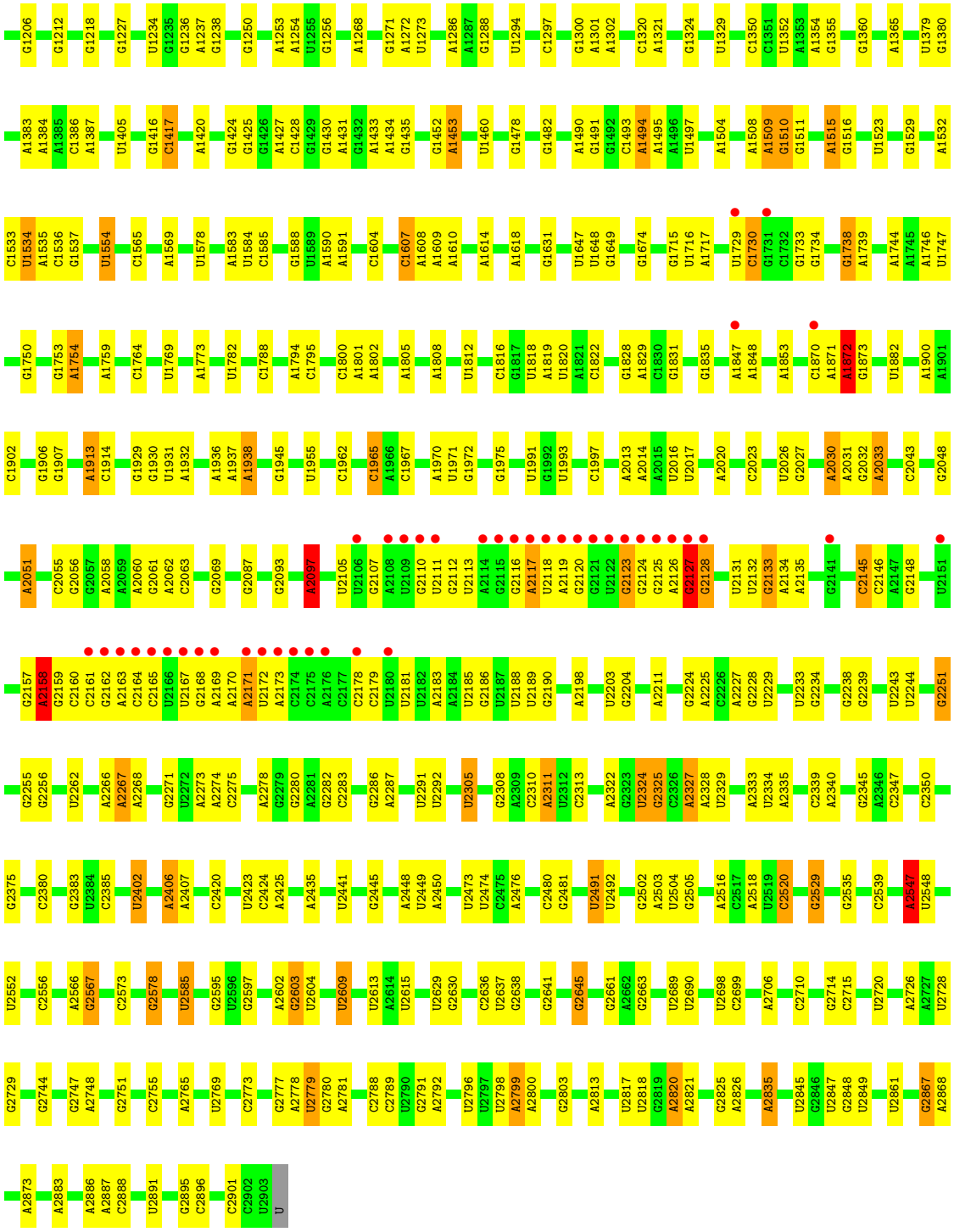
Chain DI:



• Molecule 55: 23S rRNA

Chain DA:




G1206 G1212 G1218 G1227 U1234 G1235 G1236 A1237 G1238 G1250 A1253 A1254 U1255 G1256 A1268 G1271 A1272 U1273 A1286 A1287 G1288 U1294 C1297 G1300 A1301 A1302 C1320 A1321 G1324 U1329 C1350 C1351 U1352 A1353 A1354 G1355 G1360 A1365 U1379 G1380
A1383 A1384 A1385 C1386 A1387 U1405 G1416 C1417 A1420 G1424 G1425 G1426 A1427 C1428 G1429 G1430 A1431 G1432 A1433 A1434 G1435 G1452 A1453 U1460 G1478 G1482 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 A1504 A1508 A1509 G1510 G1511 A1515 G1516 U1523 G1529 A1532
C1533 U1534 A1535 C1536 G1537 U1584 C1565 A1569 U1578 A1583 U1584 C1585 G1588 U1589 A1590 A1591 C1604 C1607 A1608 A1609 A1610 A1614 A1618 G1631 U1647 U1648 G1649 G1674 G1715 U1716 A1717 U1729 C1730 G1731 C1732 G1733 G1734 G1738 A1739 A1744 A1745 A1746 U1747
G1750 G1753 A1754 A1759 C1764 U1769 A1773 U1782 C1788 A1794 C1795 C1800 A1801 A1802 A1805 A1808 U1812 C1816 G1817 U1818 A1819 U1820 A1821 C1822 G1828 A1829 C1830 G1831 G1835 A1847 A1848 A1853 C1870 A1871 A1872 G1873 U1882 A1900 A1901
C1902 G1906 G1907 A1913 C1914 G1929 G1930 U1931 A1932 A1936 A1937 A1938 G1945 U1955 C1962 C1965 A1966 C1967 A1970 U1971 G1972 G1975 U1991 G1992 U1993 C1997 A2013 A2014 A2015 U2016 U2017 A2020 C2023 U2026 G2027 A2030 A2031 G2032 A2033 C2043 G2048
A2051 C2055 G2056 G2057 A2058 A2059 A2060 G2061 A2062 C2063 G2069 G2087 G2093 A2097 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 U2131 U2132 G2133 A2134 A2135 G2141 C2145 C2146 A2147 G2148 U2151
G2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 U2181 U2182 A2183 A2184 U2185 G2186 U2187 U2188 U2189 G2190 A2198 U2203 G2204 A2211 G2224 A2225 C2226 A2227 G2228 U2229 U2233 G2234 G2238 G2239 U2243 U2244 G2251
G2255 G2256 U2262 A2266 A2267 A2268 G2271 U2272 A2273 A2274 C2275 A2278 G2279 G2280 A2281 G2282 C2283 G2286 A2287 U2291 U2292 U2305 G2308 A2309 C2310 A2311 U2312 C2313 A2322 G2323 U2324 G2325 C2326 A2327 A2328 U2329 A2333 U2334 A2335 C2339 A2340 G2345 A2346 C2347 C2350
G2375 C2380 G2383 U2384 C2385 U2402 A2406 A2407 C2420 U2423 C2424 A2425 A2435 U2441 G2445 A2448 U2449 A2450 U2473 U2474 C2475 A2476 C2480 G2481 U2491 U2492 G2502 A2503 U2504 G2505 A2516 C2517 A2518 U2519 C2520 G2529 G2535 C2539 A2547 U2548
U2552 C2556 A2566 G2567 C2573 G2578 U2585 G2595 U2596 G2597 A2602 G2603 U2604 U2609 U2613 A2614 U2615 U2629 G2630 C2636 U2637 G2638 G2641 G2645 C2661 A2662 G2663 U2689 U2690 U2698 C2699 A2706 C2710 G2714 C2715 U2720 A2726 A2727 U2728
G2729 G2744 G2747 A2748 G2751 C2755 A2765 U2769 C2773 G2777 A2778 U2779 G2780 A2781 C2788 C2789 U2790 G2791 A2792 U2796 U2797 U2798 A2799 A2800 G2803 A2813 U2817 U2818 G2819 A2820 A2821 G2825 A2826 A2835 U2845 G2846 U2847 C2848 U2849 U2861 G2867 A2868
A2873 A2883 A2886 A2887 C2888 U2891 G2895 C2896 C2901 C2902 U2903 U

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	213.04Å 436.85Å 628.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 3.03 48.02 – 3.03	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.39-3.03) 96.8 (48.02-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 3.01Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, R_{free}	0.172 , 0.200 0.186 , 0.215	Depositor DCC
R_{free} test set	4333 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å^2)	60.4	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 92.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	295130	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

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

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	3
1	BA	0	1
20	AT	0	1

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

All (129) bond length outliers are listed below:

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

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

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

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

All (47) bond angle outliers are listed below:

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

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

There are no chirality outliers.

All (45) planarity outliers are listed below:

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

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

5.2 Too-close contacts (i)

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

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

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	DT	857	0	922	11	0
48	CU	739	0	807	5	0
48	DU	739	0	807	7	0
49	CV	780	0	831	6	0
49	DV	780	0	831	4	0
50	CW	753	0	780	4	0
50	DW	753	0	780	4	0
51	CX	569	0	581	4	0
51	DX	591	0	606	10	0
52	CY	625	0	652	8	0
52	DY	625	0	652	8	0
53	CZ	501	0	531	1	0
53	DZ	501	0	531	1	0
54	DI	1023	0	1052	19	0
55	DA	62423	0	31411	199	0
56	AA	71	0	0	0	0
56	BA	43	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	184	0	0	0	0
56	DB	9	0	0	0	0
56	DD	1	0	0	0	0
56	DM	1	0	0	0	0
56	DR	1	0	0	0	0
57	AA	13	0	18	1	0
57	BA	13	0	18	1	0
57	DA	26	0	36	2	0
57	DQ	13	0	18	1	0
57	DR	13	0	18	3	0
57	DS	13	0	18	1	0
58	AA	16	0	28	2	0
58	DA	48	0	84	4	0
58	DE	16	0	28	0	0
58	DK	8	0	14	0	0
58	DN	8	0	14	0	0
58	DS	8	0	14	3	0
58	DT	8	0	14	0	0
59	AA	24	0	48	0	0
59	DA	66	0	132	4	0
59	DM	6	0	12	0	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D1	7	0	10	1	0
61	D3	7	0	10	2	0
61	DA	35	0	50	0	0
61	DL	7	0	10	0	0
61	DP	7	0	10	1	0
61	DQ	7	0	10	1	0
62	D1	4	0	6	0	0
62	DA	36	0	54	3	0
62	DB	8	0	12	1	0
63	D1	10	0	14	3	0
63	D3	10	0	14	0	0
63	DA	40	0	56	4	0
63	DD	10	0	14	0	0
63	DS	10	0	14	0	0
63	DU	10	0	14	1	0
64	DA	40	0	76	2	0
65	DA	32	0	44	1	0
66	DA	12	0	9	0	0
67	DA	11	0	5	0	0
68	DA	8	0	12	2	0
69	AA	508	0	0	1	0
69	AC	5	0	0	0	0
69	AD	1	0	0	0	0
69	AE	5	0	0	0	0
69	AF	1	0	0	0	0
69	AG	1	0	0	0	0
69	AJ	3	0	0	0	0
69	AK	6	0	0	0	0
69	AL	10	0	0	0	0
69	AM	4	0	0	1	0
69	AN	5	0	0	2	0
69	AO	2	0	0	0	0
69	AP	2	0	0	1	0
69	AT	4	0	0	0	0
69	AU	2	0	0	0	0
69	BA	282	0	0	1	0
69	BD	12	0	0	0	0
69	BE	1	0	0	0	0
69	BF	1	0	0	0	0
69	BK	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	BL	6	0	0	0	0
69	BN	2	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	1	0
69	BR	1	0	0	0	0
69	BT	3	0	0	0	0
69	BU	3	0	0	0	0
69	C3	2	0	0	0	0
69	C4	1	0	0	0	0
69	C5	1	0	0	0	0
69	CA	693	0	0	4	0
69	CB	13	0	0	0	0
69	CC	8	0	0	0	0
69	CD	7	0	0	0	0
69	CE	4	0	0	0	0
69	CL	1	0	0	0	0
69	CM	4	0	0	0	0
69	CO	2	0	0	0	0
69	CQ	1	0	0	0	0
69	CU	3	0	0	0	0
69	CV	1	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	26	0	0	0	0
69	D1	46	0	0	1	0
69	D2	6	0	0	0	0
69	D3	28	0	0	1	0
69	D4	33	0	0	0	0
69	D5	11	0	0	0	0
69	DA	4830	0	0	20	0
69	DB	203	0	0	1	0
69	DC	102	0	0	1	0
69	DD	95	0	0	1	0
69	DE	63	0	0	2	0
69	DF	16	0	0	0	0
69	DG	7	0	0	0	0
69	DH	2	0	0	0	0
69	DK	60	0	0	1	0
69	DL	51	0	0	0	0
69	DM	68	0	0	1	0
69	DN	73	0	0	1	0
69	DO	49	0	0	0	0

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DG:42:GLU:HG3	35:DG:55:ARG:HH21	1.66	0.61
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.81	0.61
12:AL:3:THR:HB	12:AL:6:GLN:HB2	1.82	0.61
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.82	0.61
54:DI:15:VAL:HG23	54:DI:53:ARG:HH21	1.66	0.61
31:CA:2226:C:H2'	31:CA:2227:A:O4'	2.01	0.61
38:DK:9:GLU:HG2	69:DA:4873:HOH:O	2.01	0.61
38:CK:81:ILE:HG23	38:CK:82:GLY:N	2.16	0.61
55:DA:1105:U:H2'	55:DA:1106:G:C8	2.36	0.61
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.66	0.60
1:BA:841:C:H3'	1:BA:842:U:H5"	1.82	0.60
8:BH:77:ARG:NH1	8:BH:80:ARG:HA	2.16	0.60
31:CA:784:G:H5'	31:CA:785:G:OP1	2.01	0.60
31:CA:910:A:H62	41:CN:12:MET:HA	1.65	0.60
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.36	0.60
28:CB:28:C:OP1	43:CP:31:THR:HG21	2.01	0.60
17:BQ:8:LEU:HD13	17:BQ:73:TRP:CH2	2.37	0.60
31:CA:1936:A:C2	31:CA:1943:U:N3	2.51	0.60
35:CG:42:GLU:HG3	35:CG:55:ARG:HH21	1.67	0.60
49:CV:74:ASN:HD22	49:CV:77:THR:H	1.49	0.60
55:DA:2751:G:H2'	69:DA:4610:HOH:O	2.01	0.60
28:CB:89:U:C6	31:CA:958:U:H2'	2.37	0.60
31:CA:528:A:H2	31:CA:2043:C:H4'	1.66	0.60
36:CH:41:LYS:HA	36:CH:44:ILE:HG12	1.84	0.60
1:AA:1518:MA6:H103	1:AA:1519:MA6:C10	2.32	0.60
14:BN:31:ILE:HG23	14:BN:42:TRP:HZ2	1.66	0.60
31:CA:2573:C:H5	69:CA:3275:HOH:O	1.84	0.60
42:CO:33:ILE:HD12	42:CO:114:GLU:HB3	1.83	0.60
42:DO:33:ILE:HD12	42:DO:114:GLU:HB3	1.83	0.59
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.82	0.59
44:DQ:6:LYS:O	44:DQ:10:GLN:HG2	2.02	0.59
5:AE:90:THR:HG22	5:AE:91:GLY:H	1.67	0.59
29:CC:219:THR:O	31:CA:1789:A:H5"	2.02	0.59
31:CA:2065:C:H4'	31:CA:2251:OMG:HM22	1.85	0.59
41:DN:42:THR:HG22	41:DN:93:VAL:HG12	1.85	0.59
49:DV:52:LEU:HB3	49:DV:54:GLN:HB2	1.84	0.59
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.84	0.59
34:CF:31:VAL:HG11	34:CF:97:TRP:CH2	2.38	0.59
38:DK:56:VAL:HB	38:DK:124:VAL:HB	1.85	0.59
42:DO:73:ASN:HA	42:DO:76:VAL:HG13	1.84	0.59
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:CH:27:ARG:HH11	52:CY:60:ASP:HA	1.68	0.59
39:CL:103:VAL:O	39:CL:122:VAL:HB	2.02	0.59
36:DH:41:LYS:HA	36:DH:44:ILE:HG12	1.84	0.59
45:DR:6:ARG:NH1	55:DA:585:G:N7	2.50	0.59
5:AE:16:ILE:HD13	5:AE:137:VAL:HG11	1.84	0.59
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.68	0.59
5:BE:90:THR:HG22	5:BE:91:GLY:H	1.67	0.59
31:CA:822:G:O6	31:CA:943:A:H2	1.86	0.59
5:BE:16:ILE:HD13	5:BE:137:VAL:HG11	1.85	0.58
22:D1:54:VAL:HG23	22:D1:55:ILE:HG12	1.85	0.58
30:CD:1:MET:HB3	30:CD:205:PRO:HG2	1.84	0.58
34:CF:31:VAL:CG1	34:CF:97:TRP:CH2	2.86	0.58
41:CN:41:LEU:HD22	41:CN:46:ILE:HG13	1.84	0.58
5:AE:76:LEU:HD11	5:AE:120:VAL:HG22	1.85	0.58
32:DD:1:MET:HB3	32:DD:205:PRO:HG2	1.85	0.58
1:BA:202:G:H1	1:BA:215:C:H42	1.51	0.58
5:AE:157:ARG:HD2	8:AH:43:GLU:O	2.03	0.58
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	1.86	0.58
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.84	0.58
25:D4:54:ASP:HB3	40:DM:57:LEU:HD22	1.83	0.58
1:BA:1060:U:C5	3:BC:2:GLY:HA3	2.39	0.58
9:BI:12:ARG:HG3	9:BI:107:ASP:HB3	1.84	0.58
55:DA:2886[A]:A:C2	55:DA:2887[A]:A:H1'	2.39	0.58
1:BA:502:A:OP1	12:BL:115:SER:HB3	2.04	0.58
42:CO:73:ASN:HA	42:CO:76:VAL:HG13	1.85	0.58
52:DY:61:LYS:HD3	55:DA:372:G:H5"	1.86	0.58
41:CN:77:PRO:HG2	41:CN:80:VAL:HG21	1.84	0.58
47:CT:69:LEU:HG	47:CT:107:VAL:HG22	1.85	0.58
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.86	0.58
48:CU:54:GLU:HB3	48:CU:88:LYS:HD2	1.86	0.58
55:DA:11:C:H2'	55:DA:12:U:H5'	1.86	0.58
58:AA:1671:MPD:H31	20:AT:24:ARG:HH12	1.68	0.58
1:BA:923:A:OP1	5:BE:26:LYS:HG2	2.04	0.57
31:CA:396:G:H1'	52:CY:29:PHE:HB3	1.86	0.57
44:CQ:114:LEU:H	44:CQ:114:LEU:CD2	2.17	0.57
51:DX:59:LEU:HD12	51:DX:80:ILE:HD12	1.86	0.57
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	1.87	0.57
31:CA:118:A:N3	31:CA:178:G:H1'	2.19	0.57
55:DA:551:G:H8	55:DA:551:G:H5"	1.69	0.57
9:AI:12:ARG:HG3	9:AI:107:ASP:HB3	1.86	0.57
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:774:G:H21	57:AA:1670:PG4:H51	1.69	0.57
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.85	0.57
31:CA:783:A:H4'	31:CA:1779:U:O2	2.05	0.57
38:CK:56:VAL:HB	38:CK:124:VAL:HB	1.85	0.57
19:AS:32:ARG:HE	19:AS:57:HIS:CE1	2.23	0.57
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.85	0.57
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	1.86	0.57
36:CH:82:SER:HB2	36:CH:94:ILE:HD11	1.85	0.57
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.86	0.57
1:BA:1397:C:O2	1:BA:1397:C:H2'	2.05	0.57
13:BM:90:ARG:HD3	13:BM:97:VAL:HA	1.87	0.57
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.85	0.57
28:DB:85:G:H1'	62:DB:211:EDO:H11	1.87	0.57
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.40	0.57
31:CA:2796:U:H3	31:CA:2799:A:N6	1.97	0.57
44:CQ:6:LYS:O	44:CQ:10:GLN:HG2	2.04	0.56
36:DH:82:SER:HB2	36:DH:94:ILE:HD11	1.86	0.56
1:AA:677:U:H3	1:AA:713:G:H22	1.53	0.56
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.40	0.56
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.39	0.56
12:BL:65:SER:CB	12:BL:82:ILE:HD11	2.30	0.56
13:AM:90:ARG:HD3	13:AM:97:VAL:HA	1.86	0.56
23:C2:37:LYS:HG2	23:C2:48:ILE:HG13	1.86	0.56
1:BA:677:U:H3	1:BA:713:G:H22	1.50	0.56
7:BG:22:LEU:HD23	7:BG:62:PHE:HE1	1.70	0.56
1:BA:209:U:H2'	1:BA:209:U:O2	2.04	0.56
1:BA:1106:G:H5"	3:BC:172:ARG:HG3	1.87	0.56
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	1.86	0.56
1:AA:413:G:H5"	1:AA:414:A:H5'	1.88	0.56
37:CJ:19:ASN:H	37:CJ:20:PRO:HD2	1.71	0.56
39:CL:58:LEU:HD11	39:CL:86:LEU:HD13	1.87	0.56
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.87	0.56
35:CG:80:THR:HG23	35:CG:81:GLU:H	1.69	0.56
51:CX:37:ILE:HG21	51:CX:80:ILE:HG21	1.87	0.56
54:DI:50:VAL:HG11	54:DI:92:ALA:HB2	1.87	0.56
54:DI:132:TYR:H	54:DI:133:GLU:HB2	1.70	0.56
1:BA:706:A:O2'	11:BK:31:ILE:HD11	2.06	0.56
8:BH:105:SER:HB2	8:BH:126:ILE:HD11	1.87	0.56
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	1.88	0.56
41:CN:41:LEU:HD21	41:CN:124:LEU:HD22	1.88	0.56
1:AA:202:G:H1	1:AA:215:C:H42	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:502:A:OP1	12:AL:115:SER:HB3	2.06	0.56
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.40	0.56
1:BA:774:G:H21	57:BA:1642:PG4:H62	1.71	0.56
4:BD:197:GLU:HA	4:BD:200:ILE:HD12	1.88	0.56
1:BA:1219:A:H2'	1:BA:1220:G:C8	2.41	0.55
31:CA:528:A:H2'	31:CA:529:A:H5"	1.87	0.55
31:CA:1509:A:HO2'	31:CA:1510:G:H8	1.53	0.55
55:DA:1831:G:H1'	63:DA:3227:PGE:H1	1.88	0.55
4:AD:197:GLU:HA	4:AD:200:ILE:HD12	1.88	0.55
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.87	0.55
55:DA:1509:A:HO2'	55:DA:1510:G:H8	1.53	0.55
29:CC:17:VAL:HB	29:CC:204:VAL:HG13	1.88	0.55
45:CR:9:ILE:HG13	45:CR:10:ALA:N	2.22	0.55
55:DA:788:A:H5"	59:DA:3224:PUT:H12	1.87	0.55
1:BA:518:C:H2'	1:BA:530:G:C8	2.42	0.55
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	1.89	0.55
37:DJ:19:ASN:H	37:DJ:20:PRO:HD2	1.72	0.55
1:BA:1518:MA6:H103	1:BA:1519:MA6:C10	2.34	0.55
29:CC:155:ALA:HB2	29:CC:162:VAL:HG23	1.89	0.55
44:DQ:54:GLY:HA3	61:DQ:201:PEG:H22	1.88	0.55
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.88	0.55
13:AM:90:ARG:NH2	13:AM:95:LEU:HB3	2.22	0.55
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	1.88	0.55
11:BK:23:ILE:HD11	11:BK:86:VAL:HG13	1.88	0.55
19:BS:29:LYS:HB3	19:BS:30:PRO:HD2	1.89	0.55
20:BT:4:ILE:HA	20:BT:8:LYS:HE2	1.89	0.55
31:CA:751:A:H5'	47:CT:90:LYS:HA	1.89	0.55
32:DD:161:MET:HG2	69:DA:5697:HOH:O	2.07	0.55
24:D3:12:ARG:HD3	69:DA:7002:HOH:O	2.07	0.54
51:CX:59:LEU:HD12	51:CX:80:ILE:HD12	1.88	0.54
31:CA:551:G:H5"	31:CA:551:G:H8	1.71	0.54
39:DL:58:LEU:HD11	39:DL:86:LEU:HD13	1.89	0.54
48:DU:54:GLU:HB3	48:DU:88:LYS:HD2	1.90	0.54
51:DX:37:ILE:HG21	51:DX:80:ILE:HG21	1.88	0.54
1:BA:1356:G:H2'	1:BA:1357:A:C8	2.42	0.54
31:CA:1991:U:H2'	31:CA:1992:G:H5"	1.90	0.54
40:CM:28:GLY:O	40:CM:29:LYS:O	2.25	0.54
45:CR:58:ARG:NH1	45:CR:62:ILE:HD11	2.23	0.54
1:AA:1219:A:H2'	1:AA:1220:G:C8	2.43	0.54
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.43	0.54
55:DA:1417:C:H5'	55:DA:1588:G:H1'	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:1424:G:H21	63:DA:3216:PGE:H32	1.72	0.54
1:AA:1239:A:H62	1:AA:1299:A:H62	1.55	0.54
3:AC:23:PHE:CD1	3:AC:23:PHE:C	2.81	0.54
1:BA:12:U:H4'	1:BA:526:C:H4'	1.89	0.54
31:CA:2190:G:H2'	31:CA:2191:A:H8	1.71	0.54
55:DA:686:U:H2'	55:DA:788:A:N1	2.22	0.54
55:DA:2796:U:H3	55:DA:2799:A:N6	1.96	0.54
31:CA:686:U:H2'	31:CA:788:A:N1	2.22	0.54
31:CA:1131:G:OP1	38:CK:82:GLY:HA2	2.08	0.54
46:DS:85:LYS:HE3	69:DA:6504:HOH:O	2.08	0.54
9:AI:79:ILE:HG22	9:AI:83:ILE:HD11	1.90	0.54
31:CA:2502:G:H5"	31:CA:2503:2MA:H5"	1.89	0.54
42:CO:95:THR:HG21	42:CO:113:ILE:HD11	1.89	0.54
3:AC:33:LEU:HD21	14:AN:93:ILE:HG12	1.90	0.54
10:BJ:26:VAL:HG21	10:BJ:39:PRO:HD3	1.90	0.54
23:D2:6:ARG:HG2	23:D2:24:THR:HB	1.90	0.54
55:DA:2030:6MZ:H8	69:DA:6158:HOH:O	2.08	0.54
12:BL:80:ILE:HD13	12:BL:97:THR:HG22	1.91	0.53
3:AC:7:PRO:HD2	3:AC:184:TYR:CD1	2.43	0.53
2:BB:31:ILE:HG21	2:BB:39:HIS:HD2	1.74	0.53
29:CC:208:ALA:HB2	31:CA:1790:C:O2'	2.08	0.53
30:CD:133:THR:CG2	31:CA:1993:U:H4'	2.36	0.53
47:DT:17:VAL:HG11	47:DT:103:ILE:HG12	1.89	0.53
1:AA:542:G:H5'	4:AD:39:GLY:HA3	1.90	0.53
13:BM:90:ARG:NH2	13:BM:95:LEU:HB3	2.23	0.53
19:AS:29:LYS:HB3	19:AS:30:PRO:HD2	1.90	0.53
20:AT:48:GLN:HE21	20:AT:52:ASN:ND2	2.05	0.53
3:BC:43:LEU:HD13	3:BC:55:ILE:HD11	1.91	0.53
47:CT:17:VAL:HG11	47:CT:103:ILE:HG12	1.89	0.53
31:CA:2718:G:OP1	44:CQ:98:TYR:HD2	1.92	0.53
11:AK:25:ALA:HA	11:AK:30:THR:HG22	1.90	0.53
14:BN:13:ARG:HB3	14:BN:60:GLN:HG2	1.91	0.53
34:DF:132:VAL:HG22	34:DF:152:LEU:HG	1.90	0.53
1:AA:518:C:H2'	1:AA:530:G:C8	2.44	0.53
2:AB:188:ASP:HB2	2:AB:204:ASP:OD2	2.07	0.53
42:CO:2:ARG:HA	42:CO:5:LYS:HD2	1.91	0.53
11:BK:16:VAL:HG13	11:BK:79:ILE:HG13	1.89	0.53
54:DI:48:ALA:HB1	54:DI:91:ALA:HB1	1.90	0.53
34:CF:36:LEU:HD21	34:CF:91:LEU:HD11	1.91	0.53
48:CU:69:ARG:HB2	48:CU:74:ILE:HG22	1.91	0.53
44:DQ:53:ARG:HG2	44:DQ:53:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:526:A:H2'	69:DA:3655:HOH:O	2.07	0.52
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.73	0.52
1:BA:1108:G:H5"	3:BC:176:HIS:ND1	2.25	0.52
2:BB:188:ASP:HB2	2:BB:204:ASP:OD2	2.08	0.52
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.74	0.52
29:DC:155:ALA:HB2	29:DC:162:VAL:HG23	1.92	0.52
40:CM:82:LEU:HD11	40:CM:116:VAL:CG2	2.37	0.52
55:DA:62:U:O4'	58:DA:3206:MPD:H31	2.09	0.52
55:DA:118:A:N3	55:DA:178:G:H1'	2.24	0.52
1:BA:542:G:H5'	4:BD:39:GLY:HA3	1.91	0.52
5:BE:40:GLY:HA2	5:BE:45:ARG:O	2.09	0.52
31:CA:1268:A:H2'	31:CA:1269:A:O4'	2.10	0.52
1:AA:209:U:H4'	1:AA:210:C:OP2	2.09	0.52
1:AA:1052:G:H22	1:AA:1206:G:H1	1.56	0.52
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	1.92	0.52
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.90	0.52
24:D3:29:GLN:HB3	61:D3:102:PEG:H32	1.91	0.52
55:DA:2255:G:H21	68:DA:3222:TRS:H12	1.73	0.52
1:BA:1239:A:H62	1:BA:1299:A:H62	1.56	0.52
31:CA:528:A:H8	31:CA:528:A:H3'	1.75	0.52
31:CA:2788:C:H2'	31:CA:2789:C:C6	2.44	0.52
46:DS:83:TYR:CE1	55:DA:1187:G:H5"	2.45	0.52
47:DT:93:ALA:HB2	55:DA:1614:A:C2	2.44	0.52
1:AA:131:A:H2'	1:AA:132:C:C6	2.45	0.52
14:AN:13:ARG:HB3	14:AN:60:GLN:HG2	1.91	0.52
29:CC:266:PHE:CD1	29:CC:266:PHE:N	2.77	0.52
37:DJ:24:VAL:HG22	37:DJ:28:LEU:HD22	1.92	0.52
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.92	0.52
11:BK:25:ALA:HA	11:BK:30:THR:HG22	1.89	0.52
11:BK:67:ALA:HB2	11:BK:96:THR:HG23	1.92	0.52
23:D2:8:LYS:HE2	55:DA:2420:C:H5"	1.90	0.52
16:BP:21:VAL:HG12	16:BP:33:ILE:HD12	1.92	0.52
31:CA:1936:A:H62	31:CA:1963:U:H3	1.57	0.52
36:CH:9:VAL:HG22	36:CH:35:LYS:HD3	1.91	0.52
34:DF:36:LEU:CD2	34:DF:154:ILE:HG12	2.40	0.52
1:BA:1277:C:O2'	1:BA:1279:G:H8	1.93	0.52
3:BC:33:LEU:HD21	14:BN:93:ILE:HG12	1.91	0.52
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.45	0.52
32:DD:167:ASN:HD21	62:DA:3201:EDO:H11	1.73	0.52
35:CG:17:VAL:HG11	35:CG:50:LEU:HD21	1.92	0.52
37:CJ:97:LYS:HE2	37:CJ:139:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2788:C:H2'	55:DA:2789:C:C6	2.45	0.52
2:AB:111:ILE:HD12	2:AB:152:LYS:HA	1.92	0.52
11:AK:23:ILE:HD11	11:AK:86:VAL:HG13	1.90	0.52
23:C2:6:ARG:HG2	23:C2:24:THR:HB	1.90	0.52
1:BA:209:U:H4'	1:BA:210:C:OP2	2.10	0.52
9:BI:79:ILE:HG22	9:BI:83:ILE:HD11	1.91	0.52
29:CC:50:THR:O	31:CA:1805:A:H1'	2.10	0.52
31:CA:566:U:O4	46:CS:80:ARG:HD3	2.09	0.52
34:DF:122:PHE:CE1	34:DF:128:TYR:HB2	2.45	0.52
34:DF:131:GLY:HA3	55:DA:2305:U:H5"	1.92	0.52
5:AE:106:ILE:HD11	5:AE:124:LEU:HD23	1.91	0.51
1:BA:131:A:H2'	1:BA:132:C:C6	2.46	0.51
22:D1:26:THR:HG23	55:DA:2887[B]:A:H2	1.75	0.51
9:BI:7:TYR:HE1	9:BI:18:ARG:HB2	1.75	0.51
19:BS:6:LYS:HD2	19:BS:7:LYS:H	1.76	0.51
31:CA:781:A:H2'	31:CA:1777:U:O2'	2.10	0.51
53:CZ:56:LEU:HA	53:CZ:59:GLU:HG2	1.92	0.51
35:DG:17:VAL:HG11	35:DG:50:LEU:HD21	1.92	0.51
29:CC:50:THR:HB	31:CA:1805:A:N3	2.25	0.51
35:DG:86:LYS:HG2	35:DG:132:VAL:HG22	1.92	0.51
44:DQ:29:LYS:HB3	44:DQ:40:LEU:HD13	1.92	0.51
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	2.26	0.51
31:CA:2095:A:H8	31:CA:2095:A:H5"	1.74	0.51
39:DL:113:MET:SD	39:DL:116:ILE:HD11	2.51	0.51
53:DZ:56:LEU:HA	53:DZ:59:GLU:HG2	1.93	0.51
9:AI:9:THR:O	9:AI:85:ARG:HD2	2.11	0.51
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.92	0.51
18:AR:22:ASP:OD2	18:AR:24:LYS:HB2	2.10	0.51
1:BA:532:A:H61	3:BC:193:TYR:HD2	1.58	0.51
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.76	0.51
29:CC:210:ALA:HA	29:CC:213:TRP:CE2	2.45	0.51
31:CA:1141:U:H4'	31:CA:1142:A:O4'	2.11	0.51
31:CA:1931:U:H2'	31:CA:1932:A:H8	1.76	0.51
5:AE:90:THR:HG22	5:AE:91:GLY:N	2.24	0.51
1:BA:845:A:O5'	1:BA:845:A:H8	1.94	0.51
5:BE:90:THR:HG22	5:BE:91:GLY:N	2.26	0.51
39:CL:21:CYS:HB2	39:CL:39:ILE:HD12	1.93	0.51
55:DA:207:A:H2'	55:DA:208:C:O4'	2.11	0.51
6:AF:40:GLU:OE2	6:AF:99:ALA:HA	2.11	0.51
19:AS:11:ILE:HD12	19:AS:38:SER:HB3	1.93	0.51
1:BA:404:G:N7	4:BD:2:ALA:HB3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BE:74:VAL:HG11	5:BE:144:LEU:HB3	1.93	0.51
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.93	0.51
34:CF:106:ILE:HD12	34:CF:139:PRO:HG2	1.93	0.51
13:BM:16:VAL:HG13	13:BM:34:LEU:HD12	1.92	0.51
31:CA:206:U:H2'	31:CA:207:A:H8	1.74	0.51
31:CA:278:A:N3	31:CA:278:A:H2'	2.26	0.51
37:CJ:24:VAL:HG22	37:CJ:28:LEU:HD22	1.93	0.51
36:DH:9:VAL:HG22	36:DH:35:LYS:HD3	1.93	0.51
1:AA:1277:C:O2'	1:AA:1279:G:H8	1.93	0.51
33:CE:149:ILE:HG12	33:CE:188:MET:HG2	1.92	0.51
55:DA:278:A:N3	55:DA:278:A:H2'	2.25	0.51
55:DA:2603:G:H5'	69:DA:7522:HOH:O	2.11	0.51
16:AP:21:VAL:HG12	16:AP:33:ILE:HD12	1.92	0.50
46:CS:49:ILE:HD12	46:CS:52:PRO:HA	1.93	0.50
37:DJ:97:LYS:HE2	37:DJ:139:VAL:HG11	1.93	0.50
45:DR:79:PHE:CZ	45:DR:83:LEU:HD11	2.46	0.50
51:DX:21:LEU:HD11	51:DX:41[A]:ARG:HE	1.75	0.50
55:DA:493:G:H2'	55:DA:494:G:O4'	2.11	0.50
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.91	0.50
18:AR:45:THR:OG1	18:AR:47:THR:HG23	2.12	0.50
26:C5:4:ARG:HB2	31:CA:2466:C:OP1	2.11	0.50
19:BS:11:ILE:HD12	19:BS:38:SER:HB3	1.93	0.50
25:D4:9:GLY:O	25:D4:13:ARG:HD2	2.12	0.50
34:DF:36:LEU:HD23	34:DF:154:ILE:HG12	1.92	0.50
54:DI:12:VAL:HG13	54:DI:63:ALA:HB2	1.94	0.50
54:DI:69:PHE:CZ	54:DI:84:TYR:HE1	2.29	0.50
1:AA:33:A:H2'	1:AA:34:C:C6	2.46	0.50
1:BA:33:A:H2'	1:BA:34:C:C6	2.46	0.50
1:BA:1052:G:H22	1:BA:1206:G:H1	1.59	0.50
7:BG:72:THR:HG22	7:BG:96:ARG:HH12	1.76	0.50
18:BR:22:ASP:OD2	18:BR:24:LYS:HB2	2.12	0.50
55:DA:307:G:N2	55:DA:309:A:H3'	2.27	0.50
55:DA:677:A:OP1	64:DA:3226:SPD:H41	2.11	0.50
55:DA:2228:G:H2'	55:DA:2229:U:C6	2.46	0.50
9:BI:9:THR:O	9:BI:85:ARG:HD2	2.12	0.50
29:DC:50:THR:HB	55:DA:1805:A:N3	2.27	0.50
46:CS:71:LYS:HG2	46:CS:73:LYS:HE3	1.93	0.50
45:DR:20:GLN:HG3	57:DR:202:PG4:C4	2.41	0.50
17:BQ:28:PHE:HD2	17:BQ:37:PHE:HB3	1.76	0.50
29:DC:231:PRO:C	29:DC:233:GLY:H	2.15	0.50
35:CG:86:LYS:HG2	35:CG:132:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2799:A:O2'	55:DA:2800:A:H5"	2.11	0.50
1:BA:82:G:H1	1:BA:84:U:H5	1.60	0.50
3:BC:23:PHE:CD2	10:BJ:97:ASP:HB2	2.47	0.50
54:DI:126:LEU:HA	54:DI:129:LEU:HD12	1.94	0.50
1:BA:202:G:O2'	1:BA:468:A:H8	1.95	0.50
5:BE:24:THR:HA	5:BE:29:ARG:HA	1.94	0.50
34:CF:132:VAL:HG22	34:CF:152:LEU:HG	1.93	0.50
51:DX:39:ARG:HD3	69:DX:117:HOH:O	2.11	0.50
6:AF:93:LYS:HE2	6:AF:93:LYS:H	1.76	0.50
31:CA:2036:C:H2'	31:CA:2037:A:C8	2.46	0.50
55:DA:45:G:H5"	55:DA:46:G:H5'	1.94	0.50
55:DA:551:G:H5"	55:DA:551:G:C8	2.47	0.50
1:AA:404:G:N7	4:AD:2:ALA:HB3	2.27	0.50
17:BQ:8:LEU:HD13	17:BQ:73:TRP:HH2	1.74	0.50
30:CD:4:LEU:HD22	30:CD:101:PHE:CE2	2.46	0.50
31:CA:674:G:H2'	31:CA:804:A:H61	1.77	0.50
31:CA:1405:U:H2'	31:CA:1406:U:C6	2.46	0.50
5:AE:106:ILE:HG13	5:AE:124:LEU:HA	1.92	0.49
12:AL:79:VAL:HG12	12:AL:102:LEU:HD23	1.94	0.49
10:BJ:80:THR:HG22	10:BJ:82:LYS:H	1.77	0.49
39:DL:21:CYS:HB2	39:DL:39:ILE:HD12	1.93	0.49
43:DP:64:TYR:HB3	43:DP:67:ASN:HD22	1.77	0.49
1:AA:1328:C:H5"	13:AM:28:THR:HG21	1.94	0.49
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.75	0.49
5:BE:77:ASN:HB2	5:BE:82:GLN:NE2	2.27	0.49
31:CA:1955:U:H5'	31:CA:2551:C:O2'	2.13	0.49
55:DA:639:U:H2'	55:DA:640:C:C6	2.47	0.49
29:CC:76:ALA:HB2	29:CC:96:TYR:CD1	2.48	0.49
44:DQ:52:ASN:O	55:DA:2845:U:H5"	2.12	0.49
1:AA:6:G:H1	5:AE:103:THR:HG21	1.78	0.49
1:AA:1305:G:H21	1:AA:1332:A:H2	1.60	0.49
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.76	0.49
23:D2:10:LYS:HE3	23:D2:53:LYS:O	2.13	0.49
31:CA:639:U:H2'	31:CA:640:C:C6	2.47	0.49
29:DC:50:THR:O	55:DA:1805:A:H1'	2.12	0.49
34:CF:61:SER:HB2	34:CF:91:LEU:HD21	1.95	0.49
43:CP:64:TYR:HB3	43:CP:67:ASN:HD22	1.77	0.49
1:AA:47:C:H2'	69:AA:2148:HOH:O	2.13	0.49
3:AC:40:ARG:HG2	3:AC:55:ILE:HG21	1.94	0.49
22:C1:38:HIS:HE1	31:CA:2884:U:O4	1.96	0.49
30:CD:155:VAL:HG21	31:CA:2618:G:H21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:357:C:H2'	31:CA:358:U:C6	2.48	0.49
34:DF:14:LYS:O	34:DF:18:THR:HG22	2.12	0.49
14:AN:42:TRP:HD1	14:AN:44:ALA:H	1.59	0.49
31:CA:1324:G:H1'	31:CA:1616:A:N6	2.27	0.49
32:DD:84:LEU:HD22	32:DD:88:GLU:HB3	1.94	0.49
49:DV:42:VAL:O	49:DV:60:GLU:HA	2.13	0.49
3:BC:70:THR:HG21	3:BC:76:VAL:HG21	1.95	0.49
16:BP:6:LEU:HB3	16:BP:17:TYR:HB3	1.94	0.49
17:BQ:14:SER:HB3	17:BQ:22:VAL:CG1	2.42	0.49
18:BR:45:THR:OG1	18:BR:47:THR:HG23	2.11	0.49
33:CE:40:ARG:HH21	33:CE:92:HIS:CE1	2.30	0.49
55:DA:1386:C:H2'	55:DA:1387:A:C8	2.47	0.49
5:AE:115:LEU:HD13	5:AE:123:VAL:HG21	1.94	0.49
28:CB:55:U:H1'	34:CF:26:MET:HG3	1.95	0.49
31:CA:45:G:H5"	31:CA:46:G:H5'	1.94	0.49
31:CA:1556:C:H2'	31:CA:1557:C:C6	2.48	0.49
55:DA:2609:U:C5	62:DA:3197:EDO:H12	2.48	0.49
1:AA:137:U:H3	1:AA:226:G:H1	1.61	0.49
1:AA:202:G:O2'	1:AA:468:A:H8	1.96	0.49
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	1.95	0.49
10:AJ:80:THR:HG22	10:AJ:82:LYS:H	1.76	0.49
23:C2:35:GLU:HG2	23:C2:50:LYS:HG2	1.95	0.49
1:BA:769:G:H4'	1:BA:1513:A:H4'	1.93	0.49
47:CT:84:ARG:HB2	47:CT:96:ILE:HB	1.95	0.49
34:DF:61:SER:HB2	34:DF:91:LEU:HD21	1.95	0.49
43:DP:27:VAL:HG21	43:DP:40:ILE:HD12	1.95	0.49
3:AC:70:THR:HG21	3:AC:76:VAL:HG21	1.95	0.49
8:AH:77:ARG:HD2	8:AH:79:SER:O	2.13	0.49
29:CC:208:ALA:CB	31:CA:1790:C:H4'	2.42	0.49
34:DF:106:ILE:HD12	34:DF:139:PRO:HG2	1.94	0.49
45:DR:22:LYS:HE3	55:DA:20:C:OP1	2.13	0.49
55:DA:2491:U:HO2'	55:DA:2492:U:H5	1.61	0.49
1:BA:607:A:H2'	1:BA:608:A:C8	2.48	0.48
3:BC:7:PRO:HD2	3:BC:184:TYR:CD1	2.48	0.48
31:CA:12:U:H2'	31:CA:12:U:O2	2.13	0.48
31:CA:1638:C:H4'	31:CA:2710:C:O2	2.13	0.48
33:CE:108:ILE:HG22	40:CM:1:MET:SD	2.52	0.48
39:DL:113:MET:CE	39:DL:116:ILE:HD11	2.43	0.48
55:DA:357:C:H2'	55:DA:358:U:C6	2.48	0.48
1:AA:1228:C:H2'	1:AA:1229:A:C8	2.48	0.48
26:C5:16:ILE:HD13	26:C5:25:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:47:LEU:HD22	7:BG:58:GLU:HG2	1.94	0.48
29:CC:220:VAL:HG21	31:CA:782:A:N7	2.28	0.48
31:CA:729:G:H2'	31:CA:1775:U:H1'	1.94	0.48
39:DL:26:GLY:HA3	39:DL:30:ARG:HH11	1.78	0.48
11:AK:16:VAL:HG23	11:AK:79:ILE:HG13	1.95	0.48
1:BA:1273:C:H2'	1:BA:1274:A:O4'	2.14	0.48
31:CA:2262:U:H1'	31:CA:2328:A:H1'	1.96	0.48
31:CA:2799:A:O2'	31:CA:2800:A:H5"	2.13	0.48
36:DH:97:ARG:HG3	36:DH:112:LYS:HG3	1.96	0.48
55:DA:933:A:H5'	55:DA:934:U:OP2	2.13	0.48
55:DA:2063:C:O2	55:DA:2450:A:N1	2.47	0.48
1:AA:1464:U:P	44:DQ:109:ARG:HH12	2.36	0.48
1:BA:1328:C:H5"	13:BM:28:THR:HG21	1.96	0.48
31:CA:1709:U:H2'	31:CA:1710:G:C8	2.49	0.48
45:CR:90:ILE:HG22	45:CR:95:LEU:HG	1.96	0.48
55:DA:543:G:H8	55:DA:543:G:H5"	1.78	0.48
55:DA:1515:A:H2'	55:DA:1516:G:O4'	2.13	0.48
29:CC:158:ALA:O	29:CC:196:GLY:O	2.31	0.48
34:CF:44:ILE:HG21	34:CF:79:ILE:HG22	1.95	0.48
43:CP:27:VAL:HG21	43:CP:40:ILE:HD12	1.96	0.48
45:CR:79:PHE:CZ	45:CR:83:LEU:HD11	2.48	0.48
34:DF:34:ILE:HG12	34:DF:156:ILE:HG12	1.95	0.48
54:DI:69:PHE:HB3	54:DI:72:LEU:HD12	1.94	0.48
1:AA:1376:U:H2'	1:AA:1377:A:C8	2.49	0.48
23:D2:35:GLU:HG2	23:D2:50:LYS:HG2	1.96	0.48
26:D5:16:ILE:HD13	26:D5:25:VAL:HG22	1.95	0.48
31:CA:528:A:H3'	31:CA:528:A:C8	2.48	0.48
31:CA:2019:A:H4'	45:CR:34:VAL:HG21	1.96	0.48
37:DJ:30:GLN:HE22	55:DA:1095:A:H61	1.61	0.48
55:DA:1738:G:O2'	55:DA:1739:A:C8	2.65	0.48
55:DA:2547:A:H2'	55:DA:2548:U:C6	2.49	0.48
16:AP:6:LEU:HB3	16:AP:17:TYR:HB3	1.96	0.48
5:BE:72:ILE:HG13	5:BE:73:ASN:N	2.28	0.48
9:BI:19:VAL:HG11	9:BI:83:ILE:HA	1.94	0.48
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	1.94	0.48
32:DD:150[A]:MEQ:HE3	55:DA:2032:G:C8	2.49	0.48
39:CL:26:GLY:HA3	39:CL:30:ARG:HH11	1.77	0.48
49:CV:42:VAL:O	49:CV:60:GLU:HA	2.13	0.48
45:DR:40:ILE:HG12	58:DS:203:MPD:H31	1.96	0.48
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	1.96	0.48
1:BA:1228:C:H2'	1:BA:1229:A:C8	2.49	0.48

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:DL:105:ARG:HG3	39:DL:122:VAL:CG1	2.46	0.46
46:DS:44:GLY:O	46:DS:45:GLU:HG2	2.15	0.46
52:DY:2:SER:HB2	52:DY:4:VAL:HG23	1.98	0.46
2:AB:120:GLN:HE22	2:AB:137:ARG:HE	1.61	0.46
1:BA:690:G:H2'	1:BA:691:G:O4'	2.16	0.46
34:CF:34:ILE:HG12	34:CF:156:ILE:HG12	1.98	0.46
34:DF:36:LEU:HD21	34:DF:99:PHE:CZ	2.51	0.46
44:DQ:31:TRP:CD1	57:DQ:202:PG4:H31	2.51	0.46
51:DX:41[B]:ARG:HA	51:DX:41[B]:ARG:HD3	1.63	0.46
1:BA:77:A:H2'	1:BA:78:A:C8	2.51	0.45
2:BB:20:THR:HA	2:BB:39:HIS:CE1	2.51	0.45
9:BI:88:MET:SD	9:BI:95:ARG:HG2	2.56	0.45
31:CA:845:A:H61	31:CA:932:U:H3	1.63	0.45
31:CA:2425:A:H4'	31:CA:2426:A:O5'	2.16	0.45
43:CP:35:ILE:HG21	43:CP:71:ALA:HA	1.98	0.45
48:DU:2:ILE:HG21	48:DU:45:ALA:CB	2.45	0.45
49:DV:14:LEU:HD21	49:DV:71:ALA:HB2	1.98	0.45
55:DA:1168:G:H8	55:DA:1168:G:H5"	1.81	0.45
55:DA:2133:G:H21	55:DA:2158:A:N6	2.14	0.45
3:AC:91:VAL:HG21	3:AC:101:ILE:HD11	1.99	0.45
9:AI:28:ILE:HG21	9:AI:35:LEU:HD13	1.97	0.45
19:AS:52:HIS:CD2	19:AS:54:GLY:H	2.30	0.45
23:C2:15:ALA:HB2	23:C2:47:VAL:HG21	1.98	0.45
26:C5:30:GLU:HG3	26:C5:32:LYS:HB2	1.98	0.45
22:D1:23:THR:HG22	63:D1:102:PGE:H62	1.98	0.45
31:CA:1509:A:O2'	31:CA:1510:G:H8	1.99	0.45
37:DJ:103:ARG:HA	37:DJ:106:LEU:HD12	1.98	0.45
50:DW:51:GLN:HB2	50:DW:57:TYR:OH	2.16	0.45
54:DI:23:LEU:HD13	54:DI:89:PRO:HD3	1.98	0.45
55:DA:1794:A:H2'	55:DA:1795:C:C6	2.51	0.45
55:DA:2033:A:H5'	69:DA:3393:HOH:O	2.15	0.45
55:DA:2609:U:H5	62:DA:3197:EDO:H12	1.82	0.45
55:DA:2887[B]:A:O2'	55:DA:2888[B]:C:H5'	2.16	0.45
1:AA:1239:A:H62	1:AA:1299:A:N6	2.14	0.45
2:AB:31:ILE:HG21	2:AB:39:HIS:CD2	2.51	0.45
3:AC:77:ILE:HA	3:AC:84:VAL:HG22	1.98	0.45
1:BA:1347:G:N2	1:BA:1373:G:H2'	2.31	0.45
22:D1:22:LEU:HD23	61:D1:103:PEG:H31	1.98	0.45
29:CC:171:TYR:CD1	29:CC:185:GLU:HA	2.51	0.45
31:CA:1430:G:H2'	31:CA:1431:A:O4'	2.16	0.45
31:CA:1510:G:H2'	31:CA:1511:G:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:CK:140:LEU:HD11	38:CK:142:ILE:HD13	1.98	0.45
39:CL:121:GLU:HG2	39:CL:122:VAL:HG23	1.97	0.45
35:DG:4:VAL:HA	58:DA:3209:MPD:H13	1.99	0.45
44:DQ:94:LYS:CE	55:DA:1754:A:C8	3.00	0.45
45:DR:6:ARG:HD3	55:DA:1250:G:C5'	2.46	0.45
54:DI:25:ALA:HA	54:DI:83:ALA:O	2.16	0.45
11:AK:84:VAL:HG21	11:AK:97:ILE:HG23	1.99	0.45
3:BC:91:VAL:HG21	3:BC:101:ILE:HD11	1.97	0.45
17:BQ:16:LYS:HD2	17:BQ:16:LYS:HA	1.84	0.45
32:DD:169:ARG:HG2	55:DA:2773:C:H5"	1.98	0.45
54:DI:50:VAL:HG22	54:DI:85:VAL:HG13	1.99	0.45
55:DA:417:C:H2'	55:DA:418:C:H6	1.81	0.45
55:DA:2123:G:H2'	55:DA:2124:G:H8	1.81	0.45
1:AA:1348:U:H2'	1:AA:1349:A:H8	1.82	0.45
1:BA:972:C:H4'	10:BJ:59:LYS:HG2	1.98	0.45
11:BK:28:ASN:O	11:BK:57:LYS:HE3	2.16	0.45
11:BK:58:SER:O	11:BK:91:PRO:HG3	2.16	0.45
34:DF:85:ILE:HD11	55:DA:2311:A:C2	2.52	0.45
1:AA:562:U:H1'	12:AL:12:ARG:HD2	1.98	0.45
1:AA:1386:G:H2'	1:AA:1387:G:H8	1.80	0.45
13:AM:31:LYS:HA	13:AM:41:GLU:OE2	2.17	0.45
14:AN:13:ARG:HD3	14:AN:59:ARG:O	2.17	0.45
1:BA:214:C:H2'	1:BA:215:C:H6	1.81	0.45
5:BE:72:ILE:HG13	5:BE:73:ASN:H	1.82	0.45
31:CA:2642:G:H5'	38:CK:80:HIS:CG	2.51	0.45
37:CJ:55:ILE:HD12	37:CJ:74:PRO:HD3	1.98	0.45
37:CJ:103:ARG:HA	37:CJ:106:LEU:HD12	1.98	0.45
44:CQ:114:LEU:H	44:CQ:114:LEU:HD23	1.81	0.45
55:DA:244:A:H2'	55:DA:245:G:O4'	2.17	0.45
55:DA:543:G:H5"	55:DA:543:G:C8	2.52	0.45
1:AA:690:G:H2'	1:AA:691:G:O4'	2.16	0.45
5:AE:160:SER:HB2	5:AE:161:VAL:HG22	1.98	0.45
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.97	0.45
11:AK:28:ASN:O	11:AK:57:LYS:HE3	2.17	0.45
9:BI:51:PRO:HB3	9:BI:84:THR:HG23	1.99	0.45
31:CA:588:U:H2'	31:CA:589:U:C6	2.52	0.45
31:CA:2636:C:H2'	31:CA:2637:U:C6	2.52	0.45
34:CF:36:LEU:HD12	34:CF:154:ILE:HG12	1.98	0.45
34:DF:158:THR:HG23	34:DF:160:ALA:H	1.82	0.45
45:DR:19:LYS:HD3	57:DR:202:PG4:H22	1.98	0.45
47:DT:73:LYS:HD3	65:DA:3188:1PE:H232	1.98	0.45

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:20:SER:HB3	14:AN:94:PRO:HG3	2.00	0.44
22:C1:43:ILE:CG2	42:CO:98:LEU:HB3	2.48	0.44
1:BA:532:A:N6	3:BC:192:THR:HG23	2.33	0.44
1:BA:1239:A:H62	1:BA:1299:A:N6	2.15	0.44
3:BC:77:ILE:HA	3:BC:84:VAL:HG22	2.00	0.44
11:BK:21:ALA:HB2	11:BK:82:LEU:HD13	2.00	0.44
12:BL:48:ALA:HB3	12:BL:50:ARG:HE	1.83	0.44
20:BT:51:PHE:HA	20:BT:54:MET:HG2	1.99	0.44
31:CA:861:A:H2'	31:CA:862:G:O4'	2.17	0.44
47:CT:66:ILE:HA	47:CT:69:LEU:HD22	1.98	0.44
41:DN:14:LYS:HE2	69:DA:4160:HOH:O	2.17	0.44
44:DQ:53:ARG:NH2	55:DA:2720:U:OP1	2.51	0.44
55:DA:1172:C:C5	55:DA:1173:U:H1'	2.53	0.44
55:DA:1494:A:H2'	55:DA:1495:A:C8	2.52	0.44
55:DA:1733:G:H2'	55:DA:1734:G:C8	2.53	0.44
1:AA:1108:G:H5"	3:AC:176:HIS:ND1	2.32	0.44
1:AA:1320:C:OP2	19:AS:3:ARG:HD3	2.18	0.44
2:BB:12:ALA:HB1	2:BB:209:ALA:HA	1.99	0.44
5:BE:88:VAL:HG12	5:BE:93:ARG:HG2	1.99	0.44
22:D1:13:ARG:HB2	69:D1:209:HOH:O	2.17	0.44
31:CA:142:A:H2'	31:CA:143:C:C6	2.52	0.44
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.52	0.44
31:CA:2261:C:H5"	51:CX:19:LYS:NZ	2.33	0.44
44:CQ:4:ILE:HD12	44:CQ:4:ILE:H	1.82	0.44
43:DP:18:LEU:HD23	43:DP:18:LEU:HA	1.91	0.44
55:DA:136:G:H1	55:DA:143:C:N4	2.16	0.44
1:AA:845:A:O4'	1:AA:845:A:P	2.76	0.43
3:AC:138:VAL:HG13	3:AC:149:ILE:HG23	2.00	0.43
7:AG:30:LEU:HD12	7:AG:105:VAL:HG13	2.00	0.43
1:BA:23:C:H5	1:BA:561:U:O4	2.01	0.43
1:BA:815:A:H4'	1:BA:817:C:C4	2.53	0.43
1:BA:1190:G:H5'	3:BC:176:HIS:NE2	2.33	0.43
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.17	0.43
31:CA:137:U:H3	31:CA:142:A:H61	1.65	0.43
29:DC:156:ARG:NH2	55:DA:1818:U:H5	2.16	0.43
39:CL:98:ARG:HH11	39:CL:98:ARG:HG2	1.83	0.43
34:DF:88:LYS:HD3	55:DA:2313:C:H5"	2.00	0.43
35:DG:95:ARG:HG2	35:DG:128:GLN:HB3	1.99	0.43
43:DP:64:TYR:HB3	43:DP:67:ASN:ND2	2.33	0.43
54:DI:35:VAL:HA	54:DI:38:MET:HB2	2.00	0.43
55:DA:340:A:H2'	55:DA:341:C:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:503:A:H5'	55:DA:505:A:OP1	2.17	0.43
1:AA:9:G:OP2	5:AE:126:LYS:HE2	2.18	0.43
9:AI:51:PRO:HB3	9:AI:84:THR:HG23	1.99	0.43
1:BA:73:C:O2'	1:BA:74:A:H8	1.99	0.43
1:BA:1061:G:H5'	10:BJ:61:ALA:HB2	2.01	0.43
1:BA:1493:A:H8	1:BA:1493:A:OP2	2.01	0.43
2:BB:164:ILE:HD13	2:BB:186:ILE:HG13	2.00	0.43
31:CA:1810:A:H2'	31:CA:1811:G:O4'	2.16	0.43
31:CA:1938:A:C6	31:CA:2590:A:H1'	2.52	0.43
33:CE:189:THR:HG22	33:CE:192:ALA:H	1.83	0.43
37:CJ:14:ALA:HB3	37:CJ:17:MET:HB2	1.99	0.43
55:DA:2097:A:H8	55:DA:2097:A:H5"	1.83	0.43
55:DA:2266:A:H4'	55:DA:2267:A:O5'	2.19	0.43
1:AA:920:U:H2'	1:AA:921:U:C6	2.54	0.43
2:AB:129:LEU:H	2:AB:129:LEU:HG	1.58	0.43
2:AB:164:ILE:HD13	2:AB:186:ILE:HG13	2.00	0.43
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.83	0.43
11:AK:58:SER:O	11:AK:91:PRO:HG3	2.17	0.43
21:AU:51:SER:HA	21:AU:54:LYS:HE3	2.00	0.43
1:BA:920:U:H2'	1:BA:921:U:C6	2.52	0.43
22:D1:53:LYS:HE3	22:D1:55:ILE:O	2.18	0.43
24:D3:19:ARG:HG3	55:DA:126:A:O5'	2.19	0.43
31:CA:2747:G:O6	31:CA:2755:C:H5"	2.18	0.43
39:CL:113:MET:SD	39:CL:116:ILE:HD11	2.58	0.43
42:DO:2:ARG:NH1	42:DO:2:ARG:HB3	2.34	0.43
5:AE:81:LEU:HB3	5:AE:147:MET:SD	2.59	0.43
19:AS:53:ASN:HD22	19:AS:58:VAL:HG23	1.83	0.43
55:DA:2291:U:H2'	55:DA:2292:U:C6	2.53	0.43
1:BA:411:A:P	4:BD:26:ARG:HH12	2.41	0.43
5:BE:155:ALA:HB1	8:BH:66:PHE:CZ	2.54	0.43
10:BJ:15:HIS:HB3	10:BJ:70:HIS:CE1	2.54	0.43
31:CA:727:A:H2'	31:CA:728:G:C8	2.53	0.43
31:CA:1224:U:H4'	46:CS:88:GLY:O	2.19	0.43
50:CW:38:LEU:HD21	50:CW:65:VAL:HG11	2.01	0.43
44:DQ:53:ARG:HG2	44:DQ:53:ARG:NH1	2.34	0.43
1:AA:1293:C:H2'	1:AA:1294:G:C8	2.54	0.43
14:AN:53:ARG:HH21	19:AS:37:ARG:HH22	1.67	0.43
1:BA:1108:G:H5"	3:BC:176:HIS:CE1	2.54	0.43
2:BB:163:VAL:HG11	2:BB:173:ILE:HD11	2.00	0.43
7:BG:30:LEU:HD12	7:BG:105:VAL:HG13	2.01	0.43
17:BQ:27:ARG:NH2	17:BQ:40:ARG:HG2	2.33	0.43

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1144:G:H21	1:AA:1146:A:H62	1.68	0.41
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	2.03	0.41
11:BK:36:ASP:CG	11:BK:38:GLN:HG2	2.41	0.41
24:D3:19:ARG:HD3	55:DA:125:A:OP2	2.20	0.41
31:CA:2781:A:H5"	31:CA:2782:G:H5'	2.01	0.41
29:DC:207:LYS:HB2	55:DA:729:G:C5	2.55	0.41
33:CE:75:SER:OG	33:CE:77:ILE:HG12	2.20	0.41
35:CG:105:LEU:HD22	35:CG:107:LEU:HD11	2.02	0.41
35:CG:123:ALA:HB2	35:CG:133:LEU:HD23	2.03	0.41
36:CH:7:ASP:HA	36:CH:15:LEU:HD12	2.02	0.41
35:DG:12:PRO:HD2	35:DG:15:VAL:HG21	2.03	0.41
41:DN:18[B]:ARG:HG2	28:DB:91:C:P	2.60	0.41
55:DA:221:A:N1	55:DA:265:A:O2'	2.51	0.41
55:DA:1604:C:H5'	69:DA:3663:HOH:O	2.20	0.41
59:DA:3187:PUT:H12	69:DA:7225:HOH:O	2.21	0.41
1:AA:32:A:H2'	1:AA:33:A:C8	2.55	0.41
1:AA:604:G:H2'	1:AA:605:U:O4'	2.20	0.41
1:AA:1001:C:H2'	1:AA:1002:G:C8	2.56	0.41
2:AB:163:VAL:HG11	2:AB:173:ILE:HD11	2.01	0.41
14:AN:43:ASN:HA	14:AN:46:LEU:HD12	2.02	0.41
17:AQ:45:HIS:HB2	17:AQ:70:THR:O	2.21	0.41
1:BA:76:G:H22	1:BA:93:U:H3	1.68	0.41
1:BA:374:A:H5"	1:BA:452:A:C2	2.56	0.41
1:BA:844:G:N3	1:BA:844:G:H2'	2.35	0.41
1:BA:1478:U:H2'	1:BA:1479:C:C6	2.56	0.41
30:CD:146:ILE:HG12	31:CA:2051:A:H4'	2.02	0.41
31:CA:455:C:HO2'	31:CA:472:A:H2	1.66	0.41
31:CA:1638:C:H5"	31:CA:2710:C:O2'	2.20	0.41
31:CA:2845:U:H2'	31:CA:2846:G:O4'	2.21	0.41
32:DD:125:TRP:CE3	32:DD:160:LYS:HD3	2.55	0.41
35:CG:164:TYR:HB2	35:CG:167:GLU:HB2	2.01	0.41
50:CW:51:GLN:HB2	50:CW:57:TYR:OH	2.20	0.41
37:DJ:19:ASN:N	37:DJ:20:PRO:HD2	2.35	0.41
48:DU:7:LEU:HD13	48:DU:46:ALA:HA	2.02	0.41
51:DX:18:ALA:HB1	55:DA:2271:G:OP1	2.19	0.41
55:DA:352:A:H5"	55:DA:352:A:H8	1.86	0.41
55:DA:2327:A:H2'	55:DA:2328:A:C8	2.55	0.41
1:AA:946:A:H2'	1:AA:947:G:C8	2.56	0.41
1:AA:1377:A:N3	7:AG:2:PRO:HG3	2.35	0.41
29:CC:266:PHE:HD1	29:CC:266:PHE:H	1.68	0.41
31:CA:2016:U:O5'	31:CA:2016:U:H6	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2030:6MZ:N3	31:CA:2499:C:H5"	2.35	0.41
31:CA:2895:G:H2'	31:CA:2896:C:C6	2.55	0.41
29:DC:177:ARG:HG2	55:DA:1820:U:OP1	2.21	0.41
36:CH:47:PHE:O	36:CH:51:ARG:HB3	2.21	0.41
36:CH:71:LYS:HB3	36:CH:108:VAL:HG22	2.02	0.41
38:CK:36:LEU:O	38:CK:51:GLY:HA3	2.20	0.41
40:DM:21:ARG:HA	55:DA:811:U:H2'	2.03	0.41
41:DN:17:ASN:O	41:DN:38:ARG:HD3	2.21	0.41
55:DA:1730:C:O2	55:DA:1730:C:O4'	2.39	0.41
55:DA:1831:G:H5'	63:DA:3227:PGE:H62	2.02	0.41
55:DA:2273:A:H2'	55:DA:2274:A:C8	2.55	0.41
55:DA:2706:A:O5'	55:DA:2706:A:H8	2.03	0.41
1:AA:721:G:H4'	1:AA:722:G:O4'	2.21	0.41
1:AA:1190:G:H5'	3:AC:176:HIS:NE2	2.36	0.41
3:AC:5:VAL:HG21	3:AC:10:ILE:HD13	2.02	0.41
4:AD:192:SER:HB3	4:AD:195:ILE:HD12	2.02	0.41
5:AE:15:LEU:HA	5:AE:37:THR:HG22	2.02	0.41
1:BA:8:A:C6	4:BD:206:LYS:HB3	2.56	0.41
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	2.01	0.41
3:BC:123:GLN:HB3	3:BC:128:VAL:CG2	2.51	0.41
5:BE:106:ILE:HG13	5:BE:123:VAL:O	2.20	0.41
31:CA:1716:U:H2'	31:CA:1717:A:H8	1.86	0.41
31:CA:2063:C:O2	31:CA:2450:A:N1	2.53	0.41
40:CM:123:ARG:HG3	40:CM:143:GLU:HG3	2.03	0.41
51:CX:51:VAL:HG22	51:CX:82:ILE:HD12	2.02	0.41
55:DA:969:G:H2'	55:DA:970:U:C6	2.54	0.41
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	2.02	0.41
16:AP:31:ARG:HA	69:AP:101:HOH:O	2.21	0.41
1:BA:269:C:H2'	1:BA:270:A:C8	2.55	0.41
1:BA:1144:G:H21	1:BA:1146:A:H62	1.68	0.41
30:CD:187:LEU:HD21	30:CD:203:VAL:HG11	2.02	0.41
31:CA:35:G:H2'	31:CA:36:G:O4'	2.21	0.41
31:CA:321:U:H5"	33:CE:131:THR:HG23	2.02	0.41
31:CA:1101:U:H2'	31:CA:1102:C:H6	1.86	0.41
31:CA:1847:A:O5'	31:CA:1847:A:H8	2.03	0.41
35:CG:52:PHE:CD2	35:CG:52:PHE:N	2.89	0.41
48:DU:1:MET:HG2	55:DA:142:A:H1'	2.03	0.41
48:DU:2:ILE:HG21	48:DU:45:ALA:HB1	2.02	0.41
51:DX:41[A]:ARG:HG2	51:DX:41[A]:ARG:HH11	1.86	0.41
52:DY:45:ARG:HG2	52:DY:46:PHE:N	2.36	0.41
55:DA:1769:U:H5"	64:DA:3208:SPD:H32	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2243:U:H2'	55:DA:2244:U:C6	2.56	0.41
1:AA:496:A:N3	1:AA:496:A:H2'	2.36	0.41
1:AA:1171:A:H2'	1:AA:1172:C:C6	2.55	0.41
9:AI:11:ARG:HB3	9:AI:16:ALA:HA	2.02	0.41
12:AL:87:VAL:HG11	12:AL:90:LEU:HD22	2.03	0.41
14:AN:42:TRP:CD1	14:AN:43:ASN:N	2.89	0.41
14:AN:79:LEU:HD22	69:AN:205:HOH:O	2.20	0.41
1:BA:76:G:H1	1:BA:93:U:H3	1.69	0.41
1:BA:706:A:H4'	11:BK:31:ILE:HG12	2.03	0.41
1:BA:1289:A:H3'	1:BA:1290:G:H8	1.85	0.41
1:BA:1298:U:H3	7:BG:114:LYS:HA	1.86	0.41
3:BC:138:VAL:HG13	3:BC:149:ILE:HG23	2.02	0.41
19:BS:66:MET:HG2	19:BS:74:PHE:CE2	2.56	0.41
30:CD:121:THR:HB	30:CD:127:PHE:CD2	2.55	0.41
31:CA:307:G:N2	31:CA:309:A:H3'	2.34	0.41
31:CA:1072:C:H2'	31:CA:1093:G:O6	2.21	0.41
31:CA:1885:A:H2'	31:CA:1886:U:O4'	2.20	0.41
31:CA:2304:G:H22	31:CA:2312:U:H3	1.69	0.41
32:DD:187:LEU:HD21	32:DD:203:VAL:HG11	2.03	0.41
40:CM:19:LEU:HD23	40:CM:31:GLY:O	2.21	0.41
49:CV:72:ILE:H	49:CV:72:ILE:HG13	1.66	0.41
42:DO:28:LEU:HD23	42:DO:48:VAL:HG21	2.01	0.41
47:DT:72:THR:CG2	47:DT:108:SER:HB3	2.51	0.41
51:DX:51:VAL:HG22	51:DX:82:ILE:HD12	2.02	0.41
54:DI:83:ALA:HB2	54:DI:96:PHE:CZ	2.55	0.41
54:DI:129:LEU:HA	54:DI:130:PRO:HD3	1.99	0.41
55:DA:68:G:H2'	55:DA:69:C:O4'	2.20	0.41
55:DA:2255:G:H21	68:DA:3222:TRS:C1	2.34	0.41
55:DA:2262:U:H4'	55:DA:2328:A:C2	2.56	0.41
55:DA:2291:U:H5"	55:DA:2380:C:O2	2.21	0.41
55:DA:2698:U:H2'	55:DA:2699:C:C6	2.56	0.41
55:DA:2886[B]:A:N3	55:DA:2886[B]:A:H2'	2.36	0.41
1:AA:1012:A:H61	1:AA:1017:U:H3	1.67	0.41
1:AA:1250:A:O3'	9:AI:69:GLY:HA2	2.20	0.41
1:AA:1492:A:H5'	1:AA:1492:A:C8	2.47	0.41
6:AF:29:ILE:HG23	6:AF:66:ALA:HB2	2.01	0.41
14:AN:69:ARG:HA	14:AN:70:PRO:HD3	1.92	0.41
6:BF:64:VAL:HG12	6:BF:65:GLU:N	2.36	0.41
29:CC:105:LEU:HD12	29:CC:105:LEU:N	2.34	0.41
31:CA:364:C:H2'	31:CA:365:U:C6	2.55	0.41
31:CA:1587:G:H2'	31:CA:1588:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2038:G:H2'	31:CA:2039:U:O4'	2.21	0.41
36:CH:27:ARG:HH12	36:CH:38:PRO:HG3	1.86	0.41
39:CL:105:ARG:O	39:CL:108:ARG:HB2	2.19	0.41
45:CR:76:TYR:CZ	45:CR:80:ILE:HG13	2.56	0.41
42:DO:19:ALA:HB2	69:DA:6721:HOH:O	2.20	0.41
43:DP:5:SER:HA	43:DP:8:ILE:HD12	2.02	0.41
55:DA:1354:A:H2'	55:DA:1355:G:O4'	2.21	0.41
55:DA:1430:G:H2'	55:DA:1431:A:O4'	2.21	0.41
1:AA:76:G:H22	1:AA:93:U:H3	1.68	0.40
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.51	0.40
1:BA:1001:C:H2'	1:BA:1002:G:C8	2.56	0.40
15:BO:2:SER:HB3	15:BO:3:LEU:H	1.74	0.40
43:DP:1:MET:HB3	43:DP:6:ALA:HB2	2.02	0.40
1:AA:859:G:H2'	1:AA:860:A:C8	2.56	0.40
2:AB:31:ILE:HD13	2:AB:39:HIS:CD2	2.55	0.40
9:AI:57:MET:HG3	9:AI:61:LEU:HG	2.03	0.40
10:AJ:53:ILE:HG13	14:AN:85:ARG:HD2	2.02	0.40
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	2.03	0.40
4:BD:170:TRP:CD2	4:BD:186:PRO:HB3	2.56	0.40
29:CC:208:ALA:HB2	31:CA:1790:C:H4'	2.04	0.40
31:CA:674:G:H21	33:CE:69:ARG:HH12	1.69	0.40
29:DC:225:MET:O	29:DC:233:GLY:O	2.40	0.40
47:CT:20:VAL:HG11	47:CT:44:ALA:HA	2.03	0.40
41:DN:33:LEU:HD13	41:DN:117:PHE:HB3	2.03	0.40
44:DQ:10:GLN:HG2	44:DQ:10:GLN:H	1.72	0.40
44:DQ:100:LEU:HD11	44:DQ:110:ILE:HD11	2.03	0.40
47:DT:20:VAL:HG11	47:DT:44:ALA:HA	2.02	0.40
55:DA:553:G:H2'	55:DA:554:U:O4'	2.20	0.40
55:DA:1093:G:H1'	55:DA:1099:G:H22	1.87	0.40
1:AA:49:U:O2	1:AA:362:G:H1'	2.20	0.40
1:AA:1508:A:H2'	1:AA:1509:C:O4'	2.22	0.40
22:C1:41:HIS:HA	22:C1:49:TYR:OH	2.21	0.40
25:C4:23:LYS:HA	25:C4:48:ALA:O	2.21	0.40
1:BA:1081:A:H5'	5:BE:23:LYS:HG3	2.04	0.40
1:BA:1151:A:O2'	1:BA:1152:A:H8	2.03	0.40
13:BM:23:TYR:HD1	13:BM:69:LEU:HD23	1.87	0.40
31:CA:998:C:OP2	45:CR:58:ARG:NH2	2.54	0.40
31:CA:2114:A:N6	31:CA:2119:A:H62	2.19	0.40
35:DG:123:ALA:HB2	35:DG:133:LEU:HD23	2.04	0.40
55:DA:397:U:O5'	55:DA:397:U:H6	2.03	0.40
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	2.03	0.40

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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	222/224 (99%)	204 (92%)	14 (6%)	4 (2%)	8 34
2	BB	222/224 (99%)	202 (91%)	16 (7%)	4 (2%)	8 34
3	AC	204/206 (99%)	195 (96%)	8 (4%)	1 (0%)	29 65
3	BC	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	15 49
4	AD	203/205 (99%)	193 (95%)	10 (5%)	0	100 100
4	BD	203/205 (99%)	192 (95%)	11 (5%)	0	100 100
5	AE	153/155 (99%)	143 (94%)	9 (6%)	1 (1%)	22 57
5	BE	148/155 (96%)	135 (91%)	10 (7%)	3 (2%)	7 31
6	AF	104/106 (98%)	92 (88%)	12 (12%)	0	100 100
6	BF	98/106 (92%)	82 (84%)	12 (12%)	4 (4%)	3 14
7	AG	149/151 (99%)	135 (91%)	12 (8%)	2 (1%)	12 42
7	BG	149/151 (99%)	138 (93%)	10 (7%)	1 (1%)	22 57
8	AH	127/129 (98%)	120 (94%)	7 (6%)	0	100 100
8	BH	127/129 (98%)	119 (94%)	8 (6%)	0	100 100
9	AI	125/127 (98%)	112 (90%)	12 (10%)	1 (1%)	19 54
9	BI	125/127 (98%)	112 (90%)	12 (10%)	1 (1%)	19 54
10	AJ	97/99 (98%)	90 (93%)	5 (5%)	2 (2%)	7 30
10	BJ	96/99 (97%)	80 (83%)	11 (12%)	5 (5%)	2 10
11	AK	115/117 (98%)	105 (91%)	9 (8%)	1 (1%)	17 52
11	BK	115/117 (98%)	102 (89%)	12 (10%)	1 (1%)	17 52
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100 100
12	BL	120/123 (98%)	115 (96%)	4 (3%)	1 (1%)	19 54
13	AM	112/114 (98%)	97 (87%)	11 (10%)	4 (4%)	3 17
13	BM	112/114 (98%)	95 (85%)	11 (10%)	6 (5%)	2 10
14	AN	98/100 (98%)	91 (93%)	4 (4%)	3 (3%)	4 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	BN	98/100 (98%)	93 (95%)	2 (2%)	3 (3%)	4 20
15	AO	86/88 (98%)	84 (98%)	2 (2%)	0	100 100
15	BO	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	13 44
16	AP	80/82 (98%)	67 (84%)	10 (12%)	3 (4%)	3 16
16	BP	80/82 (98%)	63 (79%)	14 (18%)	3 (4%)	3 16
17	AQ	78/80 (98%)	70 (90%)	5 (6%)	3 (4%)	3 16
17	BQ	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	2 11
18	AR	53/55 (96%)	52 (98%)	1 (2%)	0	100 100
18	BR	53/55 (96%)	52 (98%)	1 (2%)	0	100 100
19	AS	77/79 (98%)	66 (86%)	9 (12%)	2 (3%)	5 24
19	BS	77/79 (98%)	64 (83%)	11 (14%)	2 (3%)	5 24
20	AT	84/86 (98%)	82 (98%)	2 (2%)	0	100 100
20	BT	83/86 (96%)	79 (95%)	2 (2%)	2 (2%)	6 26
21	AU	54/56 (96%)	51 (94%)	3 (6%)	0	100 100
21	BU	54/56 (96%)	51 (94%)	3 (6%)	0	100 100
22	C1	54/56 (96%)	47 (87%)	3 (6%)	4 (7%)	1 4
22	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100 100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	3 14
23	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100 100
24	C3	44/46 (96%)	42 (96%)	2 (4%)	0	100 100
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
25	C4	62/64 (97%)	59 (95%)	3 (5%)	0	100 100
25	D4	62/64 (97%)	59 (95%)	3 (5%)	0	100 100
26	C5	36/38 (95%)	36 (100%)	0	0	100 100
26	D5	36/38 (95%)	36 (100%)	0	0	100 100
27	C0	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	3 17
27	D0	57/58 (98%)	53 (93%)	4 (7%)	0	100 100
29	CC	269/271 (99%)	242 (90%)	21 (8%)	6 (2%)	6 28
29	DC	269/271 (99%)	249 (93%)	18 (7%)	2 (1%)	22 57
30	CD	207/209 (99%)	191 (92%)	16 (8%)	0	100 100
32	DD	206/209 (99%)	197 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
33	CE	199/201 (99%)	186 (94%)	10 (5%)	3 (2%)	10 39
33	DE	199/201 (99%)	189 (95%)	9 (4%)	1 (0%)	29 65
34	CF	175/177 (99%)	161 (92%)	12 (7%)	2 (1%)	14 47
34	DF	175/177 (99%)	160 (91%)	12 (7%)	3 (2%)	9 35
35	CG	174/176 (99%)	160 (92%)	9 (5%)	5 (3%)	4 22
35	DG	174/176 (99%)	159 (91%)	13 (8%)	2 (1%)	14 47
36	CH	147/149 (99%)	127 (86%)	15 (10%)	5 (3%)	3 18
36	DH	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	7 31
37	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	4 21
37	DJ	132/134 (98%)	126 (96%)	2 (2%)	4 (3%)	4 21
38	CK	140/142 (99%)	133 (95%)	5 (4%)	2 (1%)	11 40
38	DK	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	22 57
39	CL	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	9 35
39	DL	121/123 (98%)	115 (95%)	5 (4%)	1 (1%)	19 54
40	CM	142/144 (99%)	131 (92%)	8 (6%)	3 (2%)	7 30
40	DM	142/144 (99%)	135 (95%)	7 (5%)	0	100 100
41	CN	133/136 (98%)	125 (94%)	8 (6%)	0	100 100
41	DN	134/136 (98%)	127 (95%)	7 (5%)	0	100 100
42	CO	118/125 (94%)	110 (93%)	7 (6%)	1 (1%)	19 54
42	DO	123/125 (98%)	115 (94%)	8 (6%)	0	100 100
43	CP	114/117 (97%)	111 (97%)	3 (3%)	0	100 100
43	DP	115/117 (98%)	112 (97%)	3 (3%)	0	100 100
44	CQ	112/114 (98%)	108 (96%)	3 (3%)	1 (1%)	17 52
44	DQ	112/114 (98%)	108 (96%)	3 (3%)	1 (1%)	17 52
45	CR	115/117 (98%)	112 (97%)	2 (2%)	1 (1%)	17 52
45	DR	115/117 (98%)	112 (97%)	3 (3%)	0	100 100
46	CS	101/103 (98%)	90 (89%)	10 (10%)	1 (1%)	15 49
46	DS	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	15 49
47	CT	108/110 (98%)	102 (94%)	4 (4%)	2 (2%)	8 33
47	DT	108/110 (98%)	106 (98%)	1 (1%)	1 (1%)	17 52
48	CU	91/93 (98%)	85 (93%)	5 (6%)	1 (1%)	14 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
48	DU	91/93 (98%)	85 (93%)	5 (6%)	1 (1%)	14 47
49	CV	100/102 (98%)	86 (86%)	10 (10%)	4 (4%)	3 15
49	DV	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	7 31
50	CW	92/94 (98%)	90 (98%)	2 (2%)	0	100 100
50	DW	92/94 (98%)	91 (99%)	1 (1%)	0	100 100
51	CX	73/76 (96%)	70 (96%)	3 (4%)	0	100 100
51	DX	75/76 (99%)	72 (96%)	3 (4%)	0	100 100
52	CY	75/77 (97%)	72 (96%)	3 (4%)	0	100 100
52	DY	75/77 (97%)	73 (97%)	2 (3%)	0	100 100
53	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9 35
53	DZ	60/62 (97%)	58 (97%)	2 (3%)	0	100 100
54	DI	133/135 (98%)	112 (84%)	15 (11%)	6 (4%)	2 13
All	All	11407/11629 (98%)	10595 (93%)	661 (6%)	151 (1%)	12 42

All (151) Ramachandran outliers are listed below:

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

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

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

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

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

5.3.2 Protein sidechains (i)

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 29
2	BB	186/186 (100%)	168 (90%)	18 (10%)	8 29
3	AC	170/170 (100%)	153 (90%)	17 (10%)	7 27
3	BC	170/170 (100%)	160 (94%)	10 (6%)	19 51
4	AD	172/172 (100%)	166 (96%)	6 (4%)	36 69
4	BD	172/172 (100%)	163 (95%)	9 (5%)	23 57
5	AE	118/118 (100%)	100 (85%)	18 (15%)	2 12
5	BE	113/118 (96%)	93 (82%)	20 (18%)	2 8
6	AF	92/92 (100%)	87 (95%)	5 (5%)	22 55
6	BF	87/92 (95%)	78 (90%)	9 (10%)	7 26
7	AG	124/124 (100%)	109 (88%)	15 (12%)	5 20
7	BG	124/124 (100%)	109 (88%)	15 (12%)	5 20
8	AH	104/104 (100%)	92 (88%)	12 (12%)	5 22
8	BH	104/104 (100%)	95 (91%)	9 (9%)	10 34
9	AI	105/105 (100%)	95 (90%)	10 (10%)	8 30
9	BI	105/105 (100%)	94 (90%)	11 (10%)	7 25
10	AJ	87/87 (100%)	79 (91%)	8 (9%)	9 31
10	BJ	86/87 (99%)	76 (88%)	10 (12%)	5 21
11	AK	90/90 (100%)	84 (93%)	6 (7%)	16 46
11	BK	90/90 (100%)	82 (91%)	8 (9%)	9 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	AL	102/102 (100%)	94 (92%)	8 (8%)	12 39
12	BL	102/102 (100%)	91 (89%)	11 (11%)	6 24
13	AM	92/92 (100%)	81 (88%)	11 (12%)	5 20
13	BM	92/92 (100%)	84 (91%)	8 (9%)	10 34
14	AN	83/83 (100%)	80 (96%)	3 (4%)	35 68
14	BN	83/83 (100%)	79 (95%)	4 (5%)	25 60
15	AO	76/76 (100%)	68 (90%)	8 (10%)	7 25
15	BO	76/76 (100%)	67 (88%)	9 (12%)	5 20
16	AP	65/65 (100%)	59 (91%)	6 (9%)	9 31
16	BP	65/65 (100%)	58 (89%)	7 (11%)	6 24
17	AQ	74/74 (100%)	68 (92%)	6 (8%)	11 37
17	BQ	74/74 (100%)	63 (85%)	11 (15%)	3 13
18	AR	48/48 (100%)	43 (90%)	5 (10%)	7 25
18	BR	48/48 (100%)	44 (92%)	4 (8%)	11 37
19	AS	70/70 (100%)	62 (89%)	8 (11%)	5 22
19	BS	70/70 (100%)	63 (90%)	7 (10%)	7 27
20	AT	65/65 (100%)	55 (85%)	10 (15%)	2 12
20	BT	65/65 (100%)	56 (86%)	9 (14%)	3 15
21	AU	48/48 (100%)	47 (98%)	1 (2%)	53 80
21	BU	48/48 (100%)	47 (98%)	1 (2%)	53 80
22	C1	47/47 (100%)	44 (94%)	3 (6%)	17 48
22	D1	47/47 (100%)	46 (98%)	1 (2%)	53 80
23	C2	45/46 (98%)	43 (96%)	2 (4%)	28 63
23	D2	45/46 (98%)	42 (93%)	3 (7%)	16 46
24	C3	38/38 (100%)	35 (92%)	3 (8%)	12 39
24	D3	38/38 (100%)	36 (95%)	2 (5%)	22 56
25	C4	51/51 (100%)	48 (94%)	3 (6%)	19 51
25	D4	51/51 (100%)	48 (94%)	3 (6%)	19 51
26	C5	34/34 (100%)	32 (94%)	2 (6%)	19 51
26	D5	34/34 (100%)	33 (97%)	1 (3%)	42 74
27	C0	48/48 (100%)	42 (88%)	6 (12%)	4 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	D0	49/48 (102%)	42 (86%)	7 (14%)	3 14
29	CC	216/216 (100%)	201 (93%)	15 (7%)	15 45
29	DC	216/216 (100%)	207 (96%)	9 (4%)	30 64
30	CD	164/164 (100%)	156 (95%)	8 (5%)	25 59
32	DD	163/163 (100%)	156 (96%)	7 (4%)	29 63
33	CE	165/165 (100%)	149 (90%)	16 (10%)	8 29
33	DE	165/165 (100%)	158 (96%)	7 (4%)	30 64
34	CF	148/148 (100%)	134 (90%)	14 (10%)	8 30
34	DF	148/148 (100%)	134 (90%)	14 (10%)	8 30
35	CG	137/137 (100%)	133 (97%)	4 (3%)	42 74
35	DG	137/137 (100%)	132 (96%)	5 (4%)	35 68
36	CH	114/114 (100%)	103 (90%)	11 (10%)	8 29
36	DH	114/114 (100%)	104 (91%)	10 (9%)	10 34
37	CJ	104/104 (100%)	98 (94%)	6 (6%)	20 52
37	DJ	104/104 (100%)	98 (94%)	6 (6%)	20 52
38	CK	116/116 (100%)	113 (97%)	3 (3%)	46 76
38	DK	116/116 (100%)	112 (97%)	4 (3%)	37 70
39	CL	103/104 (99%)	96 (93%)	7 (7%)	16 46
39	DL	104/104 (100%)	96 (92%)	8 (8%)	13 40
40	CM	103/103 (100%)	94 (91%)	9 (9%)	10 34
40	DM	103/103 (100%)	97 (94%)	6 (6%)	20 52
41	CN	108/108 (100%)	101 (94%)	7 (6%)	17 47
41	DN	109/108 (101%)	103 (94%)	6 (6%)	21 54
42	CO	100/102 (98%)	91 (91%)	9 (9%)	9 33
42	DO	102/102 (100%)	95 (93%)	7 (7%)	15 45
43	CP	86/87 (99%)	79 (92%)	7 (8%)	11 37
43	DP	87/87 (100%)	79 (91%)	8 (9%)	9 31
44	CQ	99/99 (100%)	91 (92%)	8 (8%)	11 37
44	DQ	99/99 (100%)	93 (94%)	6 (6%)	18 50
45	CR	89/89 (100%)	83 (93%)	6 (7%)	16 46
45	DR	89/89 (100%)	85 (96%)	4 (4%)	27 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	CS	84/84 (100%)	81 (96%)	3 (4%)	35 68
46	DS	84/84 (100%)	82 (98%)	2 (2%)	49 78
47	CT	93/93 (100%)	88 (95%)	5 (5%)	22 55
47	DT	93/93 (100%)	91 (98%)	2 (2%)	52 79
48	CU	80/80 (100%)	72 (90%)	8 (10%)	7 27
48	DU	80/80 (100%)	74 (92%)	6 (8%)	13 41
49	CV	83/83 (100%)	77 (93%)	6 (7%)	14 43
49	DV	83/83 (100%)	80 (96%)	3 (4%)	35 68
50	CW	78/78 (100%)	73 (94%)	5 (6%)	17 48
50	DW	78/78 (100%)	75 (96%)	3 (4%)	33 67
51	CX	56/58 (97%)	50 (89%)	6 (11%)	6 24
51	DX	58/58 (100%)	49 (84%)	9 (16%)	2 12
52	CY	67/67 (100%)	62 (92%)	5 (8%)	13 41
52	DY	67/67 (100%)	62 (92%)	5 (8%)	13 41
53	CZ	54/54 (100%)	51 (94%)	3 (6%)	21 54
53	DZ	54/54 (100%)	53 (98%)	1 (2%)	57 82
54	DI	103/103 (100%)	94 (91%)	9 (9%)	10 34
All	All	9461/9478 (100%)	8736 (92%)	725 (8%)	13 40

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA

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

All (1449) RNA backbone outliers are listed below:

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

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

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Mol	Chain	Res	Type
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	382	A
1	AA	384	G
1	AA	406	G
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	414	A
1	AA	421	U
1	AA	422	C
1	AA	424	G
1	AA	429	U
1	AA	430	A
1	AA	438	U
1	AA	439	U
1	AA	457	G
1	AA	458	U
1	AA	466	A
1	AA	467	U
1	AA	468	A
1	AA	474	G
1	AA	479	U
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	496	A
1	AA	511	C
1	AA	518	C
1	AA	524	G
1	AA	527	G7M
1	AA	532	A
1	AA	533	A

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Mol	Chain	Res	Type
1	AA	547	A
1	AA	559	A
1	AA	562	U
1	AA	564	C
1	AA	568	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	579	A
1	AA	633	G
1	AA	639	G
1	AA	650	G
1	AA	653	U
1	AA	661	G
1	AA	665	A
1	AA	703	G
1	AA	721	G
1	AA	723	U
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	814	A
1	AA	815	A
1	AA	817	C
1	AA	821	G
1	AA	828	U
1	AA	836	G
1	AA	839	C
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	873	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C

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

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Mol	Chain	Res	Type
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1143	G
1	AA	1145	A
1	AA	1152	A
1	AA	1158	C
1	AA	1159	U
1	AA	1160	G
1	AA	1168	U
1	AA	1184	G
1	AA	1193	G
1	AA	1196	A
1	AA	1197	A
1	AA	1200	C
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1227	A
1	AA	1236	A
1	AA	1238	A
1	AA	1239	A
1	AA	1256	A
1	AA	1257	A
1	AA	1260	G
1	AA	1280	A
1	AA	1281	C
1	AA	1286	U
1	AA	1287	A
1	AA	1296	C
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1312	G
1	AA	1317	C
1	AA	1318	A
1	AA	1320	C
1	AA	1323	G
1	AA	1346	A

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

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

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

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Mol	Chain	Res	Type
1	BA	547	A
1	BA	559	A
1	BA	560	A
1	BA	561	U
1	BA	562	U
1	BA	564	C
1	BA	568	G
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
1	BA	579	A
1	BA	633	G
1	BA	639	G
1	BA	650	G
1	BA	653	U
1	BA	661	G
1	BA	665	A
1	BA	703	G
1	BA	721	G
1	BA	723	U
1	BA	734	G
1	BA	748	G
1	BA	755	G
1	BA	777	A
1	BA	793	U
1	BA	794	A
1	BA	814	A
1	BA	815	A
1	BA	817	C
1	BA	821	G
1	BA	828	U
1	BA	836	G
1	BA	839	C
1	BA	840	C
1	BA	841	C
1	BA	842	U
1	BA	843	U
1	BA	844	G
1	BA	845	A
1	BA	846	G
1	BA	873	A

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Mol	Chain	Res	Type
1	BA	914	A
1	BA	926	G
1	BA	927	G
1	BA	934	C
1	BA	942	G
1	BA	960	U
1	BA	963	G
1	BA	966	2MG
1	BA	969	A
1	BA	971	G
1	BA	975	A
1	BA	976	G
1	BA	977	A
1	BA	992	U
1	BA	993	G
1	BA	996	A
1	BA	1004	A
1	BA	1005	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	1026	G
1	BA	1027	C
1	BA	1030	U
1	BA	1031	C
1	BA	1032	G
1	BA	1033	G
1	BA	1036	A
1	BA	1037	C
1	BA	1043	G
1	BA	1052	G
1	BA	1053	G
1	BA	1054	C
1	BA	1065	U
1	BA	1066	C
1	BA	1070	U
1	BA	1086	U
1	BA	1094	G
1	BA	1095	U
1	BA	1101	A
1	BA	1124	G

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Mol	Chain	Res	Type
1	BA	1125	U
1	BA	1127	G
1	BA	1132	C
1	BA	1133	G
1	BA	1136	C
1	BA	1137	C
1	BA	1138	G
1	BA	1139	G
1	BA	1140	C
1	BA	1141	C
1	BA	1143	G
1	BA	1145	A
1	BA	1152	A
1	BA	1159	U
1	BA	1160	G
1	BA	1168	U
1	BA	1193	G
1	BA	1196	A
1	BA	1197	A
1	BA	1200	C
1	BA	1202	U
1	BA	1212	U
1	BA	1213	A
1	BA	1214	C
1	BA	1215	G
1	BA	1227	A
1	BA	1236	A
1	BA	1238	A
1	BA	1239	A
1	BA	1256	A
1	BA	1257	A
1	BA	1258	G
1	BA	1260	G
1	BA	1261	A
1	BA	1280	A
1	BA	1281	C
1	BA	1286	U
1	BA	1287	A
1	BA	1296	C
1	BA	1300	G
1	BA	1302	C
1	BA	1305	G

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

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Mol	Chain	Res	Type
28	CB	89	U
28	CB	90	C
28	CB	99	A
28	CB	109	A
31	CA	10	A
31	CA	14	A
31	CA	34	U
31	CA	36	G
31	CA	42	A
31	CA	46	G
31	CA	49	A
31	CA	58	G
31	CA	71	A
31	CA	74	A
31	CA	75	G
31	CA	83	A
31	CA	84	A
31	CA	86	G
31	CA	102	U
31	CA	118	A
31	CA	119	A
31	CA	120	U
31	CA	125	A
31	CA	138	U
31	CA	139	U
31	CA	140	C
31	CA	141	G
31	CA	142	A
31	CA	165	A
31	CA	177	G
31	CA	178	G
31	CA	188	G
31	CA	196	A
31	CA	197	A
31	CA	199	A
31	CA	200	U
31	CA	215	G
31	CA	216	A
31	CA	221	A
31	CA	222	A
31	CA	226	A
31	CA	248	G

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Mol	Chain	Res	Type
31	CA	264	C
31	CA	265	A
31	CA	266	G
31	CA	272	A
31	CA	276	U
31	CA	277	G
31	CA	278	A
31	CA	279	A
31	CA	285	G
31	CA	310	A
31	CA	311	A
31	CA	324	A
31	CA	329	G
31	CA	330	A
31	CA	343	C
31	CA	346	A
31	CA	352	A
31	CA	353	C
31	CA	362	A
31	CA	371	A
31	CA	372	G
31	CA	386	G
31	CA	399	U
31	CA	404	A
31	CA	405	U
31	CA	411	G
31	CA	412	A
31	CA	420	C
31	CA	424	G
31	CA	451	U
31	CA	455	C
31	CA	456	C
31	CA	457	A
31	CA	459	U
31	CA	481	G
31	CA	491	G
31	CA	501	A
31	CA	503	A
31	CA	504	A
31	CA	505	A
31	CA	508	A
31	CA	517	C

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

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

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

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

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

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

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Mol	Chain	Res	Type
31	CA	2061	G
31	CA	2062	A
31	CA	2069	G7M
31	CA	2072	C
31	CA	2092	U
31	CA	2093	G
31	CA	2095	A
31	CA	2107	G
31	CA	2110	G
31	CA	2111	U
31	CA	2112	G
31	CA	2113	U
31	CA	2114	A
31	CA	2115	G
31	CA	2117	A
31	CA	2118	U
31	CA	2119	A
31	CA	2120	G
31	CA	2123	G
31	CA	2124	G
31	CA	2125	G
31	CA	2126	A
31	CA	2127	G
31	CA	2128	G
31	CA	2131	U
31	CA	2132	U
31	CA	2133	G
31	CA	2136	G
31	CA	2146	C
31	CA	2147	A
31	CA	2157	G
31	CA	2158	A
31	CA	2159	G
31	CA	2162	G
31	CA	2164	C
31	CA	2165	C
31	CA	2171	A
31	CA	2172	U
31	CA	2173	A
31	CA	2174	C
31	CA	2183	A
31	CA	2190	G

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

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Mol	Chain	Res	Type
31	CA	2430	A
31	CA	2435	A
31	CA	2441	U
31	CA	2448	A
31	CA	2465	C
31	CA	2474	U
31	CA	2476	A
31	CA	2482	A
31	CA	2491	U
31	CA	2502	G
31	CA	2504	PSU
31	CA	2505	G
31	CA	2518	A
31	CA	2520	C
31	CA	2529	G
31	CA	2535	G
31	CA	2547	A
31	CA	2554	U
31	CA	2556	C
31	CA	2566	A
31	CA	2567	G
31	CA	2578	G
31	CA	2582	G
31	CA	2585	U
31	CA	2602	A
31	CA	2603	G
31	CA	2609	U
31	CA	2613	U
31	CA	2629	U
31	CA	2630	G
31	CA	2646	C
31	CA	2661	G
31	CA	2663	G
31	CA	2681	C
31	CA	2682	A
31	CA	2689	U
31	CA	2690	U
31	CA	2693	G
31	CA	2714	G
31	CA	2718	G
31	CA	2719	G
31	CA	2726	A

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Mol	Chain	Res	Type
31	CA	2744	G
31	CA	2748	A
31	CA	2765	A
31	CA	2777	G
31	CA	2778	A
31	CA	2779	U
31	CA	2780	G
31	CA	2791	G
31	CA	2792	A
31	CA	2794	C
31	CA	2799	A
31	CA	2803	G
31	CA	2811	G
31	CA	2813	A
31	CA	2818	U
31	CA	2820	A
31	CA	2821	A
31	CA	2835	A
31	CA	2836	U
31	CA	2850	A
31	CA	2861	U
31	CA	2865	U
31	CA	2867	G
31	CA	2868	A
31	CA	2883	A
31	CA	2886	A
31	CA	2893	A
31	CA	2894	G
31	CA	2901	C
31	CA	2904	U
28	DB	9	G
28	DB	25	U
28	DB	35	C
28	DB	44	G
28	DB	56	G
28	DB	57	A
28	DB	67	G
28	DB	88	C
28	DB	89	U
28	DB	90	C
28	DB	109	A
55	DA	10	A

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

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

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

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

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

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

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

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

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

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

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

All (216) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	70	U
1	AA	88	U
1	AA	89	U
1	AA	94	G
1	AA	209	U
1	AA	305	G
1	AA	367	U
1	AA	372	C
1	AA	413	G
1	AA	422	C
1	AA	429	U
1	AA	438	U
1	AA	653	U
1	AA	702	A
1	AA	733	G
1	AA	793	U
1	AA	841	C
1	AA	884	U
1	AA	992	U
1	AA	1086	U
1	AA	1129	C
1	AA	1136	C
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1225	A
1	AA	1239	A
1	AA	1281	C
1	AA	1297	G
1	AA	1299	A
1	AA	1301	U
1	AA	1432	G
1	AA	1447	A
1	AA	1452	C
1	BA	5	U

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Mol	Chain	Res	Type
1	BA	70	U
1	BA	89	U
1	BA	94	G
1	BA	183	C
1	BA	209	U
1	BA	246	A
1	BA	305	G
1	BA	372	C
1	BA	422	C
1	BA	429	U
1	BA	438	U
1	BA	559	A
1	BA	560	A
1	BA	561	U
1	BA	653	U
1	BA	702	A
1	BA	733	G
1	BA	793	U
1	BA	842	U
1	BA	844	G
1	BA	884	U
1	BA	992	U
1	BA	1086	U
1	BA	1129	C
1	BA	1136	C
1	BA	1137	C
1	BA	1139	G
1	BA	1140	C
1	BA	1225	A
1	BA	1281	C
1	BA	1297	G
1	BA	1299	A
1	BA	1301	U
1	BA	1362	A
1	BA	1432	G
1	BA	1447	A
1	BA	1452	C
1	BA	1493	A
31	CA	125	A
31	CA	138	U
31	CA	139	U
31	CA	141	G

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Mol	Chain	Res	Type
31	CA	177	G
31	CA	196	A
31	CA	199	A
31	CA	271	G
31	CA	278	A
31	CA	310	A
31	CA	371	A
31	CA	403	U
31	CA	404	A
31	CA	411	G
31	CA	455	C
31	CA	503	A
31	CA	527	C
31	CA	555	G
31	CA	685	A
31	CA	764	A
31	CA	784	G
31	CA	846	U
31	CA	973	A
31	CA	984	A
31	CA	1045	C
31	CA	1061	U
31	CA	1069	A
31	CA	1070	A
31	CA	1088	A
31	CA	1089	A
31	CA	1111	A
31	CA	1128	G
31	CA	1133	A
31	CA	1141	U
31	CA	1253	A
31	CA	1286	A
31	CA	1288	G
31	CA	1300	G
31	CA	1324	G
31	CA	1329	U
31	CA	1379	U
31	CA	1452	G
31	CA	1490	A
31	CA	1497	U
31	CA	1509	A
31	CA	1535	A

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Mol	Chain	Res	Type
31	CA	1536	C
31	CA	1567	G
31	CA	1607	C
31	CA	1647	U
31	CA	1818	U
31	CA	1870	C
31	CA	1900	A
31	CA	1913	A
31	CA	2035	G
31	CA	2062	A
31	CA	2095	A
31	CA	2119	A
31	CA	2126	A
31	CA	2146	C
31	CA	2157	G
31	CA	2164	C
31	CA	2225	A
31	CA	2238	G
31	CA	2275	C
31	CA	2282	G
31	CA	2286	G
31	CA	2324	U
31	CA	2326	C
31	CA	2423	U
31	CA	2425	A
31	CA	2581	G
31	CA	2680	U
31	CA	2779	U
31	CA	2820	A
31	CA	2849	U
31	CA	2867	G
31	CA	2873	A
31	CA	2893	A
55	DA	125	A
55	DA	138	U
55	DA	141	G
55	DA	196	A
55	DA	199	A
55	DA	271	G
55	DA	278	A
55	DA	310	A
55	DA	371	A

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

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

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

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	$\#\|Z\| > 2$
32	MEQ	DD	150[A]	32	8,9,10	0.53	0	5,10,12	0.46	0
55	OMC	DA	2498	55,56	19,22,23	0.52	0	26,31,34	0.60	0
1	5MC	AA	1407	1	18,22,23	0.47	0	26,32,35	0.53	0
1	2MG	AA	966	1	18,26,27	0.86	1 (5%)	16,38,41	0.46	0
31	3TD	CA	1915	31	18,22,23	0.54	0	22,32,35	0.53	0
55	5MU	DA	747	55	19,22,23	0.32	0	28,32,35	0.35	0
55	OMU	DA	2552	55	19,22,23	0.62	1 (5%)	26,31,34	0.24	0
31	1MG	CA	745	31	18,26,27	0.82	0	19,39,42	0.50	0
31	PSU	CA	1911	31	18,21,22	0.33	0	22,30,33	0.43	0
55	PSU	DA	955	55	18,21,22	0.73	1 (5%)	22,30,33	0.53	0
31	2MA	CA	2503	31	17,25,26	1.00	2 (11%)	17,37,40	0.38	0
31	G7M	CA	2069	31	20,26,27	0.50	0	17,39,42	0.52	0
12	D2T	BL	89	12	7,9,10	2.03	2 (28%)	6,11,13	0.79	0
55	PSU	DA	2457	55	18,21,22	0.53	0	22,30,33	0.49	0
1	PSU	AA	516	1,56	18,21,22	0.46	0	22,30,33	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	OMG	CA	2251	31	18,26,27	0.85	0	19,38,41	0.58	0
1	2MG	BA	1516	1	18,26,27	0.77	0	16,38,41	0.54	0
31	PSU	CA	2504	31	18,21,22	0.55	0	22,30,33	0.42	0
55	1MG	DA	745	55	18,26,27	1.04	0	19,39,42	0.44	0
55	PSU	DA	2605	55	18,21,22	0.69	0	22,30,33	0.66	0
55	PSU	DA	746	55,56	18,21,22	1.08	1 (5%)	22,30,33	0.34	0
1	2MG	BA	1207	1	18,26,27	0.84	1 (5%)	16,38,41	0.53	0
31	PSU	CA	1917	31	18,21,22	0.31	0	22,30,33	0.46	0
1	5MC	BA	1407	1	18,22,23	0.52	0	26,32,35	0.52	0
55	5MC	DA	1962	55	18,22,23	0.74	1 (5%)	26,32,35	0.45	0
55	H2U	DA	2449	55	18,21,22	0.40	0	21,30,33	0.59	1 (4%)
32	MEQ	DD	150[B]	32	8,9,10	1.15	1 (12%)	5,10,12	0.89	0
55	PSU	DA	2604	55	18,21,22	0.95	1 (5%)	22,30,33	0.57	0
55	PSU	DA	2580	55	18,21,22	0.76	0	22,30,33	0.69	0
31	OMC	CA	2498	31,56	19,22,23	0.45	0	26,31,34	0.38	0
1	4OC	BA	1402	1	20,23,24	0.36	0	26,32,35	0.41	0
1	4OC	AA	1402	1	20,23,24	0.31	0	26,32,35	0.40	0
1	2MG	AA	1516	1	18,26,27	0.84	1 (5%)	16,38,41	0.57	0
1	G7M	AA	527	1	20,26,27	0.82	1 (5%)	17,39,42	0.89	1 (5%)
1	UR3	BA	1498	1	19,22,23	0.37	0	26,32,35	0.38	0
31	5MU	CA	1939	31	19,22,23	0.40	0	28,32,35	0.33	0
31	PSU	CA	2605	31	18,21,22	0.44	0	22,30,33	0.58	0
55	2MG	DA	2445	55	18,26,27	1.35	4 (22%)	16,38,41	0.67	0
31	OMU	CA	2552	31	19,22,23	0.39	0	26,31,34	0.28	0
31	PSU	CA	955	31	18,21,22	0.33	0	22,30,33	0.53	0
31	2MG	CA	2445	31	18,26,27	0.96	1 (5%)	16,38,41	0.58	0
1	2MG	BA	966	1	18,26,27	0.81	0	16,38,41	0.51	0
41	4D4	DN	81[A]	-	9,11,12	1.92	2 (22%)	8,13,15	2.27	2 (25%)
55	PSU	DA	1917	55	18,21,22	0.46	0	22,30,33	0.46	0
1	MA6	AA	1518	1	19,26,27	0.85	0	18,38,41	0.95	1 (5%)
31	6MZ	CA	2030	31	18,25,26	0.91	0	16,36,39	1.02	2 (12%)
31	PSU	CA	2580	31	18,21,22	0.57	0	22,30,33	0.77	2 (9%)
55	3TD	DA	1915	55	18,22,23	0.52	0	22,32,35	0.55	0
55	G7M	DA	2069	55	20,26,27	0.66	0	17,39,42	0.69	0
1	UR3	AA	1498	1	19,22,23	0.65	0	26,32,35	0.29	0
31	6MZ	CA	1618	31	18,25,26	0.87	1 (5%)	16,36,39	0.87	0
31	PSU	CA	746	31,56	18,21,22	0.57	0	22,30,33	0.35	0
31	5MC	CA	1962	31	18,22,23	0.42	0	26,32,35	0.38	0
1	5MC	BA	967	1	18,22,23	0.26	0	26,32,35	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MC	AA	967	1	18,22,23	0.31	0	26,32,35	0.37	0
55	PSU	DA	1911	55	18,21,22	0.30	0	22,30,33	0.42	0
55	6MZ	DA	2030	55	18,25,26	1.38	3 (16%)	16,36,39	0.96	2 (12%)
55	2MA	DA	2503	55,56	17,25,26	1.10	3 (17%)	17,37,40	0.44	0
41	4D4	CN	81	41	9,11,12	2.05	2 (22%)	8,13,15	2.45	2 (25%)
31	2MG	CA	1835	31	18,26,27	0.90	1 (5%)	16,38,41	0.47	0
31	PSU	CA	2457	31	18,21,22	0.70	0	22,30,33	0.48	0
55	6MZ	DA	1618	55	18,25,26	0.95	1 (5%)	16,36,39	1.37	1 (6%)
55	5MU	DA	1939	55	19,22,23	0.57	0	28,32,35	0.39	0
1	PSU	BA	516	1	18,21,22	0.46	0	22,30,33	0.46	0
55	OMG	DA	2251	55	18,26,27	0.89	2 (11%)	19,38,41	0.52	0
55	PSU	DA	2504	55	18,21,22	0.53	0	22,30,33	0.48	0
1	MA6	BA	1519	1	19,26,27	1.01	0	18,38,41	1.09	1 (5%)
1	MA6	AA	1519	1	19,26,27	1.03	1 (5%)	18,38,41	1.12	1 (5%)
1	G7M	BA	527	1	20,26,27	0.72	0	17,39,42	0.44	0
31	5MU	CA	747	31	19,22,23	0.33	0	28,32,35	0.27	0
41	4D4	DN	81[B]	-	9,11,12	1.62	2 (22%)	8,13,15	2.65	2 (25%)
55	2MG	DA	1835	55	18,26,27	0.91	1 (5%)	16,38,41	0.63	0
1	MA6	BA	1518	1	19,26,27	0.84	0	18,38,41	0.90	1 (5%)
1	2MG	AA	1207	1	18,26,27	0.84	0	16,38,41	0.50	0
12	D2T	AL	89	12	7,9,10	1.63	2 (28%)	6,11,13	0.96	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
32	MEQ	DD	150[A]	32	-	3/8/9/11	-
55	OMC	DA	2498	55,56	-	0/9/27/28	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
55	5MU	DA	747	55	-	1/7/25/26	0/2/2/2
55	OMU	DA	2552	55	-	0/9/27/28	0/2/2/2
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
55	PSU	DA	955	55	-	0/7/25/26	0/2/2/2
31	2MA	CA	2503	31	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	G7M	CA	2069	31	-	1/3/25/26	0/3/3/3
12	D2T	BL	89	12	-	4/7/12/14	-
55	PSU	DA	2457	55	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	1,56	-	0/7/25/26	0/2/2/2
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
31	PSU	CA	2504	31	-	2/7/25/26	0/2/2/2
55	1MG	DA	745	55	-	0/3/25/26	0/3/3/3
55	PSU	DA	2605	55	-	0/7/25/26	0/2/2/2
55	PSU	DA	746	55,56	-	4/7/25/26	0/2/2/2
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
55	5MC	DA	1962	55	-	2/7/25/26	0/2/2/2
55	H2U	DA	2449	55	-	0/7/38/39	0/2/2/2
32	MEQ	DD	150[B]	32	-	6/8/9/11	-
55	PSU	DA	2604	55	-	0/7/25/26	0/2/2/2
55	PSU	DA	2580	55	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	31,56	-	0/9/27/28	0/2/2/2
1	4OC	BA	1402	1	-	1/9/29/30	0/2/2/2
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
55	2MG	DA	2445	55	-	0/5/27/28	0/3/3/3
31	OMU	CA	2552	31	-	0/9/27/28	0/2/2/2
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
31	2MG	CA	2445	31	-	1/5/27/28	0/3/3/3
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
41	4D4	DN	81[A]	-	-	2/11/12/14	-
55	PSU	DA	1917	55	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
31	6MZ	CA	2030	31	-	2/5/27/28	0/3/3/3
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
55	3TD	DA	1915	55	-	0/7/25/26	0/2/2/2
55	G7M	DA	2069	55	-	1/3/25/26	0/3/3/3
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PSU	CA	746	31,56	-	4/7/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
55	PSU	DA	1911	55	-	0/7/25/26	0/2/2/2
55	6MZ	DA	2030	55	-	1/5/27/28	0/3/3/3
55	2MA	DA	2503	55,56	-	2/3/25/26	0/3/3/3
41	4D4	CN	81	41	-	2/11/12/14	-
31	2MG	CA	1835	31	-	1/5/27/28	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
55	6MZ	DA	1618	55	-	0/5/27/28	0/3/3/3
55	5MU	DA	1939	55	-	0/7/25/26	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
55	OMG	DA	2251	55	-	1/5/27/28	0/3/3/3
55	PSU	DA	2504	55	-	2/7/25/26	0/2/2/2
1	MA6	BA	1519	1	-	2/7/29/30	0/3/3/3
1	MA6	AA	1519	1	-	2/7/29/30	0/3/3/3
1	G7M	BA	527	1	-	2/3/25/26	0/3/3/3
31	5MU	CA	747	31	-	1/7/25/26	0/2/2/2
41	4D4	DN	81[B]	-	-	3/11/12/14	-
55	2MG	DA	1835	55	-	2/5/27/28	0/3/3/3
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
12	D2T	AL	89	12	-	2/7/12/14	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	CN	81	4D4	CZ-NE	5.64	1.44	1.33
41	DN	81[A]	4D4	CZ-NE	4.79	1.42	1.33
41	DN	81[B]	4D4	CZ-NE	4.14	1.41	1.33
12	BL	89	D2T	CB-SB	3.89	1.86	1.82
55	DA	746	PSU	O4'-C1'	-3.72	1.38	1.43
12	BL	89	D2T	CB-CG	3.53	1.58	1.52
55	DA	2030	6MZ	C2'-C1'	-3.45	1.48	1.53
32	DD	150[B]	MEQ	CB-CA	3.12	1.57	1.53
55	DA	2503	2MA	C8-N7	-3.11	1.29	1.35
55	DA	2445	2MG	O5'-C5'	-3.09	1.37	1.44
12	AL	89	D2T	CB-SB	2.98	1.85	1.82
55	DA	2030	6MZ	O4'-C1'	-2.87	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	AL	89	D2T	CB-CG	2.79	1.56	1.52
31	CA	2503	2MA	C8-N7	-2.77	1.30	1.35
41	DN	81[A]	4D4	CZ-NH1	2.72	1.46	1.34
55	DA	2445	2MG	C5-C4	-2.62	1.36	1.43
55	DA	1962	5MC	O5'-C5'	-2.43	1.38	1.44
55	DA	1835	2MG	C5-C4	-2.30	1.37	1.43
31	CA	1618	6MZ	C8-N7	-2.26	1.30	1.34
55	DA	2552	OMU	O5'-C5'	-2.25	1.39	1.44
55	DA	2604	PSU	O3'-C3'	-2.21	1.37	1.43
1	AA	1516	2MG	C5-C4	-2.20	1.37	1.43
55	DA	1618	6MZ	C8-N7	-2.20	1.30	1.34
55	DA	955	PSU	C2'-C1'	-2.20	1.50	1.53
1	AA	966	2MG	C8-N7	-2.17	1.31	1.35
1	AA	527	G7M	O3'-C3'	-2.17	1.37	1.43
55	DA	2030	6MZ	O5'-C5'	-2.13	1.39	1.44
55	DA	2445	2MG	C8-N7	-2.11	1.31	1.35
55	DA	2503	2MA	O5'-C5'	-2.08	1.39	1.44
55	DA	2251	OMG	C5-C6	-2.08	1.43	1.47
41	CN	81	4D4	CZ-NH1	2.06	1.43	1.34
55	DA	2251	OMG	C8-N7	-2.05	1.31	1.35
31	CA	2503	2MA	C5-C4	-2.04	1.37	1.43
1	AA	1519	MA6	O3'-C3'	-2.04	1.38	1.43
41	DN	81[B]	4D4	CZ-NH1	2.03	1.43	1.34
55	DA	2503	2MA	C5-C4	-2.03	1.37	1.43
1	BA	1207	2MG	C8-N7	-2.03	1.31	1.35
31	CA	1835	2MG	C8-N7	-2.03	1.31	1.35
31	CA	2445	2MG	O4'-C1'	2.02	1.43	1.41
55	DA	2445	2MG	C2'-C1'	-2.02	1.50	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	DN	81[B]	4D4	NE-CZ-NH2	5.85	130.98	120.70
41	CN	81	4D4	NE-CZ-NH2	5.80	130.89	120.70
41	DN	81[A]	4D4	NE-CZ-NH2	5.08	129.62	120.70
55	DA	1618	6MZ	C9-N6-C6	-4.89	118.66	122.87
41	DN	81[B]	4D4	NH1-CZ-NE	-4.33	109.20	119.19
41	DN	81[A]	4D4	NH1-CZ-NE	-3.44	111.25	119.19
1	AA	1519	MA6	N1-C6-N6	-3.40	113.47	117.06
1	BA	1519	MA6	N1-C6-N6	-3.30	113.59	117.06
41	CN	81	4D4	NH1-CZ-NE	-3.22	111.75	119.19
1	AA	527	G7M	O4'-C1'-C2'	-3.02	102.51	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	CA	2030	6MZ	C9-N6-C6	2.91	125.38	122.87
1	AA	1518	MA6	N1-C6-N6	-2.40	114.53	117.06
1	BA	1518	MA6	N1-C6-N6	-2.38	114.55	117.06
55	DA	2030	6MZ	C2-N1-C6	2.36	118.61	116.59
31	CA	2030	6MZ	C2-N1-C6	2.19	118.47	116.59
31	CA	2580	PSU	C3'-C2'-C1'	2.16	104.15	101.64
55	DA	2449	H2U	O4'-C1'-N1	-2.06	106.49	109.30
55	DA	2030	6MZ	O4'-C1'-C2'	-2.04	103.94	106.93
31	CA	2580	PSU	O4'-C1'-C2'	2.04	108.02	105.14

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	AL	89	D2T	SB-CB-CG-OD2
1	BA	527	G7M	O4'-C4'-C5'-O5'
1	BA	527	G7M	C3'-C4'-C5'-O5'
12	BL	89	D2T	CA-CB-CG-OD1
12	BL	89	D2T	CA-CB-CG-OD2
31	CA	746	PSU	C2'-C1'-C5-C4
31	CA	746	PSU	C2'-C1'-C5-C6
31	CA	746	PSU	O4'-C1'-C5-C6
32	DD	150[B]	MEQ	N-CA-CB-CG
32	DD	150[B]	MEQ	O-C-CA-CB
55	DA	746	PSU	C2'-C1'-C5-C4
55	DA	746	PSU	C2'-C1'-C5-C6
55	DA	2251	OMG	C1'-C2'-O2'-CM2
41	DN	81[B]	4D4	N-CA-CB-CG
41	DN	81[B]	4D4	CA-CB-CG-CD
1	AA	527	G7M	C3'-C4'-C5'-O5'
31	CA	2030	6MZ	O4'-C4'-C5'-O5'
31	CA	2030	6MZ	C3'-C4'-C5'-O5'
1	AA	527	G7M	O4'-C4'-C5'-O5'
32	DD	150[A]	MEQ	NE2-CD-CG-CB
32	DD	150[A]	MEQ	OE1-CD-CG-CB
32	DD	150[B]	MEQ	CG-CD-NE2-CE
41	DN	81[B]	4D4	OB-CB-CG-CD
32	DD	150[B]	MEQ	OE1-CD-NE2-CE
32	DD	150[B]	MEQ	C-CA-CB-CG
1	BA	1519	MA6	O4'-C4'-C5'-O5'
55	DA	2504	PSU	O4'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
31	CA	2504	PSU	O4'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
12	BL	89	D2T	CG-CB-SB-CB1
32	DD	150[A]	MEQ	N-CA-CB-CG
55	DA	747	5MU	C3'-C4'-C5'-O5'
32	DD	150[B]	MEQ	CA-CB-CG-CD
31	CA	2503	2MA	O4'-C4'-C5'-O5'
41	CN	81	4D4	CG-CD-NE-CZ
41	DN	81[A]	4D4	CG-CD-NE-CZ
55	DA	2503	2MA	O4'-C4'-C5'-O5'
31	CA	746	PSU	O4'-C1'-C5-C4
55	DA	746	PSU	O4'-C1'-C5-C4
31	CA	747	5MU	C3'-C4'-C5'-O5'
55	DA	2030	6MZ	O4'-C4'-C5'-O5'
55	DA	1962	5MC	C2'-C1'-N1-C6
12	BL	89	D2T	SB-CB-CG-OD2
1	AA	1519	MA6	C3'-C4'-C5'-O5'
1	BA	1519	MA6	C3'-C4'-C5'-O5'
55	DA	1962	5MC	O4'-C1'-N1-C6
55	DA	2069	G7M	O4'-C4'-C5'-O5'
55	DA	746	PSU	O4'-C1'-C5-C6
31	CA	2503	2MA	C4'-C5'-O5'-P
1	BA	1402	4OC	O4'-C4'-C5'-O5'
31	CA	2069	G7M	O4'-C4'-C5'-O5'
31	CA	2445	2MG	C3'-C4'-C5'-O5'
31	CA	2504	PSU	C3'-C4'-C5'-O5'
55	DA	1835	2MG	O4'-C4'-C5'-O5'
55	DA	2504	PSU	C3'-C4'-C5'-O5'
55	DA	2503	2MA	C4'-C5'-O5'-P
31	CA	1835	2MG	O4'-C4'-C5'-O5'
55	DA	1835	2MG	C3'-C4'-C5'-O5'
41	CN	81	4D4	O-C-CA-CB
41	DN	81[A]	4D4	O-C-CA-CB

There are no ring outliers.

14 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	DD	150[A]	MEQ	2	0
55	DA	747	5MU	1	0
31	CA	2503	2MA	1	0
31	CA	2251	OMG	1	0

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
61	PEG	D1	103	-	6,6,6	0.28	0	5,5,5	0.17	0
67	GUN	DA	3213	-	7,12,12	0.43	0	8,17,17	0.69	0
62	EDO	DA	3211	-	3,3,3	0.69	0	2,2,2	0.19	0
58	MPD	DA	3004	-	7,7,7	0.64	0	9,10,10	0.26	0
61	PEG	DA	3203	-	6,6,6	0.30	0	5,5,5	0.19	0
59	PUT	DA	3187	-	5,5,5	0.46	0	4,4,4	0.28	0
58	MPD	DA	3209	-	7,7,7	0.73	0	9,10,10	0.52	0
64	SPD	DA	3208	-	9,9,9	0.20	0	8,8,8	0.18	0
63	PGE	DD	301	-	9,9,9	0.18	0	8,8,8	0.17	0
62	EDO	D1	101	-	3,3,3	0.62	0	2,2,2	0.21	0
58	MPD	DT	201	-	7,7,7	0.81	0	9,10,10	0.47	0
61	PEG	AL	201	-	6,6,6	0.26	0	5,5,5	0.24	0
61	PEG	DP	201	-	6,6,6	0.29	0	5,5,5	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
59	PUT	AA	1672	-	5,5,5	0.25	0	4,4,4	0.15	0
64	SPD	DA	3190	-	9,9,9	0.13	0	8,8,8	0.18	0
59	PUT	DA	3224	-	5,5,5	0.45	0	4,4,4	0.68	0
58	MPD	DA	3212	-	7,7,7	0.83	0	9,10,10	0.42	0
59	PUT	DA	3221	-	5,5,5	0.15	0	4,4,4	0.11	0
62	EDO	DB	210	-	3,3,3	0.69	0	2,2,2	0.06	0
59	PUT	AA	1673	-	5,5,5	0.14	0	4,4,4	0.12	0
61	PEG	DA	3202	-	6,6,6	0.21	0	5,5,5	0.15	0
58	MPD	DE	301	-	7,7,7	0.73	0	9,10,10	0.49	0
58	MPD	AA	1671	-	7,7,7	0.72	0	9,10,10	0.41	0
57	PG4	DS	202	-	12,12,12	0.38	0	11,11,11	0.33	0
61	PEG	DQ	201	-	6,6,6	0.33	0	5,5,5	0.29	0
58	MPD	DS	203	-	7,7,7	0.50	0	9,10,10	0.44	0
63	PGE	D3	101	-	9,9,9	0.30	0	8,8,8	0.29	0
59	PUT	DA	3215	-	5,5,5	0.27	0	4,4,4	0.19	0
59	PUT	DA	3191	-	5,5,5	0.11	0	4,4,4	0.19	0
61	PEG	DA	3220	-	6,6,6	0.20	0	5,5,5	0.08	0
64	SPD	DA	3186	-	9,9,9	0.19	0	8,8,8	0.15	0
59	PUT	AA	1675	-	5,5,5	0.21	0	4,4,4	0.10	0
64	SPD	DA	3226	-	9,9,9	0.34	0	8,8,8	0.44	0
66	ACY	DA	3204	-	3,3,3	0.63	0	3,3,3	1.13	0
62	EDO	DA	3005	-	3,3,3	0.58	0	2,2,2	0.30	0
59	PUT	DA	3223	-	5,5,5	0.27	0	4,4,4	0.21	0
59	PUT	DA	3214	-	5,5,5	0.23	0	4,4,4	0.08	0
59	PUT	AA	1674	-	5,5,5	0.18	0	4,4,4	0.11	0
57	PG4	DR	202	-	12,12,12	0.31	0	11,11,11	0.35	0
63	PGE	DA	3219	-	9,9,9	0.22	0	8,8,8	0.27	0
68	TRS	DA	3222	-	7,7,7	0.29	0	9,9,9	0.31	0
59	PUT	DA	3198	-	5,5,5	0.24	0	4,4,4	0.21	0
58	MPD	DA	3195	-	7,7,7	0.66	0	9,10,10	0.64	0
57	PG4	BA	1642	-	12,12,12	0.34	0	11,11,11	0.27	0
58	MPD	DE	302	-	7,7,7	1.07	1 (14%)	9,10,10	0.49	0
57	PG4	AA	1670	-	12,12,12	0.36	0	11,11,11	0.35	0
61	PEG	DA	3229	-	6,6,6	0.38	0	5,5,5	0.24	0
57	PG4	DA	3218	-	12,12,12	0.20	0	11,11,11	0.25	0
58	MPD	DK	201	-	7,7,7	0.67	0	9,10,10	0.39	0
63	PGE	D1	102	-	9,9,9	0.27	0	8,8,8	0.25	0
65	1PE	DA	3205	-	15,15,15	0.41	0	14,14,14	0.49	0
58	MPD	DN	201	-	7,7,7	1.15	1 (14%)	9,10,10	0.63	0
62	EDO	DA	3197	-	3,3,3	1.08	0	2,2,2	0.35	0
61	PEG	D3	102	-	6,6,6	0.50	0	5,5,5	0.39	0
57	PG4	DA	3196	-	12,12,12	0.38	0	11,11,11	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
62	EDO	DA	3003	-	3,3,3	0.64	0	2,2,2	0.27	0
58	MPD	AA	1676	-	7,7,7	0.69	0	9,10,10	0.31	0
59	PUT	DA	3225	-	5,5,5	0.26	0	4,4,4	0.19	0
59	PUT	DA	3192	-	5,5,5	0.37	0	4,4,4	0.42	0
65	1PE	DA	3188	-	15,15,15	0.19	0	14,14,14	0.29	0
62	EDO	DA	3002	-	3,3,3	0.69	0	2,2,2	0.15	0
61	PEG	DA	3228	-	6,6,6	0.40	0	5,5,5	0.32	0
61	PEG	DL	201	-	6,6,6	0.18	0	5,5,5	0.13	0
62	EDO	DA	3201	-	3,3,3	0.52	0	2,2,2	0.45	0
63	PGE	DA	3216	-	9,9,9	0.30	0	8,8,8	0.34	0
59	PUT	DA	3207	-	5,5,5	0.21	0	4,4,4	0.16	0
62	EDO	DA	3217	-	3,3,3	0.64	0	2,2,2	0.27	0
63	PGE	DA	3227	-	9,9,9	0.18	0	8,8,8	0.23	0
63	PGE	DU	101	-	9,9,9	0.29	0	8,8,8	0.21	0
62	EDO	DA	3200	-	3,3,3	0.75	0	2,2,2	0.10	0
63	PGE	DA	3189	-	9,9,9	0.42	0	8,8,8	0.30	0
66	ACY	DA	3194	-	3,3,3	0.60	0	3,3,3	1.10	0
59	PUT	DM	201	-	5,5,5	0.17	0	4,4,4	0.17	0
62	EDO	DA	3210	-	3,3,3	0.67	0	2,2,2	0.26	0
58	MPD	DA	3193	-	7,7,7	0.31	0	9,10,10	0.46	0
57	PG4	DQ	202	-	12,12,12	0.28	0	11,11,11	0.25	0
58	MPD	DA	3206	-	7,7,7	0.95	0	9,10,10	0.72	0
63	PGE	DS	201	-	9,9,9	0.39	0	8,8,8	0.31	0
66	ACY	DA	3199	-	3,3,3	2.13	1 (33%)	3,3,3	2.28	2 (66%)
62	EDO	DB	211	-	3,3,3	0.73	0	2,2,2	0.13	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
61	PEG	D1	103	-	-	0/4/4/4	-
67	GUN	DA	3213	-	-	-	0/2/2/2
62	EDO	DA	3211	-	-	0/1/1/1	-
58	MPD	DA	3004	-	-	3/5/5/5	-
61	PEG	DA	3203	-	-	3/4/4/4	-
59	PUT	DA	3187	-	-	0/3/3/3	-
58	MPD	DA	3209	-	-	3/5/5/5	-
64	SPD	DA	3208	-	-	2/7/7/7	-
63	PGE	DD	301	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	EDO	D1	101	-	-	0/1/1/1	-
58	MPD	DT	201	-	-	1/5/5/5	-
61	PEG	AL	201	-	-	2/4/4/4	-
61	PEG	DP	201	-	-	2/4/4/4	-
59	PUT	AA	1672	-	-	1/3/3/3	-
64	SPD	DA	3190	-	-	2/7/7/7	-
59	PUT	DA	3224	-	-	0/3/3/3	-
58	MPD	DA	3212	-	-	0/5/5/5	-
59	PUT	DA	3221	-	-	0/3/3/3	-
62	EDO	DB	210	-	-	0/1/1/1	-
59	PUT	AA	1673	-	-	0/3/3/3	-
61	PEG	DA	3202	-	-	2/4/4/4	-
58	MPD	DE	301	-	-	2/5/5/5	-
58	MPD	AA	1671	-	-	0/5/5/5	-
57	PG4	DS	202	-	-	6/10/10/10	-
61	PEG	DQ	201	-	-	0/4/4/4	-
58	MPD	DS	203	-	-	1/5/5/5	-
63	PGE	D3	101	-	-	3/7/7/7	-
59	PUT	DA	3215	-	-	0/3/3/3	-
59	PUT	DA	3191	-	-	0/3/3/3	-
61	PEG	DA	3220	-	-	2/4/4/4	-
64	SPD	DA	3186	-	-	1/7/7/7	-
59	PUT	AA	1675	-	-	1/3/3/3	-
64	SPD	DA	3226	-	-	4/7/7/7	-
62	EDO	DA	3005	-	-	0/1/1/1	-
59	PUT	DA	3223	-	-	0/3/3/3	-
59	PUT	DA	3214	-	-	1/3/3/3	-
59	PUT	AA	1674	-	-	0/3/3/3	-
57	PG4	DR	202	-	-	6/10/10/10	-
63	PGE	DA	3219	-	-	3/7/7/7	-
68	TRS	DA	3222	-	-	1/9/9/9	-
59	PUT	DA	3198	-	-	1/3/3/3	-
58	MPD	DA	3195	-	-	2/5/5/5	-
57	PG4	BA	1642	-	-	3/10/10/10	-
58	MPD	DE	302	-	-	1/5/5/5	-
57	PG4	AA	1670	-	-	6/10/10/10	-
61	PEG	DA	3229	-	-	1/4/4/4	-
57	PG4	DA	3218	-	-	4/10/10/10	-
58	MPD	DK	201	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PGE	D1	102	-	-	3/7/7/7	-
65	1PE	DA	3205	-	-	4/13/13/13	-
58	MPD	DN	201	-	-	1/5/5/5	-
62	EDO	DA	3197	-	-	0/1/1/1	-
61	PEG	D3	102	-	-	2/4/4/4	-
57	PG4	DA	3196	-	-	5/10/10/10	-
62	EDO	DA	3003	-	-	0/1/1/1	-
58	MPD	AA	1676	-	-	0/5/5/5	-
59	PUT	DA	3225	-	-	1/3/3/3	-
59	PUT	DA	3192	-	-	0/3/3/3	-
65	1PE	DA	3188	-	-	4/13/13/13	-
62	EDO	DA	3002	-	-	0/1/1/1	-
61	PEG	DA	3228	-	-	3/4/4/4	-
61	PEG	DL	201	-	-	2/4/4/4	-
62	EDO	DA	3201	-	-	0/1/1/1	-
63	PGE	DA	3216	-	-	2/7/7/7	-
59	PUT	DA	3207	-	-	0/3/3/3	-
62	EDO	DA	3217	-	-	0/1/1/1	-
63	PGE	DA	3227	-	-	3/7/7/7	-
63	PGE	DU	101	-	-	2/7/7/7	-
62	EDO	DA	3200	-	-	1/1/1/1	-
63	PGE	DA	3189	-	-	1/7/7/7	-
59	PUT	DM	201	-	-	0/3/3/3	-
62	EDO	DA	3210	-	-	1/1/1/1	-
58	MPD	DA	3193	-	-	2/5/5/5	-
57	PG4	DQ	202	-	-	3/10/10/10	-
58	MPD	DA	3206	-	-	1/5/5/5	-
63	PGE	DS	201	-	-	2/7/7/7	-
62	EDO	DB	211	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	DA	3199	ACY	O-C	3.44	1.38	1.22
58	DN	201	MPD	C3-C2	2.58	1.60	1.53
58	DE	302	MPD	C3-C2	2.48	1.60	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
66	DA	3199	ACY	OXT-C-CH3	2.97	127.47	115.18
66	DA	3199	ACY	O-C-CH3	-2.56	112.36	122.33

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	DA	3209	MPD	C2-C3-C4-O4
57	DR	202	PG4	O2-C3-C4-O3
65	DA	3205	1PE	OH5-C14-C24-OH4
61	D3	102	PEG	O1-C1-C2-O2
65	DA	3205	1PE	OH4-C13-C23-OH3
64	DA	3186	SPD	C4-C5-N6-C7
57	DS	202	PG4	O1-C1-C2-O2
63	DU	101	PGE	O1-C1-C2-O2
63	DA	3227	PGE	O2-C3-C4-O3
64	DA	3208	SPD	C8-C7-N6-C5
64	DA	3226	SPD	C8-C7-N6-C5
57	DR	202	PG4	O4-C7-C8-O5
63	D3	101	PGE	O3-C5-C6-O4
61	DA	3220	PEG	O1-C1-C2-O2
64	DA	3226	SPD	C4-C5-N6-C7
63	DA	3227	PGE	O3-C5-C6-O4
57	AA	1670	PG4	O2-C3-C4-O3
57	AA	1670	PG4	O1-C1-C2-O2
57	BA	1642	PG4	O1-C1-C2-O2
57	DQ	202	PG4	O1-C1-C2-O2
61	DL	201	PEG	O1-C1-C2-O2
59	AA	1672	PUT	C1-C2-C3-C4
57	DS	202	PG4	O4-C7-C8-O5
59	DA	3225	PUT	C1-C2-C3-C4
63	DD	301	PGE	O2-C3-C4-O3
61	DP	201	PEG	O1-C1-C2-O2
61	DA	3202	PEG	O2-C3-C4-O4
62	DA	3200	EDO	O1-C1-C2-O2
58	DA	3004	MPD	O2-C2-C3-C4
64	DA	3208	SPD	C4-C5-N6-C7
61	DA	3228	PEG	C4-C3-O2-C2
63	DA	3189	PGE	O3-C5-C6-O4
57	DA	3196	PG4	C6-C5-O3-C4
65	DA	3188	1PE	C24-C14-OH5-C25
63	DA	3219	PGE	C1-C2-O2-C3
63	DA	3216	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
61	DL	201	PEG	C4-C3-O2-C2
63	DA	3219	PGE	C4-C3-O2-C2
63	DD	301	PGE	C4-C3-O2-C2
63	D3	101	PGE	C1-C2-O2-C3
57	DR	202	PG4	C5-C6-O4-C7
61	AL	201	PEG	C1-C2-O2-C3
65	DA	3188	1PE	C12-C22-OH3-C23
57	DQ	202	PG4	C3-C4-O3-C5
61	DP	201	PEG	C4-C3-O2-C2
63	DU	101	PGE	C6-C5-O3-C4
57	AA	1670	PG4	C8-C7-O4-C6
57	DR	202	PG4	O3-C5-C6-O4
57	DA	3218	PG4	C1-C2-O2-C3
61	DA	3203	PEG	C1-C2-O2-C3
57	DA	3218	PG4	C3-C4-O3-C5
59	DA	3214	PUT	C1-C2-C3-C4
61	DA	3203	PEG	C4-C3-O2-C2
57	AA	1670	PG4	C5-C6-O4-C7
58	DE	301	MPD	C2-C3-C4-C5
58	DT	201	MPD	C2-C3-C4-C5
58	DA	3195	MPD	C2-C3-C4-C5
58	DA	3206	MPD	C2-C3-C4-C5
58	DA	3209	MPD	C2-C3-C4-C5
65	DA	3205	1PE	C12-C22-OH3-C23
57	BA	1642	PG4	C4-C3-O2-C2
64	DA	3226	SPD	C2-C3-C4-C5
57	DA	3218	PG4	O1-C1-C2-O2
57	AA	1670	PG4	C3-C4-O3-C5
57	DA	3196	PG4	C4-C3-O2-C2
63	DA	3227	PGE	C6-C5-O3-C4
58	DA	3195	MPD	C2-C3-C4-O4
63	DD	301	PGE	C3-C4-O3-C5
64	DA	3190	SPD	C2-C3-C4-C5
61	D3	102	PEG	O2-C3-C4-O4
58	DA	3004	MPD	C1-C2-C3-C4
58	DA	3004	MPD	CM-C2-C3-C4
63	DD	301	PGE	C1-C2-O2-C3
63	D1	102	PGE	O2-C3-C4-O3
61	DA	3202	PEG	C4-C3-O2-C2
59	AA	1675	PUT	C1-C2-C3-C4
57	DS	202	PG4	C4-C3-O2-C2
65	DA	3188	1PE	C16-C26-OH6-C15

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Mol	Chain	Res	Type	Atoms
63	DS	201	PGE	O2-C3-C4-O3
57	BA	1642	PG4	C1-C2-O2-C3
57	DS	202	PG4	C1-C2-O2-C3
57	DR	202	PG4	C3-C4-O3-C5
57	DA	3196	PG4	C1-C2-O2-C3
61	DA	3220	PEG	C1-C2-O2-C3
61	DA	3229	PEG	C1-C2-O2-C3
61	AL	201	PEG	C4-C3-O2-C2
57	DQ	202	PG4	O3-C5-C6-O4
64	DA	3190	SPD	C7-C8-C9-N10
57	DS	202	PG4	C5-C6-O4-C7
57	DA	3196	PG4	O3-C5-C6-O4
63	D1	102	PGE	C3-C4-O3-C5
63	DA	3219	PGE	C3-C4-O3-C5
61	DA	3228	PEG	O2-C3-C4-O4
64	DA	3226	SPD	N6-C7-C8-C9
58	DN	201	MPD	O2-C2-C3-C4
58	DA	3209	MPD	O2-C2-C3-C4
57	AA	1670	PG4	C4-C3-O2-C2
63	D1	102	PGE	O3-C5-C6-O4
57	DS	202	PG4	C8-C7-O4-C6
63	D3	101	PGE	C3-C4-O3-C5
59	DA	3198	PUT	C1-C2-C3-C4
62	DA	3210	EDO	O1-C1-C2-O2
65	DA	3188	1PE	OH6-C15-C25-OH5
63	DS	201	PGE	C6-C5-O3-C4
57	DA	3196	PG4	O2-C3-C4-O3
68	DA	3222	TRS	C1-C-C2-O2
61	DA	3228	PEG	O1-C1-C2-O2
58	DA	3193	MPD	C2-C3-C4-C5
63	DA	3216	PGE	O2-C3-C4-O3
61	DA	3203	PEG	O2-C3-C4-O4
58	DE	301	MPD	C2-C3-C4-O4
58	DE	302	MPD	C2-C3-C4-O4
58	DS	203	MPD	C2-C3-C4-O4
58	DA	3193	MPD	C2-C3-C4-O4
57	DR	202	PG4	C4-C3-O2-C2
57	DA	3218	PG4	C8-C7-O4-C6
65	DA	3205	1PE	OH2-C12-C22-OH3

There are no ring outliers.

30 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	D1	103	PEG	1	0
59	DA	3187	PUT	1	0
58	DA	3209	MPD	1	0
64	DA	3208	SPD	1	0
61	DP	201	PEG	1	0
59	DA	3224	PUT	2	0
59	DA	3221	PUT	1	0
58	AA	1671	MPD	2	0
57	DS	202	PG4	1	0
61	DQ	201	PEG	1	0
58	DS	203	MPD	3	0
64	DA	3226	SPD	1	0
57	DR	202	PG4	3	0
68	DA	3222	TRS	2	0
58	DA	3195	MPD	1	0
57	BA	1642	PG4	1	0
57	AA	1670	PG4	1	0
57	DA	3218	PG4	1	0
63	D1	102	PGE	3	0
62	DA	3197	EDO	2	0
61	D3	102	PEG	2	0
57	DA	3196	PG4	1	0
65	DA	3188	1PE	1	0
62	DA	3201	EDO	1	0
63	DA	3216	PGE	1	0
63	DA	3227	PGE	3	0
63	DU	101	PGE	1	0
57	DQ	202	PG4	1	0
58	DA	3206	MPD	2	0
62	DB	211	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.00	31 (2%) 65 36	37, 95, 237, 293	0
1	BA	1522/1534 (99%)	0.48	146 (9%) 8 2	58, 133, 255, 272	0
2	AB	224/224 (100%)	0.49	16 (7%) 16 5	76, 123, 192, 236	0
2	BB	224/224 (100%)	0.71	34 (15%) 2 0	101, 145, 205, 239	0
3	AC	206/206 (100%)	-0.12	3 (1%) 73 46	65, 93, 121, 147	0
3	BC	206/206 (100%)	0.19	8 (3%) 39 16	86, 121, 150, 169	0
4	AD	205/205 (100%)	-0.20	1 (0%) 91 75	69, 97, 128, 136	0
4	BD	205/205 (100%)	-0.19	0 100 100	68, 101, 127, 138	0
5	AE	155/155 (100%)	-0.19	1 (0%) 89 72	60, 84, 120, 175	0
5	BE	150/155 (96%)	0.28	6 (4%) 38 16	72, 106, 138, 202	0
6	AF	106/106 (100%)	0.11	7 (6%) 18 5	69, 103, 126, 144	0
6	BF	100/106 (94%)	0.46	4 (4%) 38 16	82, 115, 140, 149	0
7	AG	151/151 (100%)	0.92	26 (17%) 1 0	106, 150, 177, 189	0
7	BG	151/151 (100%)	1.89	65 (43%) 0 0	137, 190, 215, 221	0
8	AH	129/129 (100%)	0.04	4 (3%) 49 22	68, 91, 119, 130	0
8	BH	129/129 (100%)	0.11	5 (3%) 39 16	98, 126, 151, 161	0
9	AI	127/127 (100%)	1.07	25 (19%) 1 0	75, 144, 180, 187	0
9	BI	127/127 (100%)	1.20	30 (23%) 0 0	111, 162, 195, 202	0
10	AJ	99/99 (100%)	0.46	10 (10%) 7 2	82, 112, 142, 147	0
10	BJ	98/99 (98%)	2.21	44 (44%) 0 0	111, 152, 181, 187	0
11	AK	117/117 (100%)	0.38	6 (5%) 28 10	54, 104, 138, 152	0
11	BK	117/117 (100%)	0.12	3 (2%) 56 27	62, 97, 134, 165	0
12	AL	122/123 (99%)	-0.05	1 (0%) 86 65	48, 65, 106, 141	0
12	BL	122/123 (99%)	0.65	10 (8%) 11 3	82, 102, 129, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	114/114 (100%)	1.82	39 (34%) 0 0	126, 159, 182, 189	0
13	BM	114/114 (100%)	2.77	74 (64%) 0 0	187, 224, 236, 244	0
14	AN	100/100 (100%)	0.60	7 (7%) 16 5	72, 110, 177, 184	0
14	BN	100/100 (100%)	1.49	33 (33%) 0 0	107, 167, 215, 218	0
15	AO	88/88 (100%)	0.04	1 (1%) 80 56	63, 91, 115, 142	0
15	BO	88/88 (100%)	0.68	10 (11%) 5 1	84, 114, 143, 156	0
16	AP	82/82 (100%)	0.54	7 (8%) 10 3	68, 85, 126, 145	0
16	BP	82/82 (100%)	1.78	28 (34%) 0 0	100, 125, 161, 175	0
17	AQ	80/80 (100%)	0.02	2 (2%) 57 28	63, 87, 116, 138	0
17	BQ	80/80 (100%)	1.11	21 (26%) 0 0	101, 142, 165, 173	0
18	AR	55/55 (100%)	0.93	9 (16%) 1 0	73, 97, 142, 174	0
18	BR	55/55 (100%)	0.10	2 (3%) 42 18	67, 90, 125, 166	0
19	AS	79/79 (100%)	1.24	17 (21%) 0 0	138, 162, 179, 182	0
19	BS	79/79 (100%)	2.25	39 (49%) 0 0	197, 221, 238, 243	0
20	AT	86/86 (100%)	-0.04	1 (1%) 79 53	63, 85, 116, 128	0
20	BT	85/86 (98%)	2.02	37 (43%) 0 0	110, 143, 164, 169	0
21	AU	56/56 (100%)	0.13	1 (1%) 68 40	75, 113, 153, 163	0
21	BU	56/56 (100%)	0.25	1 (1%) 68 40	69, 94, 123, 138	0
22	C1	56/56 (100%)	1.45	16 (28%) 0 0	93, 155, 176, 188	0
22	D1	56/56 (100%)	-0.48	0 100 100	21, 45, 74, 114	0
23	C2	50/51 (98%)	2.22	22 (44%) 0 0	150, 178, 190, 205	0
23	D2	51/51 (100%)	0.02	0 100 100	47, 63, 89, 108	0
24	C3	46/46 (100%)	1.80	18 (39%) 0 0	100, 132, 149, 173	0
24	D3	46/46 (100%)	-0.28	0 100 100	25, 35, 54, 118	0
25	C4	64/64 (100%)	0.69	6 (9%) 8 2	95, 116, 139, 151	0
25	D4	64/64 (100%)	-0.33	0 100 100	29, 39, 57, 68	0
26	C5	38/38 (100%)	0.57	4 (10%) 6 2	97, 115, 133, 149	0
26	D5	38/38 (100%)	-0.28	0 100 100	32, 45, 71, 83	0
27	C0	58/58 (100%)	1.46	20 (34%) 0 0	99, 121, 149, 157	0
27	D0	58/58 (100%)	-0.51	0 100 100	23, 34, 54, 88	0
28	CB	118/120 (98%)	0.75	16 (13%) 3 1	104, 167, 221, 231	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DB	120/120 (100%)	-0.31	0 100 100	28, 53, 86, 134	0
29	CC	271/271 (100%)	0.25	9 (3%) 46 20	76, 98, 120, 132	0
29	DC	271/271 (100%)	-0.36	1 (0%) 92 79	23, 52, 80, 100	0
30	CD	209/209 (100%)	1.10	50 (23%) 0 0	88, 118, 149, 165	0
31	CA	2876/2904 (99%)	0.62	285 (9%) 7 2	65, 132, 252, 292	0
32	DD	208/209 (99%)	-0.48	0 100 100	18, 38, 71, 100	0
33	CE	201/201 (100%)	1.06	40 (19%) 1 0	88, 159, 186, 195	0
33	DE	201/201 (100%)	-0.41	1 (0%) 91 75	20, 52, 98, 127	0
34	CF	177/177 (100%)	2.65	107 (60%) 0 0	186, 212, 225, 231	0
34	DF	177/177 (100%)	-0.11	0 100 100	45, 78, 126, 139	0
35	CG	176/176 (100%)	2.46	92 (52%) 0 0	138, 164, 187, 198	0
35	DG	176/176 (100%)	-0.13	2 (1%) 80 56	45, 74, 105, 131	0
36	CH	149/149 (100%)	1.15	32 (21%) 0 0	81, 148, 176, 186	0
36	DH	149/149 (100%)	0.92	28 (18%) 1 0	60, 158, 195, 208	0
37	CJ	134/134 (100%)	4.61	106 (79%) 0 0	237, 258, 270, 275	0
37	DJ	134/134 (100%)	3.61	84 (62%) 0 0	204, 238, 246, 254	0
38	CK	142/142 (100%)	0.38	5 (3%) 44 19	91, 108, 135, 150	0
38	DK	142/142 (100%)	-0.50	0 100 100	18, 36, 58, 94	0
39	CL	122/123 (99%)	0.42	9 (7%) 14 4	91, 114, 148, 163	0
39	DL	123/123 (100%)	-0.48	0 100 100	29, 43, 72, 106	0
40	CM	144/144 (100%)	1.63	49 (34%) 0 0	87, 146, 186, 214	0
40	DM	144/144 (100%)	-0.37	0 100 100	19, 50, 81, 115	0
41	CN	135/136 (99%)	0.46	8 (5%) 22 7	75, 113, 134, 162	0
41	DN	135/136 (99%)	-0.58	0 100 100	25, 39, 68, 99	0
42	CO	120/125 (96%)	0.77	13 (10%) 5 2	107, 124, 146, 197	0
42	DO	125/125 (100%)	-0.37	1 (0%) 86 65	23, 37, 73, 145	0
43	CP	116/117 (99%)	2.38	65 (56%) 0 0	132, 154, 173, 181	0
43	DP	117/117 (100%)	-0.22	0 100 100	36, 54, 81, 96	0
44	CQ	114/114 (100%)	1.27	24 (21%) 1 0	110, 127, 146, 168	0
44	DQ	114/114 (100%)	-0.38	1 (0%) 84 62	28, 50, 84, 119	0
45	CR	117/117 (100%)	0.57	11 (9%) 8 2	76, 107, 129, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
45	DR	117/117 (100%)	-0.43	1 (0%) 84 62	15, 30, 49, 85	0
46	CS	103/103 (100%)	1.62	36 (34%) 0 0	94, 127, 152, 164	0
46	DS	103/103 (100%)	-0.56	0 100 100	21, 41, 70, 99	0
47	CT	110/110 (100%)	0.71	16 (14%) 2 1	99, 123, 157, 176	0
47	DT	110/110 (100%)	-0.50	0 100 100	17, 32, 61, 114	0
48	CU	93/93 (100%)	1.67	34 (36%) 0 0	129, 147, 176, 181	0
48	DU	93/93 (100%)	-0.05	2 (2%) 62 33	31, 52, 115, 130	0
49	CV	102/102 (100%)	2.88	58 (56%) 0 0	148, 166, 201, 204	0
49	DV	102/102 (100%)	-0.27	1 (0%) 82 59	40, 62, 97, 129	0
50	CW	94/94 (100%)	0.98	15 (15%) 1 0	114, 140, 159, 164	0
50	DW	94/94 (100%)	-0.49	1 (1%) 80 56	31, 52, 84, 96	0
51	CX	75/76 (98%)	1.07	18 (24%) 0 0	92, 120, 134, 183	0
51	DX	76/76 (100%)	-0.50	1 (1%) 77 51	24, 39, 67, 116	0
52	CY	77/77 (100%)	0.39	3 (3%) 39 16	78, 117, 147, 166	0
52	DY	77/77 (100%)	-0.35	0 100 100	32, 53, 93, 111	0
53	CZ	62/62 (100%)	1.92	28 (45%) 0 0	133, 169, 183, 190	0
53	DZ	62/62 (100%)	0.17	2 (3%) 47 21	42, 70, 110, 138	0
54	DI	135/135 (100%)	1.57	37 (27%) 0 0	81, 152, 215, 229	1 (0%)
55	DA	2873/2904 (98%)	-0.02	89 (3%) 49 22	19, 44, 227, 299	0
All	All	20634/20745 (99%)	0.48	2282 (11%) 5 1	15, 106, 233, 299	1 (0%)

All (2282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	DJ	135	SER	21.4
37	DJ	54	PRO	17.3
37	CJ	13	VAL	17.0
31	CA	2172	U	16.1
37	CJ	59	ILE	15.3
37	CJ	23	PRO	13.3
37	CJ	57	VAL	13.1
37	CJ	9	VAL	13.0
31	CA	1067	A	12.9
37	CJ	11	LEU	12.8
31	CA	1068	G	12.3

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Mol	Chain	Res	Type	RSRZ
37	CJ	69	PHE	12.2
37	DJ	53	LEU	11.9
37	CJ	54	PRO	11.1
37	CJ	12	GLN	10.9
37	CJ	53	LEU	10.7
55	DA	2120	G	10.6
37	DJ	96	ASP	10.6
46	CS	50	GLY	10.6
37	CJ	87	LYS	10.6
37	DJ	94	ASN	10.5
37	CJ	75	PRO	10.5
37	CJ	21	SER	10.3
54	DI	131	THR	10.3
37	DJ	23	PRO	9.9
37	DJ	67	PHE	9.9
31	CA	1537	G	9.7
49	CV	20	GLY	9.7
37	CJ	14	ALA	9.6
44	CQ	115	ASN	9.5
37	DJ	133	ALA	9.4
55	DA	2163	A	9.2
1	BA	82	G	9.1
37	DJ	79	LEU	9.0
31	CA	2174	C	9.0
37	CJ	20	PRO	9.0
37	CJ	56	PRO	9.0
9	BI	128	SER	8.9
23	C2	18	GLY	8.9
31	CA	2402	U	8.9
31	CA	2173	A	8.8
40	CM	81	ASP	8.8
35	CG	33	LEU	8.8
14	BN	35	ASN	8.7
37	CJ	17	MET	8.7
19	BS	4	SER	8.6
54	DI	128	THR	8.6
37	DJ	138	LEU	8.4
1	BA	1030	U	8.4
54	DI	130	PRO	8.4
10	BJ	76	ILE	8.4
37	DJ	24	VAL	8.4
31	CA	2126	A	8.4

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Mol	Chain	Res	Type	RSRZ
1	BA	211	G	8.3
34	CF	153	ASP	8.3
55	DA	884	U	8.2
37	DJ	55	ILE	8.2
35	CG	103	ILE	8.2
2	AB	123	ASP	8.2
55	DA	1065	U	8.1
37	DJ	76	ALA	8.1
37	DJ	13	VAL	8.1
1	AA	844	G	8.1
37	CJ	22	PRO	8.0
35	CG	105	LEU	8.0
10	BJ	74	VAL	8.0
49	CV	32	GLY	8.0
55	DA	1064	C	7.9
34	CF	176	PRO	7.9
37	CJ	120	ALA	7.9
51	CX	54	GLY	7.9
37	CJ	89	GLY	7.9
37	CJ	118	THR	7.9
49	CV	80	ALA	7.8
37	DJ	66	SER	7.8
35	CG	32	GLU	7.8
49	CV	29	LEU	7.8
37	DJ	88	SER	7.7
49	CV	33	LYS	7.7
37	CJ	126	THR	7.7
1	AA	1030	U	7.6
37	CJ	60	THR	7.6
1	AA	86	G	7.6
49	CV	89	ASP	7.6
13	BM	10	PRO	7.5
31	CA	1087	G	7.5
19	BS	74	PHE	7.5
55	DA	2125	G	7.5
17	BQ	70	THR	7.5
37	DJ	137	GLY	7.5
13	BM	95	LEU	7.5
55	DA	892	A	7.5
37	CJ	82	LYS	7.4
37	DJ	132	THR	7.4
16	BP	16	PHE	7.4

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Mol	Chain	Res	Type	RSRZ
55	DA	2124	G	7.3
37	CJ	121	ASP	7.3
20	BT	4	ILE	7.3
10	BJ	75	ASP	7.3
31	CA	1104	C	7.2
37	CJ	90	SER	7.2
40	CM	114	GLY	7.2
37	CJ	47	ASP	7.2
31	CA	1103	A	7.2
35	CG	84	THR	7.1
35	CG	111	HIS	7.1
13	AM	24	GLY	7.1
55	DA	881	G	7.1
37	CJ	61	VAL	7.0
37	CJ	80	LEU	7.0
34	CF	116	GLY	7.0
43	CP	51	ALA	7.0
49	CV	79	LYS	7.0
9	AI	130	ARG	7.0
55	DA	2127	G	6.9
34	CF	132	VAL	6.9
37	CJ	76	ALA	6.9
37	CJ	68	THR	6.9
31	CA	2163	A	6.9
49	CV	31	SER	6.9
31	CA	2125	G	6.9
14	AN	21	PHE	6.9
31	CA	1175	A	6.8
31	CA	1066	U	6.8
55	DA	2110	G	6.8
49	CV	3	ALA	6.8
49	CV	13	VAL	6.8
37	DJ	78	VAL	6.8
34	CF	154	ILE	6.8
16	BP	17	TYR	6.8
19	BS	49	ILE	6.8
37	DJ	98	VAL	6.8
31	CA	1057	A	6.8
37	DJ	114	ALA	6.8
13	AM	64	VAL	6.8
55	DA	1172	C	6.7
37	DJ	80	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
13	BM	65	VAL	6.7
34	CF	152	LEU	6.7
37	DJ	68	THR	6.7
7	BG	62	PHE	6.7
31	CA	2127	G	6.7
35	CG	106	SER	6.6
34	CF	40	VAL	6.6
37	DJ	69	PHE	6.6
31	CA	75	G	6.6
10	BJ	39	PRO	6.6
20	BT	3	ASN	6.6
31	CA	329	G	6.6
31	CA	2120	G	6.6
13	AM	13	LYS	6.5
48	CU	57	VAL	6.5
34	CF	175	PHE	6.5
43	CP	53	THR	6.5
31	CA	2171	A	6.5
13	BM	96	PRO	6.5
37	DJ	12	GLN	6.5
36	CH	11	ASN	6.4
19	BS	60	VAL	6.4
13	AM	33	ILE	6.4
34	CF	85	ILE	6.4
55	DA	2172	U	6.4
34	CF	36	LEU	6.4
31	CA	1084	A	6.4
10	BJ	40	ILE	6.3
34	CF	136	ILE	6.3
49	CV	78	GLY	6.3
10	BJ	102	LEU	6.3
7	BG	4	ARG	6.3
19	BS	39	THR	6.3
31	CA	331	C	6.3
49	CV	30	SER	6.3
55	DA	2121	G	6.3
31	CA	1065	U	6.2
37	CJ	79	LEU	6.2
1	BA	94	G	6.2
31	CA	2119	A	6.2
55	DA	882	G	6.2
10	BJ	25	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
37	CJ	74	PRO	6.2
37	DJ	19	ASN	6.2
1	AA	87	C	6.2
34	CF	135	GLN	6.1
10	BJ	26	VAL	6.1
55	DA	1067	A	6.1
23	C2	16	GLY	6.1
31	CA	1056	G	6.1
37	DJ	20	PRO	6.1
35	CG	110	SER	6.1
55	DA	879	G	6.1
35	CG	82	GLY	6.1
37	CJ	88	SER	6.0
10	BJ	77	VAL	6.0
13	AM	30	SER	6.0
43	CP	65	THR	6.0
37	DJ	93	PRO	6.0
31	CA	2128	G	6.0
34	CF	65	PRO	6.0
37	DJ	134	ARG	6.0
23	C2	45	GLN	6.0
31	CA	2161	C	6.0
37	CJ	28	LEU	6.0
19	BS	24	GLU	5.9
9	AI	32	GLN	5.9
14	BN	31	ILE	5.9
37	DJ	99	GLY	5.9
55	DA	883	G	5.9
1	BA	1236	A	5.9
31	CA	549	G	5.9
13	BM	2	ALA	5.9
43	CP	64	TYR	5.9
35	CG	121	ILE	5.9
49	CV	36	VAL	5.9
30	CD	26	VAL	5.8
46	CS	96	VAL	5.8
55	DA	2111	U	5.8
34	CF	34	ILE	5.8
34	CF	144	ASP	5.8
13	AM	19	LEU	5.8
35	CG	30	ASN	5.8
7	BG	151	PHE	5.8

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Mol	Chain	Res	Type	RSRZ
43	CP	34	HIS	5.8
7	BG	116	MET	5.8
10	BJ	8	ILE	5.8
31	CA	2164	C	5.8
35	CG	148	LEU	5.8
55	DA	880	G	5.7
16	BP	57	ILE	5.7
34	CF	128	TYR	5.7
19	BS	3	ARG	5.7
54	DI	134	GLU	5.7
31	CA	2116	G	5.7
31	CA	2110	G	5.7
37	DJ	28	LEU	5.7
37	CJ	86	ILE	5.7
37	CJ	119	GLY	5.7
35	CG	83	PHE	5.7
55	DA	896	A	5.6
34	CF	174	ASP	5.6
37	CJ	58	VAL	5.6
43	CP	52	SER	5.6
53	CZ	45	GLN	5.6
51	CX	52	GLY	5.6
16	BP	11	ALA	5.6
37	CJ	52	GLY	5.6
18	BR	20	GLU	5.6
35	CG	31	GLY	5.6
55	DA	2174	C	5.6
1	AA	1032	G	5.6
40	CM	82	LEU	5.5
14	BN	33	ASP	5.5
55	DA	1068	G	5.5
34	CF	156	ILE	5.5
55	DA	2167	U	5.5
31	CA	318	C	5.5
55	DA	885	C	5.5
34	CF	130	MET	5.5
35	CG	80	THR	5.5
23	C2	43	VAL	5.5
55	DA	2175	C	5.5
1	BA	85	U	5.5
37	CJ	8	TYR	5.5
40	CM	79	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
43	CP	35	ILE	5.5
16	BP	39	PHE	5.5
37	DJ	38	PHE	5.5
55	DA	1077	A	5.5
31	CA	1086	A	5.4
43	CP	24	THR	5.4
37	CJ	29	GLY	5.4
9	AI	20	PHE	5.4
31	CA	2123	G	5.4
49	CV	5	ILE	5.4
7	BG	148	ASN	5.4
43	CP	40	ILE	5.4
20	BT	77	ALA	5.4
35	CG	104	ASN	5.4
55	DA	2126	A	5.4
35	CG	2	SER	5.4
43	CP	63	LYS	5.4
55	DA	2162	G	5.4
43	CP	26	LEU	5.4
7	BG	123	GLU	5.4
10	BJ	38	GLY	5.3
31	CA	2802	G	5.3
34	CF	157	THR	5.3
46	CS	20	VAL	5.3
1	BA	84	U	5.3
35	CG	117	LEU	5.3
37	CJ	46	THR	5.3
31	CA	878	A	5.3
31	CA	1095	A	5.3
34	CF	106	ILE	5.3
40	CM	144	GLU	5.3
16	BP	52	LEU	5.3
49	CV	15	THR	5.3
49	CV	88	GLU	5.3
55	DA	1062	G	5.3
31	CA	1083	U	5.3
55	DA	2123	G	5.3
14	BN	36	ALA	5.3
7	BG	5	ARG	5.3
10	BJ	42	LEU	5.3
13	BM	97	VAL	5.3
7	BG	8	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
37	DJ	11	LEU	5.3
20	BT	60	ARG	5.3
44	CQ	91	ALA	5.3
31	CA	931	U	5.3
1	BA	1314	C	5.2
54	DI	136	ILE	5.2
43	CP	78	VAL	5.2
10	BJ	73	LEU	5.2
49	CV	40	ASN	5.2
55	DA	2109	U	5.2
54	DI	132	TYR	5.2
18	AR	20	GLU	5.2
47	CT	43	ALA	5.2
31	CA	1105	U	5.2
13	BM	99	GLY	5.2
31	CA	1536	C	5.2
37	CJ	71	THR	5.2
14	BN	39	GLU	5.2
1	BA	1032	G	5.2
13	BM	29	ARG	5.2
31	CA	330	A	5.2
13	BM	25	VAL	5.2
49	CV	35	ILE	5.2
55	DA	1063	G	5.2
55	DA	2116	G	5.2
31	CA	2666	C	5.2
37	DJ	22	PRO	5.1
31	CA	2162	G	5.1
2	BB	34	ALA	5.1
33	CE	144	GLU	5.1
9	BI	16	ALA	5.1
44	CQ	111	LYS	5.1
48	DU	1	MET	5.1
31	CA	1085	A	5.1
13	BM	41	GLU	5.1
37	CJ	115	ALA	5.1
44	CQ	85	SER	5.1
43	CP	58	ILE	5.1
46	CS	27	ILE	5.1
37	CJ	24	VAL	5.1
35	CG	151	TYR	5.1
49	CV	6	ARG	5.1

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Mol	Chain	Res	Type	RSRZ
14	BN	60	GLN	5.1
31	CA	1210	G	5.1
40	CM	89	VAL	5.1
7	BG	43	VAL	5.0
14	BN	30	ILE	5.0
31	CA	2170	A	5.0
7	AG	6	VAL	5.0
13	BM	47	GLU	5.0
23	C2	47	VAL	5.0
24	C3	32	ALA	5.0
35	CG	102	VAL	5.0
7	AG	61	ALA	5.0
34	CF	35	THR	5.0
1	BA	202	G	5.0
13	BM	56	LEU	5.0
53	CZ	42	LEU	5.0
30	CD	6	GLY	5.0
37	CJ	129	ILE	5.0
53	CZ	15	ASN	5.0
13	BM	48	LEU	5.0
10	BJ	41	PRO	5.0
40	CM	80	SER	5.0
13	AM	7	ILE	5.0
19	BS	80	TYR	5.0
35	CG	112	PRO	5.0
37	DJ	42	PHE	4.9
9	BI	38	TYR	4.9
13	BM	17	ILE	4.9
37	DJ	59	ILE	4.9
13	BM	60	VAL	4.9
34	CF	32	GLU	4.9
33	CE	124	PHE	4.9
9	BI	7	TYR	4.9
1	BA	4	U	4.9
43	CP	66	GLY	4.9
34	CF	117	LEU	4.9
49	CV	28	VAL	4.9
22	C1	11	SER	4.9
26	C5	38	GLY	4.9
40	CM	101	ILE	4.8
23	C2	52	ALA	4.8
19	BS	29	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
55	DA	1078	U	4.8
53	CZ	49	ASP	4.8
12	AL	124	ALA	4.8
37	CJ	122	ILE	4.8
31	CA	2169	A	4.8
14	AN	23	LYS	4.8
54	DI	96	PHE	4.8
44	CQ	8	LEU	4.8
10	AJ	35	GLN	4.8
31	CA	1071	G	4.8
49	CV	87	PHE	4.8
34	CF	105	THR	4.8
13	BM	39	ILE	4.8
49	CV	75	ALA	4.8
27	C0	56	LYS	4.8
1	BA	1302	C	4.8
50	CW	48	MET	4.8
1	BA	203	G	4.8
17	BQ	45	HIS	4.8
30	CD	186	LEU	4.7
37	DJ	136	MET	4.7
54	DI	104	ALA	4.7
43	CP	37	ALA	4.7
49	CV	77	THR	4.7
13	AM	43	VAL	4.7
31	CA	1090	A	4.7
9	BI	130	ARG	4.7
49	CV	83	VAL	4.7
13	BM	30	SER	4.7
7	AG	5	ARG	4.7
7	BG	152	ALA	4.7
7	BG	42	ILE	4.7
37	CJ	33	VAL	4.7
34	CF	158	THR	4.7
31	CA	1535	A	4.7
31	CA	2121	G	4.7
40	CM	10	GLU	4.7
37	CJ	45	LYS	4.7
37	CJ	67	PHE	4.7
13	BM	40	ALA	4.7
20	BT	36	TYR	4.6
43	CP	38	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
20	BT	76	LYS	4.6
1	BA	209	U	4.6
31	CA	1094	U	4.6
53	CZ	63	ALA	4.6
24	C3	35	ARG	4.6
13	BM	115	PRO	4.6
37	CJ	98	VAL	4.6
48	CU	43	ILE	4.6
37	CJ	132	THR	4.6
31	CA	1863	G	4.6
1	AA	84	U	4.6
7	AG	8	GLY	4.5
48	CU	56	GLU	4.5
54	DI	133	GLU	4.5
1	BA	1296	C	4.5
35	CG	75	MET	4.5
37	DJ	92	LYS	4.5
36	DH	137	GLU	4.5
51	CX	53	CYS	4.5
55	DA	2168	G	4.5
54	DI	129	LEU	4.5
7	BG	144	MET	4.5
1	AA	1031	C	4.5
31	CA	2124	G	4.5
35	CG	131	ILE	4.5
14	BN	21	PHE	4.5
37	CJ	38	PHE	4.5
16	BP	42	ILE	4.5
34	CF	113	ASP	4.5
14	BN	49	GLN	4.5
34	CF	67	ILE	4.5
17	BQ	63	GLU	4.4
20	BT	52	ASN	4.4
34	CF	93	GLY	4.4
10	BJ	37	ARG	4.4
34	CF	138	PHE	4.4
37	CJ	116	ASP	4.4
37	CJ	99	GLY	4.4
35	CG	10	VAL	4.4
22	C1	55	ILE	4.4
37	CJ	55	ILE	4.4
40	CM	100	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
10	BJ	91	ASP	4.4
40	CM	78	ARG	4.4
54	DI	55	VAL	4.4
12	BL	124	ALA	4.4
35	CG	96	ALA	4.4
31	CA	1167	C	4.4
13	BM	42	ASP	4.4
20	BT	59	ASP	4.4
53	CZ	40	SER	4.4
13	BM	4	ILE	4.4
35	CG	26	ILE	4.4
54	DI	94	ARG	4.4
34	CF	111	ILE	4.4
1	BA	83	C	4.4
9	BI	5	GLN	4.4
55	DA	1060	U	4.3
2	BB	35	ARG	4.3
7	AG	62	PHE	4.3
2	BB	130	THR	4.3
7	BG	72	THR	4.3
49	CV	19	LYS	4.3
43	CP	36	TYR	4.3
9	BI	4	ASN	4.3
31	CA	88	G	4.3
31	CA	312	G	4.3
13	AM	99	GLY	4.3
23	C2	48	ILE	4.3
30	CD	4	LEU	4.3
37	CJ	62	TYR	4.3
2	BB	33	GLY	4.3
16	BP	41	PRO	4.3
1	BA	983	A	4.3
37	CJ	31	GLN	4.3
49	CV	12	ILE	4.3
37	DJ	87	LYS	4.3
7	AG	58	GLU	4.3
7	AG	4	ARG	4.3
36	DH	67	ALA	4.3
41	CN	136	MET	4.3
7	AG	112	GLY	4.3
37	DJ	95	LYS	4.3
12	BL	70	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
44	CQ	9	GLU	4.3
10	BJ	6	ILE	4.3
37	CJ	51	LYS	4.3
21	AU	2	PRO	4.3
31	CA	103	A	4.3
1	BA	1024	G	4.3
20	BT	75	HIS	4.3
23	C2	24	THR	4.3
35	CG	40	ALA	4.3
10	AJ	75	ASP	4.3
34	CF	129	SER	4.3
44	CQ	84	ILE	4.3
46	CS	32	THR	4.2
15	BO	89	ARG	4.2
20	BT	72	ALA	4.2
36	DH	94	ILE	4.2
34	CF	94	GLU	4.2
7	BG	16	PRO	4.2
43	CP	92	PHE	4.2
1	BA	470	C	4.2
31	CA	2803	G	4.2
43	CP	117	PHE	4.2
34	CF	102	ARG	4.2
48	CU	15	HIS	4.2
53	CZ	37	LEU	4.2
44	CQ	12	GLN	4.2
50	CW	94	ALA	4.2
9	AI	22	LYS	4.2
1	BA	1031	C	4.2
19	BS	76	PRO	4.2
7	BG	120	LEU	4.2
10	BJ	7	ARG	4.2
13	AM	23	TYR	4.2
37	CJ	95	LYS	4.2
37	CJ	78	VAL	4.2
46	CS	63	VAL	4.2
31	CA	1061	U	4.2
54	DI	38	MET	4.2
37	CJ	42	PHE	4.2
13	AM	16	VAL	4.1
40	CM	8	PRO	4.1
53	CZ	41	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
16	BP	53	ASP	4.1
31	CA	613	A	4.1
55	DA	2173	A	4.1
9	BI	32	GLN	4.1
34	CF	95	ARG	4.1
7	BG	52	GLN	4.1
30	CD	179	ARG	4.1
7	BG	48	GLU	4.1
37	CJ	26	PRO	4.1
55	DA	893	C	4.1
14	BN	55	SER	4.1
16	AP	47	GLU	4.1
34	CF	151	GLY	4.1
17	BQ	73	TRP	4.1
10	BJ	90	LEU	4.1
1	AA	88	U	4.1
55	DA	2166	U	4.1
34	CF	97	TRP	4.1
40	CM	92	LEU	4.1
31	CA	546	U	4.1
34	CF	83	TYR	4.1
34	CF	86	GLY	4.1
35	CG	81	GLU	4.1
43	CP	33	ARG	4.1
49	CV	81	ASP	4.1
54	DI	121	SER	4.1
2	BB	9	MET	4.1
55	DA	1088	A	4.1
19	BS	31	LEU	4.1
40	CM	118	THR	4.1
35	CG	166	ASP	4.1
31	CA	2797	U	4.1
20	BT	24	ARG	4.0
11	AK	19	GLY	4.0
13	AM	5	ALA	4.0
54	DI	135	ALA	4.0
38	CK	142	ILE	4.0
31	CA	2667	C	4.0
49	CV	4	LYS	4.0
34	CF	38	MET	4.0
35	CG	86	LYS	4.0
7	BG	129	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
20	BT	35	VAL	4.0
27	C0	43	ALA	4.0
48	CU	16	VAL	4.0
49	CV	51	ALA	4.0
1	BA	1034	G	4.0
23	C2	31	PRO	4.0
55	DA	1087	G	4.0
1	BA	80	A	4.0
46	CS	7	SER	4.0
55	DA	1731	G	4.0
7	BG	6	VAL	4.0
43	CP	39	VAL	4.0
37	DJ	115	ALA	4.0
31	CA	2665	A	4.0
31	CA	879	G	4.0
40	CM	126	ARG	4.0
7	BG	88	PRO	4.0
1	BA	208	U	4.0
1	BA	81	A	4.0
33	CE	172	ALA	4.0
34	CF	131	GLY	4.0
37	DJ	110	ALA	4.0
2	BB	213	TYR	4.0
7	BG	145	ALA	4.0
13	AM	32	ALA	4.0
43	CP	54	VAL	4.0
7	AG	50	LEU	4.0
14	BN	27	LEU	4.0
19	BS	66	MET	4.0
37	CJ	83	ALA	4.0
9	BI	129	LYS	4.0
31	CA	138	U	4.0
33	CE	33	VAL	4.0
55	DA	1072	C	4.0
36	DH	87	GLU	3.9
1	BA	68	G	3.9
10	BJ	10	LEU	3.9
24	C3	31	LEU	3.9
1	BA	469	C	3.9
31	CA	1106	G	3.9
27	C0	8	THR	3.9
31	CA	311	A	3.9

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Mol	Chain	Res	Type	RSRZ
31	CA	12	U	3.9
35	CG	132	VAL	3.9
43	CP	62	LEU	3.9
36	CH	140	ALA	3.9
31	CA	1064	C	3.9
37	CJ	96	ASP	3.9
1	AA	82	G	3.9
37	DJ	100	LYS	3.9
22	C1	15	MET	3.9
23	C2	35	GLU	3.9
13	BM	31	LYS	3.9
35	CG	76	VAL	3.9
37	CJ	113	LYS	3.9
7	BG	109	ARG	3.9
34	CF	112	ARG	3.9
46	CS	95	ASP	3.9
30	CD	25	THR	3.9
35	CG	116	GLN	3.9
44	CQ	2	SER	3.9
33	CE	8	ALA	3.9
7	AG	7	ILE	3.9
13	BM	21	SER	3.9
13	BM	16	VAL	3.9
43	CP	41	ALA	3.9
34	CF	143	TYR	3.9
37	CJ	32	GLY	3.9
37	DJ	131	GLY	3.9
13	BM	100	GLN	3.9
14	BN	40	ASP	3.9
40	CM	132	ARG	3.9
33	CE	190	ALA	3.9
37	CJ	73	THR	3.9
53	CZ	33	ALA	3.9
19	BS	59	PRO	3.9
19	BS	37	ARG	3.9
37	DJ	36	MET	3.9
55	DA	1066	U	3.9
51	CX	63	ALA	3.9
31	CA	262	A	3.9
49	CV	84	GLY	3.9
1	BA	844	G	3.9
9	AI	21	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
50	CW	11	GLU	3.9
1	BA	1242	G	3.9
13	BM	105	ASN	3.9
37	CJ	18	ALA	3.9
34	CF	31	VAL	3.8
20	BT	48	GLN	3.8
35	CG	136	ALA	3.8
49	CV	27	ASN	3.8
1	BA	632	U	3.8
31	CA	267	C	3.8
24	C3	42	LEU	3.8
7	BG	71	PRO	3.8
13	AM	25	VAL	3.8
33	CE	30	GLN	3.8
37	CJ	138	LEU	3.8
37	DJ	21	SER	3.8
37	DJ	89	GLY	3.8
53	CZ	29	ARG	3.8
9	BI	67	VAL	3.8
43	CP	115	LEU	3.8
40	CM	133	ALA	3.8
13	BM	23	TYR	3.8
31	CA	356	G	3.8
51	CX	85	GLU	3.8
2	BB	131	LYS	3.8
36	DH	99	ILE	3.8
37	CJ	10	LYS	3.8
40	CM	77	ILE	3.8
13	BM	32	ALA	3.8
13	BM	37	ALA	3.8
19	AS	56	GLN	3.8
1	BA	134	G	3.8
28	CB	51	G	3.8
34	CF	170	LEU	3.8
55	DA	2128	G	3.8
10	BJ	19	ASP	3.8
31	CA	892	A	3.8
26	C5	10	LEU	3.8
30	CD	77	ARG	3.8
49	CV	39	ILE	3.8
35	CG	113	VAL	3.8
20	BT	53	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
37	CJ	43	ASN	3.8
7	AG	109	ARG	3.8
5	BE	91	GLY	3.7
37	CJ	91	GLY	3.7
43	CP	67	ASN	3.7
9	BI	66	THR	3.7
24	C3	30	VAL	3.7
55	DA	2165	C	3.7
31	CA	1538	G	3.7
13	BM	103	LYS	3.7
20	BT	49	LYS	3.7
55	DA	654	A	3.7
31	CA	2168	G	3.7
13	BM	85	CYS	3.7
55	DA	138	U	3.7
34	CF	23	ASN	3.7
35	CG	27	LYS	3.7
14	BN	37	SER	3.7
34	CF	60	ILE	3.7
1	AA	81	A	3.7
48	CU	55	VAL	3.7
17	BQ	53	CYS	3.7
31	CA	1049	C	3.7
6	BF	8	PHE	3.7
13	AM	58	ASP	3.7
40	CM	120	VAL	3.7
31	CA	74	A	3.7
31	CA	76	C	3.7
34	CF	173	PHE	3.7
20	BT	56	PRO	3.7
37	CJ	84	ALA	3.7
34	CF	139	PRO	3.7
53	CZ	17	GLU	3.7
19	BS	56	GLN	3.7
48	CU	85	VAL	3.7
30	CD	200	ASP	3.7
15	BO	22	THR	3.7
19	BS	48	THR	3.7
31	CA	877	A	3.7
55	DA	897	C	3.7
55	DA	1089	A	3.7
36	CH	132	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
49	CV	21	LYS	3.6
19	AS	77	THR	3.6
10	BJ	72	ARG	3.6
47	CT	97	LEU	3.6
1	BA	121	U	3.6
1	BA	472	U	3.6
31	CA	846	U	3.6
2	BB	40	ILE	3.6
13	BM	49	SER	3.6
13	BM	101	ARG	3.6
35	CG	115	HIS	3.6
35	CG	73	ASN	3.6
2	BB	201	PRO	3.6
44	CQ	110	ILE	3.6
43	CP	46	GLU	3.6
48	CU	87	LEU	3.6
24	C3	28	ARG	3.6
31	CA	1069	A	3.6
13	BM	24	GLY	3.6
36	DH	93	SER	3.6
31	CA	1107	G	3.6
31	CA	1238	G	3.6
23	C2	21	TYR	3.6
33	CE	119	ILE	3.6
35	CG	152	ARG	3.6
1	BA	191	G	3.6
31	CA	2410	G	3.6
48	CU	60	THR	3.6
37	CJ	44	ALA	3.6
16	BP	60	TRP	3.6
14	BN	32	SER	3.6
19	BS	12	ASP	3.6
46	CS	35	PHE	3.6
31	CA	1211	C	3.6
12	BL	48	ALA	3.6
49	CV	50	PRO	3.6
19	AS	74	PHE	3.6
7	AG	54	SER	3.6
9	BI	58	VAL	3.6
13	BM	9	ILE	3.6
22	C1	36	GLU	3.6
33	CE	7	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
55	DA	878	A	3.6
1	BA	1026	G	3.6
13	BM	34	LEU	3.6
17	BQ	46	VAL	3.6
13	BM	108	THR	3.6
9	BI	90	TYR	3.6
31	CA	896	A	3.5
33	CE	143	LEU	3.5
35	CG	94	TYR	3.5
54	DI	106	PHE	3.5
7	AG	42	ILE	3.5
35	CG	97	ALA	3.5
13	BM	19	LEU	3.5
35	CG	108	GLY	3.5
45	CR	81	ASN	3.5
49	CV	95	PHE	3.5
2	BB	206	ALA	3.5
31	CA	431	U	3.5
49	CV	18	ASP	3.5
14	BN	53	ARG	3.5
31	CA	1870	C	3.5
37	DJ	10	LYS	3.5
25	C4	61	CYS	3.5
47	CT	94	ASP	3.5
13	BM	22	ILE	3.5
34	CF	155	THR	3.5
46	CS	49	ILE	3.5
31	CA	1111	A	3.5
1	BA	218	U	3.5
20	BT	8	LYS	3.5
1	BA	1033	G	3.5
10	BJ	35	GLN	3.5
37	CJ	128	SER	3.5
54	DI	80	THR	3.5
10	BJ	81	GLU	3.5
2	BB	14	VAL	3.5
10	BJ	87	LEU	3.5
23	C2	40	ASP	3.5
9	AI	6	TYR	3.5
23	C2	37	LYS	3.5
2	BB	82	ASP	3.5
31	CA	1048	A	3.5

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Mol	Chain	Res	Type	RSRZ
40	CM	1	MET	3.5
7	BG	41	SER	3.5
24	C3	33	ARG	3.5
31	CA	2129	C	3.5
31	CA	317	G	3.5
31	CA	1731	G	3.5
31	CA	1046	A	3.5
2	BB	135	LEU	3.5
27	C0	29	LEU	3.5
30	CD	188	LEU	3.5
35	CG	24	ILE	3.5
30	CD	1	MET	3.5
31	CA	316	C	3.4
54	DI	103	ASN	3.4
30	CD	180	VAL	3.4
35	CG	162	VAL	3.4
13	BM	5	ALA	3.4
27	C0	39	GLU	3.4
40	CM	113	ALA	3.4
2	BB	37	LYS	3.4
10	AJ	74	VAL	3.4
35	CG	141	ILE	3.4
37	DJ	128	SER	3.4
9	BI	127	PHE	3.4
1	BA	1241	G	3.4
27	C0	47	MET	3.4
55	DA	1071	G	3.4
34	CF	142	ASP	3.4
37	DJ	40	LYS	3.4
19	BS	40	ILE	3.4
40	CM	115	GLU	3.4
55	DA	2171	A	3.4
30	CD	45	TYR	3.4
13	AM	29	ARG	3.4
47	CT	5	ALA	3.4
49	CV	14	LEU	3.4
11	AK	81	ASN	3.4
30	CD	42	ASN	3.4
33	CE	183	PHE	3.4
35	CG	85	LYS	3.4
9	BI	9	THR	3.4
1	AA	85	U	3.4

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Mol	Chain	Res	Type	RSRZ
1	BA	1038	C	3.4
35	CG	133	LEU	3.4
34	CF	114	PHE	3.4
43	CP	69	ASP	3.4
37	CJ	19	ASN	3.4
44	CQ	34	GLU	3.4
13	AM	8	ASN	3.4
31	CA	1089	A	3.4
49	CV	70	VAL	3.4
18	AR	32	TYR	3.4
24	C3	18	PHE	3.4
51	CX	60	PHE	3.4
13	BM	112	PRO	3.4
10	BJ	21	ALA	3.4
14	AN	47	LYS	3.4
37	CJ	139	VAL	3.4
1	BA	325	A	3.4
35	CG	45	HIS	3.4
37	DJ	25	GLY	3.4
31	CA	313	G	3.4
19	BS	61	PHE	3.4
31	CA	1868	C	3.4
35	CG	109	PHE	3.4
30	CD	76	GLY	3.4
31	CA	309	A	3.4
31	CA	1169	A	3.4
35	CG	59	ALA	3.4
40	CM	90	VAL	3.4
48	CU	35	ALA	3.4
43	CP	99	TYR	3.4
10	BJ	24	GLU	3.4
31	CA	183	C	3.4
55	DA	1074	G	3.4
55	DA	2161	C	3.4
13	BM	12	HIS	3.4
34	CF	80	ARG	3.4
9	AI	17	ALA	3.3
20	BT	50	ALA	3.3
36	CH	18	GLN	3.3
36	DH	95	GLY	3.3
34	CF	110	ARG	3.3
28	CB	97	C	3.3

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Mol	Chain	Res	Type	RSRZ
9	AI	39	PHE	3.3
37	CJ	133	ALA	3.3
13	BM	50	GLU	3.3
8	AH	121	LEU	3.3
14	BN	2	ALA	3.3
27	C0	2	ALA	3.3
30	CD	209	ALA	3.3
37	CJ	27	ALA	3.3
30	CD	10	GLY	3.3
30	CD	43	ASP	3.3
13	AM	63	PHE	3.3
48	CU	37	ASP	3.3
6	BF	39	LEU	3.3
31	CA	308	G	3.3
36	DH	66	ASN	3.3
10	AJ	6	ILE	3.3
16	BP	77	GLU	3.3
34	CF	147	ASP	3.3
37	DJ	58	VAL	3.3
55	DA	1729	U	3.3
34	CF	141	ILE	3.3
36	DH	70	GLU	3.3
14	BN	3	LYS	3.3
53	CZ	31	GLN	3.3
13	AM	45	ILE	3.3
46	CS	31	GLU	3.3
7	BG	45	SER	3.3
14	BN	48	LEU	3.3
37	DJ	33	VAL	3.3
7	BG	108	ALA	3.3
35	CG	62	TRP	3.3
7	BG	39	ALA	3.3
20	BT	85	LYS	3.3
33	CE	104	ALA	3.3
46	CS	62	GLU	3.3
37	CJ	85	GLY	3.3
47	CT	84	ARG	3.3
14	BN	51	LEU	3.3
35	CG	107	LEU	3.3
1	BA	473	U	3.3
7	BG	69	VAL	3.3
43	CP	103	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	AB	46	THR	3.3
49	CV	98	SER	3.3
13	BM	113	ARG	3.3
31	CA	476	G	3.3
35	CG	126	PRO	3.3
34	CF	96	MET	3.3
10	BJ	36	VAL	3.3
1	BA	1441	A	3.2
7	AG	45	SER	3.2
37	DJ	37	GLU	3.2
1	BA	54	C	3.2
37	DJ	84	ALA	3.2
1	AA	1016	A	3.2
36	DH	63	ALA	3.2
13	BM	13	LYS	3.2
9	AI	19	VAL	3.2
36	CH	107	GLY	3.2
43	CP	29	HIS	3.2
45	CR	71	GLN	3.2
7	BG	66	LEU	3.2
37	DJ	83	ALA	3.2
53	CZ	22	LEU	3.2
55	DA	2115	G	3.2
33	CE	10	SER	3.2
54	DI	84	TYR	3.2
7	BG	7	ILE	3.2
30	CD	8	LYS	3.2
55	DA	1847	A	3.2
13	BM	26	GLY	3.2
23	C2	36	LEU	3.2
45	CR	73	GLY	3.2
17	BQ	72	SER	3.2
36	CH	108	VAL	3.2
49	CV	49	VAL	3.2
1	BA	1002	G	3.2
6	AF	97	THR	3.2
3	BC	159	GLY	3.2
7	BG	111	ARG	3.2
13	BM	98	ARG	3.2
9	AI	90	TYR	3.2
24	C3	37	LYS	3.2
31	CA	1044	C	3.2

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Mol	Chain	Res	Type	RSRZ
37	CJ	135	SER	3.2
13	BM	28	THR	3.2
19	BS	27	ASP	3.2
50	CW	27	PRO	3.2
20	BT	19	LYS	3.2
13	BM	84	GLY	3.2
31	CA	1963	U	3.2
31	CA	2122	U	3.2
34	CF	59	ALA	3.2
36	CH	72	ILE	3.2
10	BJ	22	THR	3.2
37	DJ	60	THR	3.2
40	CM	142	ILE	3.2
1	BA	79	G	3.2
37	CJ	36	MET	3.2
22	C1	46	ASP	3.2
35	CG	56	ASP	3.2
7	BG	60	GLU	3.2
55	DA	546	U	3.2
29	CC	249	GLY	3.2
22	C1	18	SER	3.2
13	BM	102	THR	3.2
45	CR	91	ASP	3.2
55	DA	1175	A	3.2
1	AA	1302	C	3.1
51	CX	55	ARG	3.1
30	CD	41	ALA	3.1
37	DJ	34	ASN	3.1
40	CM	138	ALA	3.1
43	CP	91	SER	3.1
7	BG	49	THR	3.1
20	BT	68	HIS	3.1
34	CF	150	ARG	3.1
43	CP	90	VAL	3.1
18	AR	74	HIS	3.1
23	C2	23	THR	3.1
24	C3	24	THR	3.1
19	BS	41	PHE	3.1
29	CC	30	PHE	3.1
7	BG	73	VAL	3.1
31	CA	1077	A	3.1
42	CO	116	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	BA	204	G	3.1
31	CA	335	C	3.1
40	CM	108	ALA	3.1
43	CP	87	ILE	3.1
46	CS	92	TRP	3.1
37	CJ	77	ALA	3.1
3	BC	53	SER	3.1
7	AG	57	SER	3.1
27	C0	7	ILE	3.1
31	CA	876	C	3.1
31	CA	1075	C	3.1
7	AG	49	THR	3.1
31	CA	548	G	3.1
50	CW	32	GLY	3.1
43	CP	93	ASP	3.1
13	BM	38	GLY	3.1
2	BB	187	VAL	3.1
27	C0	24	LEU	3.1
33	CE	157	LEU	3.1
34	CF	149	VAL	3.1
36	DH	142	VAL	3.1
1	BA	1226	C	3.1
31	CA	2860	A	3.1
19	BS	5	LEU	3.1
1	BA	212	G	3.1
31	CA	1168	G	3.1
46	CS	37	GLU	3.1
40	CM	134	ALA	3.1
41	CN	8	LYS	3.1
50	CW	6	ALA	3.1
55	DA	2108	A	3.1
36	CH	110	VAL	3.1
46	CS	14	VAL	3.1
6	AF	61	LEU	3.1
36	CH	136	SER	3.1
14	BN	9	ARG	3.1
1	BA	1201	A	3.1
2	BB	44	GLU	3.1
34	CF	140	GLU	3.1
37	CJ	50	GLU	3.1
42	CO	120	GLU	3.1
35	CG	101	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
43	CP	102	ARG	3.1
2	AB	32	PHE	3.1
46	CS	55	ASP	3.1
31	CA	1873	G	3.1
31	CA	2801	G	3.1
14	BN	45	VAL	3.1
37	CJ	70	VAL	3.1
31	CA	53	A	3.1
35	CG	87	LEU	3.1
55	DA	2169	A	3.1
12	BL	113	ALA	3.1
14	BN	43	ASN	3.0
34	CF	76	GLY	3.0
37	DJ	116	ASP	3.0
46	CS	15	SER	3.0
10	BJ	71	LEU	3.0
53	CZ	32	ALA	3.0
1	BA	135	C	3.0
55	DA	1073	A	3.0
1	BA	1025	U	3.0
31	CA	369	U	3.0
35	CG	122	THR	3.0
37	CJ	136	MET	3.0
9	BI	39	PHE	3.0
34	CF	84	PRO	3.0
9	AI	128	SER	3.0
34	CF	115	ARG	3.0
55	DA	2164	C	3.0
31	CA	1078	U	3.0
35	CG	129	THR	3.0
47	CT	103	ILE	3.0
35	CG	17	VAL	3.0
1	BA	86	G	3.0
7	BG	137	LYS	3.0
9	AI	63	LEU	3.0
34	CF	56	ASP	3.0
10	BJ	28	THR	3.0
31	CA	2175	C	3.0
40	CM	117	THR	3.0
1	BA	843	U	3.0
2	BB	21	ARG	3.0
20	BT	32	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
16	BP	15	PRO	3.0
33	CE	193	VAL	3.0
14	BN	4	GLN	3.0
20	BT	6	SER	3.0
5	BE	140	THR	3.0
19	AS	39	THR	3.0
1	BA	174	A	3.0
31	CA	2862	G	3.0
33	CE	25	GLU	3.0
7	BG	118	LEU	3.0
20	BT	79	LEU	3.0
9	BI	31	ASN	3.0
30	CD	91	THR	3.0
31	CA	646	U	3.0
31	CA	1015	U	3.0
43	CP	74	VAL	3.0
55	DA	2180	U	3.0
31	CA	86	G	3.0
9	AI	38	TYR	3.0
9	AI	129	LYS	3.0
12	BL	117	TYR	3.0
15	BO	26	GLU	3.0
22	C1	34	SER	3.0
35	CG	130	GLU	3.0
2	BB	210	VAL	3.0
13	BM	20	THR	3.0
46	CS	12	HIS	3.0
31	CA	228	C	3.0
31	CA	2165	C	3.0
7	BG	85	TYR	3.0
9	BI	6	TYR	3.0
28	CB	98	G	3.0
31	CA	81	G	3.0
31	CA	1869	G	3.0
37	DJ	52	GLY	3.0
43	CP	22	GLY	3.0
46	CS	38	VAL	3.0
6	BF	97	THR	3.0
50	CW	12	GLN	3.0
31	CA	2891	U	3.0
37	CJ	25	GLY	3.0
37	CJ	123	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
13	AM	36	ALA	3.0
13	BM	35	ALA	3.0
13	BM	45	ILE	3.0
1	BA	1005	A	3.0
7	BG	130	ASN	3.0
19	AS	55	ARG	3.0
35	CG	52	PHE	3.0
1	BA	1029	U	3.0
46	CS	59	ILE	3.0
34	CF	122	PHE	3.0
48	CU	59	ASN	3.0
14	BN	26	GLU	3.0
1	BA	1048	G	2.9
28	CB	117	G	2.9
34	CF	75	ALA	2.9
30	CD	39	ASP	2.9
33	CE	47	LYS	2.9
35	CG	137	ASP	2.9
13	BM	46	SER	2.9
40	CM	7	SER	2.9
7	AG	118	LEU	2.9
36	CH	9	VAL	2.9
49	CV	11	VAL	2.9
1	BA	1240	U	2.9
33	CE	140	ASP	2.9
24	C3	26	ASN	2.9
25	C4	28	ASN	2.9
37	DJ	90	SER	2.9
1	BA	1004	A	2.9
3	BC	71	ALA	2.9
7	BG	134	ALA	2.9
13	BM	27	LYS	2.9
22	C1	33	THR	2.9
48	CU	67	VAL	2.9
31	CA	264	C	2.9
31	CA	1076	C	2.9
1	BA	1362	A	2.9
7	BG	70	ARG	2.9
39	CL	112	PHE	2.9
31	CA	501	A	2.9
17	BQ	69	LYS	2.9
43	CP	88	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	AA	121	U	2.9
22	C1	5	GLN	2.9
51	CX	33	ALA	2.9
53	CZ	56	LEU	2.9
20	BT	51	PHE	2.9
35	DG	177	LYS	2.9
40	CM	139	GLY	2.9
1	BA	1049	U	2.9
31	CA	1060	U	2.9
36	CH	78	VAL	2.9
9	AI	31	ASN	2.9
48	CU	76	ARG	2.9
47	CT	98	LYS	2.9
13	AM	41	GLU	2.9
28	CB	116	G	2.9
31	CA	1072	C	2.9
52	CY	49	LEU	2.9
1	BA	459	A	2.9
1	BA	468	A	2.9
16	AP	43	ALA	2.9
31	CA	1070	A	2.9
33	CE	135	ALA	2.9
31	CA	1082	U	2.9
31	CA	2167	U	2.9
31	CA	2861	U	2.9
3	BC	192	THR	2.9
48	CU	80	TRP	2.9
40	CM	3	LEU	2.9
37	DJ	51	LYS	2.9
18	AR	51	TYR	2.9
31	CA	2892	G	2.9
16	BP	40	ASN	2.9
31	CA	1098	A	2.9
7	BG	119	ARG	2.9
15	BO	25	THR	2.9
30	CD	59	ARG	2.9
34	CF	145	LYS	2.9
53	CZ	54	LYS	2.9
20	BT	82	GLN	2.9
28	CB	49	C	2.9
43	CP	32	PRO	2.9
1	BA	69	G	2.9

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Mol	Chain	Res	Type	RSRZ
1	BA	213	G	2.9
33	CE	24	ASN	2.9
34	CF	33	LYS	2.9
37	CJ	125	MET	2.9
43	CP	106	LEU	2.9
48	CU	24	MET	2.9
48	CU	47	VAL	2.9
3	BC	193	TYR	2.9
10	BJ	86	ALA	2.9
2	BB	133	GLU	2.9
16	BP	10	GLY	2.9
37	DJ	85	GLY	2.9
31	CA	1729	U	2.9
31	CA	1047	G	2.9
31	CA	1059	G	2.9
34	CF	79	ILE	2.8
34	CF	37	ASN	2.8
1	AA	1286	U	2.8
31	CA	2160	C	2.8
13	BM	66	GLU	2.8
25	C4	37	ALA	2.8
42	DO	125	ALA	2.8
13	BM	58	ASP	2.8
31	CA	117	G	2.8
40	CM	130	GLY	2.8
53	CZ	6	LEU	2.8
54	DI	72	LEU	2.8
55	DA	2117	A	2.8
37	DJ	49	ILE	2.8
30	CD	90	PHE	2.8
34	CF	92	ARG	2.8
16	BP	80	LYS	2.8
13	BM	104	THR	2.8
33	CE	154	ASP	2.8
54	DI	124	ASP	2.8
36	DH	138	VAL	2.8
7	BG	3	ARG	2.8
15	BO	17	ARG	2.8
16	BP	56	ARG	2.8
7	BG	58	GLU	2.8
37	CJ	48	SER	2.8
37	DJ	48	SER	2.8

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Mol	Chain	Res	Type	RSRZ
19	BS	79	THR	2.8
1	AA	1037	C	2.8
13	AM	62	LYS	2.8
43	CP	27	VAL	2.8
48	CU	10	VAL	2.8
55	DA	613	A	2.8
38	CK	131	ASN	2.8
44	DQ	115	ASN	2.8
19	BS	68	GLY	2.8
23	C2	44	ARG	2.8
1	BA	1224	U	2.8
25	C4	41	LYS	2.8
40	CM	135	ILE	2.8
13	BM	11	ASP	2.8
31	CA	893	C	2.8
31	CA	2117	A	2.8
2	AB	30	PHE	2.8
19	BS	33	THR	2.8
40	CM	5	THR	2.8
44	CQ	86	VAL	2.8
31	CA	235	U	2.8
37	DJ	77	ALA	2.8
7	AG	110	LYS	2.8
37	DJ	91	GLY	2.8
46	CS	22	LEU	2.8
20	BT	70	ASN	2.8
34	CF	99	PHE	2.8
2	BB	132	LYS	2.8
7	BG	15	ASP	2.8
36	CH	12	LEU	2.8
1	BA	1003	G	2.8
31	CA	277	G	2.8
13	AM	39	ILE	2.8
31	CA	2300	C	2.8
35	CG	43	VAL	2.8
37	CJ	112	THR	2.8
17	BQ	44	LEU	2.8
34	CF	58	ALA	2.8
34	CF	107	ALA	2.8
43	CP	79	ALA	2.8
9	BI	126	GLN	2.8
35	CG	169	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
9	AI	28	ILE	2.8
39	CL	21	CYS	2.8
49	CV	72	ILE	2.8
7	BG	143	ARG	2.8
5	BE	125	ALA	2.8
25	C4	43	HIS	2.8
50	CW	13	GLY	2.8
16	BP	38	PHE	2.8
31	CA	1174	U	2.8
48	CU	58	VAL	2.8
55	DA	2118	U	2.8
55	DA	2176	A	2.8
13	AM	57	ARG	2.8
20	BT	5	LYS	2.8
51	CX	59	LEU	2.8
1	BA	201	G	2.8
35	CG	54	PRO	2.8
48	DU	91	GLN	2.8
53	CZ	24	GLU	2.8
1	BA	1067	A	2.8
13	AM	48	LEU	2.8
22	C1	27	SER	2.8
37	DJ	106	LEU	2.8
37	DJ	14	ALA	2.8
9	BI	68	LYS	2.8
19	BS	69	HIS	2.8
20	BT	29	ARG	2.8
36	DH	108	VAL	2.8
46	CS	29	THR	2.8
13	BM	33	ILE	2.7
28	CB	27	C	2.8
31	CA	139	U	2.7
1	BA	609	A	2.7
9	BI	17	ALA	2.7
9	BI	20	PHE	2.7
20	BT	63	ALA	2.7
43	CP	25	ARG	2.7
53	CZ	7	ARG	2.7
36	CH	142	VAL	2.7
40	CM	119	PRO	2.7
16	BP	18	GLN	2.7
49	CV	66	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
31	CA	1454	C	2.7
51	CX	62	LYS	2.7
33	CE	150	THR	2.7
55	DA	2119	A	2.7
22	C1	52	ARG	2.7
16	BP	7	ALA	2.7
7	BG	115	SER	2.7
21	BU	2	PRO	2.7
44	CQ	11	GLU	2.7
31	CA	1055	G	2.7
31	CA	2107	G	2.7
37	DJ	97	LYS	2.7
13	AM	26	GLY	2.7
7	BG	89	VAL	2.7
30	CD	203	VAL	2.7
1	BA	67	C	2.7
1	BA	153	C	2.7
34	CF	42	GLU	2.7
7	BG	56	LYS	2.7
34	CF	69	LYS	2.7
43	CP	56	LYS	2.7
1	BA	108	G	2.7
30	CD	44	GLY	2.7
31	CA	1142	A	2.7
36	CH	47	PHE	2.7
33	CE	128	ALA	2.7
48	CU	23	ALA	2.7
13	BM	109	ARG	2.7
19	BS	28	LYS	2.7
50	CW	89	ILE	2.7
30	CD	55	LYS	2.7
37	DJ	27	ALA	2.7
1	BA	460	A	2.7
31	CA	502	A	2.7
7	AG	68	ASN	2.7
31	CA	854	C	2.7
50	CW	34	LYS	2.7
54	DI	32	GLY	2.7
31	CA	1460	U	2.7
48	CU	62	VAL	2.7
7	AG	48	GLU	2.7
55	DA	2151	U	2.7

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Mol	Chain	Res	Type	RSRZ
13	BM	36	ALA	2.7
31	CA	2178	C	2.7
44	CQ	114	LEU	2.7
49	CV	52	LEU	2.7
13	AM	103	LYS	2.7
33	CE	186	VAL	2.7
35	CG	135	GLY	2.7
43	CP	30	ARG	2.7
1	BA	1035	A	2.7
14	AN	25	ALA	2.7
43	CP	89	ASP	2.7
45	CR	90	ILE	2.7
1	BA	90	C	2.7
1	BA	107	G	2.7
31	CA	1017	G	2.7
34	CF	91	LEU	2.7
16	AP	39	PHE	2.7
34	CF	26	MET	2.7
30	CD	29	VAL	2.7
36	DH	88	GLY	2.7
54	DI	26	VAL	2.7
37	CJ	41	ALA	2.7
22	C1	57	LYS	2.7
55	DA	895	U	2.7
55	DA	2114	A	2.7
34	CF	27	GLN	2.7
31	CA	1407	G	2.7
40	CM	102	GLY	2.7
43	CP	86	GLY	2.7
22	C1	6	ASN	2.6
1	BA	89	U	2.6
1	BA	1126	U	2.6
1	BA	1235	U	2.6
31	CA	355	U	2.6
31	CA	1143	A	2.6
34	CF	25	VAL	2.6
50	CW	67	GLY	2.6
7	AG	129	GLU	2.6
1	BA	210	C	2.6
1	BA	1028	C	2.6
31	CA	357	C	2.6
31	CA	1531	C	2.6

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Mol	Chain	Res	Type	RSRZ
55	DA	1076	C	2.6
18	AR	68	LEU	2.6
30	CD	199	SER	2.6
31	CA	361	G	2.6
37	CJ	34	ASN	2.6
11	AK	15	GLN	2.6
30	CD	35	THR	2.6
20	BT	34	LYS	2.6
33	CE	127	GLU	2.6
43	CP	28	VAL	2.6
44	CQ	92	VAL	2.6
13	AM	15	ALA	2.6
31	CA	236	C	2.6
2	AB	221	VAL	2.6
5	AE	10	GLU	2.6
36	CH	41	LYS	2.6
48	CU	68	LYS	2.6
9	AI	18	ARG	2.6
27	C0	9	GLN	2.6
37	CJ	30	GLN	2.6
31	CA	1340	U	2.6
33	CE	138	LEU	2.6
34	CF	137	ILE	2.6
49	CV	73	PHE	2.6
1	BA	207	C	2.6
13	AM	6	GLY	2.6
31	CA	885	C	2.6
48	CU	36	LYS	2.6
52	CY	35	SER	2.6
53	CZ	44	LYS	2.6
2	BB	57	LEU	2.6
14	BN	50	THR	2.6
31	CA	2668	G	2.6
34	CF	43	ALA	2.6
35	CG	72	LEU	2.6
1	BA	92	U	2.6
1	BA	102	G	2.6
17	AQ	53	CYS	2.6
31	CA	315	G	2.6
31	CA	776	G	2.6
31	CA	1016	G	2.6
31	CA	1606	C	2.6

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Mol	Chain	Res	Type	RSRZ
14	BN	20	TYR	2.6
52	CY	20	HIS	2.6
1	BA	250	A	2.6
29	CC	251	GLN	2.6
15	BO	19	ALA	2.6
31	CA	550	C	2.6
31	CA	1741	C	2.6
17	BQ	66	PRO	2.6
19	BS	42	PRO	2.6
3	AC	190	HIS	2.6
27	C0	55	VAL	2.6
35	CG	79	VAL	2.6
2	BB	164	ILE	2.6
36	CH	133	GLN	2.6
41	CN	41	LEU	2.6
31	CA	85	G	2.6
40	CM	85	VAL	2.6
51	CX	83	GLU	2.6
53	CZ	46	VAL	2.6
31	CA	850	U	2.6
7	BG	54	SER	2.6
8	BH	2	SER	2.6
33	CE	191	ASP	2.6
19	BS	51	VAL	2.6
35	CG	134	LYS	2.6
54	DI	88	HIS	2.6
1	BA	1303	C	2.6
12	BL	112	GLN	2.6
31	CA	2111	U	2.6
55	DA	2122	U	2.6
17	BQ	64	CYS	2.6
19	BS	58	VAL	2.6
42	CO	62	ASN	2.6
1	BA	55	A	2.6
1	BA	471	U	2.6
31	CA	611	C	2.6
31	CA	1170	C	2.6
33	CE	23	PHE	2.6
34	CF	172	ALA	2.6
23	C2	53	LYS	2.6
24	C3	45	SER	2.6
53	CZ	5	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
54	DI	90	GLY	2.6
2	AB	225	ARG	2.6
7	AG	53	ARG	2.6
19	BS	15	LEU	2.6
44	CQ	4	ILE	2.6
48	CU	84	TYR	2.5
1	BA	186	C	2.5
1	BA	1305	G	2.5
2	BB	139	ARG	2.5
10	AJ	7	ARG	2.5
24	C3	34	ARG	2.5
33	CE	32	VAL	2.5
35	CG	95	ARG	2.5
45	CR	30	ARG	2.5
55	DA	1090	A	2.5
31	CA	880	G	2.5
8	BH	121	LEU	2.5
37	DJ	117	MET	2.5
19	BS	14	HIS	2.5
10	BJ	12	ALA	2.5
46	CS	18	GLN	2.5
24	C3	27	GLY	2.5
7	BG	37	SER	2.5
17	BQ	21	ILE	2.5
30	CD	96	ILE	2.5
31	CA	1215	G	2.5
37	DJ	50	GLU	2.5
43	CP	82	ALA	2.5
44	CQ	75	GLN	2.5
49	CV	60	GLU	2.5
54	DI	92	ALA	2.5
30	CD	166	GLY	2.5
31	CA	1539	U	2.5
31	CA	2796	U	2.5
37	CJ	35	ILE	2.5
1	BA	1145	A	2.5
1	BA	1320	C	2.5
7	BG	106	GLU	2.5
31	CA	332	A	2.5
16	BP	58	ALA	2.5
36	CH	76	GLU	2.5
42	CO	111	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
43	CP	75	GLY	2.5
6	AF	62	MET	2.5
6	AF	90	MET	2.5
19	AS	78	ARG	2.5
30	CD	101	PHE	2.5
31	CA	596	U	2.5
45	CR	29	SER	2.5
13	BM	64	VAL	2.5
14	BN	16	LEU	2.5
16	BP	50	THR	2.5
31	CA	237	C	2.5
35	CG	25	THR	2.5
35	CG	138	LYS	2.5
37	CJ	16	GLY	2.5
55	DA	1075	C	2.5
37	DJ	65	ARG	2.5
9	BI	92	GLU	2.5
14	AN	55	SER	2.5
42	CO	119	SER	2.5
54	DI	107	GLU	2.5
14	BN	47	LYS	2.5
48	CU	61	LEU	2.5
30	CD	14	ILE	2.5
31	CA	1073	A	2.5
31	CA	1171	G	2.5
35	CG	161	GLY	2.5
44	CQ	19	SER	2.5
46	CS	103	ALA	2.5
55	DA	1094	U	2.5
39	CL	89	ASN	2.5
27	C0	44	ILE	2.5
2	AB	131	LYS	2.5
13	AM	3	ARG	2.5
42	CO	66	ALA	2.5
31	CA	1524	G	2.5
33	CE	173	THR	2.5
40	CM	74	THR	2.5
7	BG	150	ALA	2.5
24	C3	23	ALA	2.5
40	CM	131	ALA	2.5
51	CX	34	GLY	2.5
31	CA	477	A	2.5

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Mol	Chain	Res	Type	RSRZ
38	CK	141	ASP	2.5
1	AA	4	U	2.5
2	BB	208	ARG	2.5
31	CA	2109	U	2.5
34	CF	133	ARG	2.5
42	CO	96	ARG	2.5
1	BA	326	G	2.5
12	BL	93	VAL	2.5
16	BP	54	LEU	2.5
19	AS	50	ALA	2.5
23	C2	42	VAL	2.5
28	CB	24	G	2.5
7	AG	18	PHE	2.5
1	BA	1322	C	2.5
29	CC	272	SER	2.5
33	CE	75	SER	2.5
24	C3	22	MET	2.5
36	CH	27	ARG	2.5
31	CA	895	U	2.5
34	CF	74	VAL	2.5
34	CF	119	ALA	2.5
43	CP	50	ALA	2.5
34	CF	109	PRO	2.5
46	CS	93	PHE	2.5
10	BJ	78	GLU	2.5
23	C2	46	HIS	2.5
28	CB	23	G	2.5
37	CJ	37	GLU	2.5
1	BA	175	C	2.4
31	CA	2766	A	2.4
49	CV	90	GLY	2.4
53	CZ	4	LYS	2.4
3	BC	50	ALA	2.4
20	BT	80	THR	2.4
37	DJ	46	THR	2.4
15	AO	17	ARG	2.4
9	BI	91	ASP	2.4
30	CD	28	GLU	2.4
47	CT	82	MET	2.4
1	BA	380	G	2.4
31	CA	1052	C	2.4
31	CA	1074	G	2.4

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Mol	Chain	Res	Type	RSRZ
43	CP	49	VAL	2.4
1	BA	461	A	2.4
49	CV	48	PRO	2.4
10	BJ	92	LEU	2.4
40	CM	140	GLY	2.4
46	CS	51	VAL	2.4
20	AT	2	ALA	2.4
20	BT	45	ALA	2.4
36	DH	74	ALA	2.4
43	CP	107	ALA	2.4
17	BQ	50	ASN	2.4
37	CJ	94	ASN	2.4
44	CQ	3	ASN	2.4
31	CA	2367	G	2.4
45	CR	74	ILE	2.4
31	CA	1328	A	2.4
17	BQ	23	VAL	2.4
30	CD	50	VAL	2.4
34	CF	4	LEU	2.4
51	CX	57	HIS	2.4
47	CT	44	ALA	2.4
1	BA	95	C	2.4
19	AS	30	PRO	2.4
9	BI	40	GLY	2.4
17	BQ	78	VAL	2.4
31	CA	1053	C	2.4
42	CO	93	GLY	2.4
47	CT	95	ARG	2.4
31	CA	289	G	2.4
45	CR	25	TYR	2.4
49	CV	17	LYS	2.4
19	BS	23	VAL	2.4
29	CC	233	GLY	2.4
37	DJ	61	VAL	2.4
1	BA	316	C	2.4
9	AI	64	TYR	2.4
30	CD	176	ASP	2.4
31	CA	1045	C	2.4
37	DJ	64	ASP	2.4
31	CA	310	A	2.4
1	AA	1015	G	2.4
1	BA	378	G	2.4

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Mol	Chain	Res	Type	RSRZ
39	CL	22	ILE	2.4
43	CP	60	GLU	2.4
33	CE	164	LEU	2.4
33	CE	199	MET	2.4
35	DG	101	ASN	2.4
45	CR	117	LEU	2.4
36	DH	89	LYS	2.4
41	CN	69	PRO	2.4
1	BA	219	U	2.4
30	CD	30	GLU	2.4
33	DE	7	ASP	2.4
35	CG	124	GLU	2.4
36	DH	82	SER	2.4
13	AM	97	VAL	2.4
36	CH	58	LEU	2.4
47	CT	105	VAL	2.4
48	CU	50	LEU	2.4
1	AA	1026	G	2.4
1	AA	1127	G	2.4
1	BA	251	G	2.4
31	CA	307	G	2.4
31	CA	597	G	2.4
35	CG	100	GLY	2.4
34	CF	77	PHE	2.4
19	BS	65	GLU	2.4
31	CA	87	U	2.4
31	CA	1864	U	2.4
7	BG	141	VAL	2.4
13	AM	44	LYS	2.4
14	BN	23	LYS	2.4
19	AS	25	SER	2.4
30	CD	84	LEU	2.4
13	BM	63	PHE	2.4
2	BB	46	THR	2.4
7	BG	68	ASN	2.4
27	C0	23	THR	2.4
36	CH	67	ALA	2.4
35	CG	16	ASP	2.4
42	CO	52	ILE	2.4
47	CT	96	ILE	2.4
47	CT	36	LEU	2.4
48	CU	81	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
10	BJ	101	SER	2.4
34	CF	89	VAL	2.4
1	BA	1460	C	2.4
10	AJ	5	ARG	2.4
16	BP	51	ARG	2.4
30	CD	88	GLU	2.4
40	CM	136	GLU	2.4
50	CW	37	PRO	2.4
5	BE	124	LEU	2.4
8	BH	90	ASP	2.4
7	BG	105	VAL	2.4
1	BA	993	G	2.4
35	CG	120	GLY	2.4
37	CJ	117	MET	2.4
1	BA	222	C	2.4
27	C0	48	ILE	2.4
54	DI	127	ALA	2.4
2	BB	123	ASP	2.3
42	CO	84	GLY	2.3
51	CX	64	ASP	2.3
55	DA	1103	A	2.3
48	CU	1	MET	2.3
19	AS	24	GLU	2.3
50	CW	10	LYS	2.3
10	BJ	79	PRO	2.3
35	CG	174	ALA	2.3
48	CU	83	ALA	2.3
17	BQ	8	LEU	2.3
31	CA	2368	C	2.3
35	CG	9	VAL	2.3
49	CV	69	ASN	2.3
51	CX	25	ARG	2.3
3	AC	80	LYS	2.3
48	CU	33	LYS	2.3
1	AA	994	A	2.3
1	BA	1125	U	2.3
30	CD	46	ARG	2.3
1	AA	1305	G	2.3
1	BA	354	G	2.3
31	CA	1179	G	2.3
34	CF	64	LYS	2.3
49	DV	56	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
12	BL	14	ARG	2.3
27	C0	53	PHE	2.3
33	CE	103	GLY	2.3
33	CE	121	VAL	2.3
35	CG	78	GLY	2.3
37	DJ	139	VAL	2.3
19	AS	44	MET	2.3
54	DI	52	MET	2.3
1	BA	388	G	2.3
19	BS	78	ARG	2.3
7	BG	47	LEU	2.3
31	CA	930	G	2.3
31	CA	1862	G	2.3
36	CH	4	ILE	2.3
36	DH	64	ALA	2.3
41	CN	124	LEU	2.3
16	BP	13	LYS	2.3
47	CT	101	SER	2.3
29	CC	180	GLU	2.3
10	BJ	83	THR	2.3
54	DI	120	ALA	2.3
1	BA	1243	C	2.3
1	AA	1020	G	2.3
28	CB	96	G	2.3
55	DA	1059	G	2.3
31	CA	2118	U	2.3
44	CQ	112	GLU	2.3
35	CG	34	THR	2.3
36	CH	10	ALA	2.3
8	AH	120	GLY	2.3
36	DH	139	PHE	2.3
1	BA	1317	C	2.3
19	BS	38	SER	2.3
28	CB	19	C	2.3
31	CA	1043	C	2.3
31	CA	1874	C	2.3
35	CG	167	GLU	2.3
47	CT	6	LYS	2.3
9	AI	83	ILE	2.3
11	AK	97	ILE	2.3
31	CA	327	G	2.3
53	CZ	14	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
19	BS	63	THR	2.3
36	DH	96	THR	2.3
44	CQ	30	VAL	2.3
50	CW	65	VAL	2.3
2	AB	27	MET	2.3
48	CU	21	SER	2.3
7	BG	91	VAL	2.3
14	BN	44	ALA	2.3
15	BO	15	PHE	2.3
16	BP	20	VAL	2.3
31	CA	1018	U	2.3
34	CF	55	ALA	2.3
36	CH	100	ALA	2.3
9	AI	89	GLU	2.3
15	BO	14	GLU	2.3
31	CA	180	G	2.3
31	CA	514	A	2.3
13	BM	83	LEU	2.3
36	CH	14	SER	2.3
7	BG	103	TRP	2.3
19	AS	40	ILE	2.3
13	BM	61	ALA	2.3
14	BN	25	ALA	2.3
36	CH	144	VAL	2.3
39	CL	33	ALA	2.3
1	AA	984	C	2.3
1	BA	88	U	2.3
9	BI	22	LYS	2.3
13	BM	114	LYS	2.3
6	AF	98	GLU	2.3
23	C2	17	THR	2.3
27	C0	19	LYS	2.3
34	CF	29	PRO	2.3
1	BA	260	G	2.3
31	CA	1633	G	2.3
46	CS	98	ILE	2.3
2	AB	4	VAL	2.3
9	AI	27	LYS	2.3
13	AM	60	VAL	2.3
36	DH	84	ALA	2.3
43	CP	59	ALA	2.3
1	BA	1148	U	2.3

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Mol	Chain	Res	Type	RSRZ
23	C2	22	THR	2.3
28	CB	22	U	2.3
31	CA	328	U	2.3
31	CA	2166	U	2.3
54	DI	29	ASP	2.3
55	DA	2106	U	2.3
1	BA	197	A	2.3
2	BB	217	VAL	2.3
6	BF	10	VAL	2.3
17	BQ	83	VAL	2.3
28	CB	73	A	2.3
31	CA	1872	A	2.3
35	CG	74	SER	2.3
36	CH	61	VAL	2.3
37	CJ	63	ALA	2.3
49	CV	76	ALA	2.3
10	BJ	9	ARG	2.2
7	AG	2	PRO	2.2
31	CA	2795	C	2.2
55	DA	1870	C	2.2
9	AI	104	VAL	2.2
49	CV	71	ALA	2.2
1	AA	205	A	2.2
17	BQ	17	MET	2.2
25	C4	36	LYS	2.2
31	CA	2876	G	2.2
39	CL	20	MET	2.2
16	AP	4	ILE	2.2
17	BQ	5	ILE	2.2
40	CM	94	THR	2.2
31	CA	2449	U	2.2
1	BA	1037	C	2.2
20	BT	81	ALA	2.2
31	CA	2150	C	2.2
33	CE	101	TYR	2.2
34	CF	98	GLU	2.2
37	CJ	15	ALA	2.2
37	CJ	124	ALA	2.2
45	DR	118	ALA	2.2
49	CV	16	GLY	2.2
51	CX	61	ALA	2.2
55	DA	898	C	2.2

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Mol	Chain	Res	Type	RSRZ
19	AS	35	SER	2.2
43	CP	85	LYS	2.2
1	BA	172	A	2.2
31	CA	345	A	2.2
19	AS	76	PRO	2.2
36	CH	77	THR	2.2
40	CM	121	THR	2.2
10	BJ	95	GLY	2.2
19	AS	22	ALA	2.2
31	CA	1529	G	2.2
34	CF	126	GLY	2.2
54	DI	2	ALA	2.2
7	BG	50	LEU	2.2
7	BG	57	SER	2.2
10	AJ	102	LEU	2.2
31	CA	2078	C	2.2
16	AP	16	PHE	2.2
1	AA	1332	A	2.2
9	BI	11	ARG	2.2
12	BL	109	ASP	2.2
13	AM	82	ASP	2.2
46	CS	64	VAL	2.2
13	AM	115	PRO	2.2
13	BM	3	ARG	2.2
35	CG	13	ALA	2.2
36	CH	74	ALA	2.2
43	CP	76	LYS	2.2
45	CR	118	ALA	2.2
49	CV	62	GLU	2.2
53	CZ	8	GLU	2.2
31	CA	1108	U	2.2
1	BA	1020	G	2.2
1	BA	1312	G	2.2
31	CA	68	G	2.2
1	BA	1147	C	2.2
2	BB	31	ILE	2.2
28	CB	63	C	2.2
17	AQ	83	VAL	2.2
11	AK	18	ASP	2.2
44	CQ	35	GLY	2.2
54	DI	105	LYS	2.2
7	AG	46	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
20	BT	78	ASN	2.2
35	CG	118	PRO	2.2
38	CK	78	THR	2.2
1	BA	1146	A	2.2
27	C0	17	LEU	2.2
30	CD	201	LEU	2.2
33	CE	200	LEU	2.2
10	AJ	76	ILE	2.2
15	BO	12	VAL	2.2
35	CG	18	LYS	2.2
27	C0	42	PRO	2.2
30	CD	132	ALA	2.2
31	CA	882	G	2.2
31	CA	2852	G	2.2
40	CM	88	GLY	2.2
43	CP	23	ALA	2.2
55	DA	2178	C	2.2
10	BJ	80	THR	2.2
11	BK	64	GLN	2.2
37	DJ	43	ASN	2.2
43	CP	104	GLN	2.2
51	CX	32	LEU	2.2
46	CS	78	ARG	2.2
1	BA	1286	U	2.2
9	BI	21	ILE	2.2
13	AM	17	ILE	2.2
18	AR	21	ILE	2.2
29	DC	272	SER	2.2
31	CA	429	A	2.2
31	CA	2833	U	2.2
31	CA	2904	U	2.2
13	BM	67	GLY	2.2
43	CP	20	GLU	2.2
7	BG	65	ALA	2.2
18	AR	23	TYR	2.2
1	BA	1336	C	2.2
3	BC	144	LEU	2.2
41	CN	72	PRO	2.2
54	DI	3	LEU	2.2
31	CA	7	G	2.2
31	CA	1455	G	2.2
2	AB	136	MET	2.2

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Mol	Chain	Res	Type	RSRZ
11	AK	34	ILE	2.2
18	BR	74	HIS	2.2
30	CD	189	VAL	2.2
47	CT	7	HIS	2.2
1	BA	96	U	2.2
31	CA	112	U	2.2
31	CA	894	U	2.2
42	CO	59	SER	2.2
41	CN	116	ALA	2.2
50	DW	94	ALA	2.2
15	BO	21	ASP	2.2
2	BB	186	ILE	2.2
28	CB	118	C	2.2
31	CA	1319	C	2.2
33	CE	131	THR	2.2
33	CE	122	GLU	2.2
46	CS	33	VAL	2.2
17	BQ	54	GLY	2.2
38	CK	83	GLY	2.2
3	AC	189	ALA	2.2
10	BJ	34	ALA	2.2
13	BM	44	LYS	2.2
36	DH	68	ARG	2.2
1	AA	1441	A	2.2
2	BB	88	ASP	2.2
31	CA	101	A	2.2
55	DA	1057	A	2.2
2	BB	36	ASN	2.2
30	CD	9	VAL	2.2
1	BA	1237	C	2.2
2	AB	17	GLY	2.2
31	CA	314	C	2.2
31	CA	1172	C	2.2
46	CS	24	LYS	2.2
13	AM	21	SER	2.2
1	BA	455	G	2.2
9	BI	51	PRO	2.2
31	CA	1530	G	2.2
14	BN	54	ASP	2.2
16	BP	45	GLU	2.2
18	AR	48	ARG	2.2
31	CA	213	A	2.2

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Mol	Chain	Res	Type	RSRZ
35	CG	69	ARG	2.2
14	BN	42	TRP	2.1
40	CM	70	LYS	2.2
40	CM	141	LYS	2.2
29	CC	244	PRO	2.1
30	CD	103	ASP	2.1
35	CG	77	ILE	2.1
36	CH	109	GLU	2.1
36	DH	86	ASP	2.1
48	CU	31	VAL	2.1
54	DI	114	GLU	2.1
1	BA	1297	G	2.1
31	CA	45	G	2.1
29	CC	33	LEU	2.1
31	CA	2800	A	2.1
34	CF	68	THR	2.1
37	DJ	118	THR	2.1
43	CP	57	ALA	2.1
4	AD	189	SER	2.1
16	BP	47	GLU	2.1
26	C5	32	LYS	2.1
31	CA	902	C	2.1
41	CN	50	ARG	2.1
46	CS	52	PRO	2.1
53	CZ	48	ARG	2.1
1	AA	89	U	2.1
31	CA	1058	U	2.1
34	CF	62	GLY	2.1
43	CP	108	ASP	2.1
43	CP	48	LEU	2.1
20	BT	47	ALA	2.1
35	CG	49	THR	2.1
36	DH	11	ASN	2.1
48	CU	28	ASN	2.1
2	BB	67	ILE	2.1
16	BP	48	GLU	2.1
31	CA	2660	A	2.1
1	BA	1325	C	2.1
36	DH	107	GLY	2.1
49	CV	57	GLY	2.1
31	CA	2245	U	2.1
54	DI	60	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
11	BK	21	ALA	2.1
30	CD	182	ALA	2.1
35	CG	119	ALA	2.1
51	DX	10	THR	2.1
44	CQ	5	ILE	2.1
1	BA	1271	A	2.1
31	CA	474	G	2.1
2	BB	12	ALA	2.1
22	C1	56	ALA	2.1
24	C3	36	ALA	2.1
31	CA	61	C	2.1
53	DZ	63	ALA	2.1
13	BM	55	THR	2.1
36	DH	110	VAL	2.1
46	CS	19	THR	2.1
18	AR	55	LEU	2.1
9	BI	64	TYR	2.1
22	C1	24	ALA	2.1
1	BA	1212	U	2.1
1	BA	352	C	2.1
1	BA	1228	C	2.1
6	AF	42	TRP	2.1
2	BB	42	ASN	2.1
6	AF	63	ASN	2.1
7	BG	87	VAL	2.1
34	CF	39	GLY	2.1
26	C5	2	LYS	2.1
16	AP	81	ALA	2.1
37	CJ	114	ALA	2.1
46	CS	28	ALA	2.1
20	BT	58	VAL	2.1
1	BA	91	U	2.1
31	CA	654	A	2.1
31	CA	1325	U	2.1
7	BG	101	MET	2.1
14	AN	24	ARG	2.1
16	AP	74	LEU	2.1
31	CA	1212	G	2.1
31	CA	1236	G	2.1
31	CA	2325	G	2.1
37	DJ	81	LYS	2.1
37	DJ	103	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
48	CU	77	ARG	2.1
49	CV	47	LYS	2.1
55	DA	2141	G	2.1
5	BE	92	SER	2.1
36	CH	25	TYR	2.1
9	AI	59	GLU	2.1
36	DH	106	ALA	2.1
53	CZ	59	GLU	2.1
19	AS	21	LYS	2.1
44	CQ	24	ASP	2.1
1	AA	1025	U	2.1
27	C0	27	LEU	2.1
1	BA	196	A	2.1
9	AI	5	GLN	2.1
10	BJ	99	GLN	2.1
42	CO	28	LEU	2.1
49	CV	38	GLY	2.1
8	BH	55	THR	2.1
36	DH	77	THR	2.1
31	CA	2693	G	2.1
34	CF	12	VAL	2.1
34	CF	28	VAL	2.1
34	CF	61	SER	2.1
39	CL	111	LYS	2.1
2	AB	157	LEU	2.1
10	AJ	73	LEU	2.1
24	C3	1	MET	2.1
31	CA	2106	U	2.1
33	CE	17	THR	2.1
7	BG	79	ARG	2.1
8	AH	108	LYS	2.1
22	C1	16	ARG	2.1
30	CD	7	LYS	2.1
30	CD	85	ALA	2.1
1	BA	984	C	2.1
2	AB	14	VAL	2.1
2	AB	134	ALA	2.1
35	CG	8	PRO	2.1
17	BQ	61	ILE	2.1
31	CA	413	C	2.1
54	DI	54	VAL	2.1
46	CS	101	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	AA	1276	G	2.1
8	BH	120	GLY	2.1
31	CA	1112	G	2.1
40	CM	91	ASP	2.1
51	CX	42	GLY	2.1
9	AI	9	THR	2.1
12	BL	110	ARG	2.1
13	BM	93	ARG	2.1
23	C2	25	LYS	2.1
35	CG	48	ASN	2.1
37	CJ	97	LYS	2.1
53	CZ	47	ARG	2.1
1	BA	78	A	2.1
10	AJ	8	ILE	2.1
19	AS	71	LEU	2.1
31	CA	515	A	2.1
1	BA	931	C	2.1
55	DA	1092	C	2.1
46	CS	48	LYS	2.0
1	BA	953	G	2.0
31	CA	619	G	2.0
31	CA	881	G	2.0
31	CA	1166	G	2.0
34	CF	134	GLU	2.0
7	BG	46	ALA	2.0
1	BA	467	U	2.0
29	CC	95	LEU	2.0
31	CA	150	U	2.0
34	CF	166	GLY	2.0
39	CL	15	GLY	2.0
31	CA	2108	A	2.0
34	CF	47	LYS	2.0
7	AG	52	GLN	2.0
11	BK	112	ASP	2.0
13	AM	11	ASP	2.0
1	BA	194	C	2.0
2	AB	44	GLU	2.0
13	BM	43	VAL	2.0
40	CM	122	VAL	2.0
43	CP	110	ALA	2.0
10	BJ	32	THR	2.0
36	CH	122	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
37	CJ	101	ILE	2.0
37	DJ	74	PRO	2.0
42	CO	83	LEU	2.0
1	BA	954	G	2.0
31	CA	1534	U	2.0
31	CA	2115	G	2.0
55	DA	1061	U	2.0
1	AA	1022	A	2.0
31	CA	1054	A	2.0
31	CA	1532	A	2.0
1	BA	1218	C	2.0
5	BE	110	ALA	2.0
30	CD	75	ALA	2.0
34	CF	7	TYR	2.0
30	CD	187	LEU	2.0
31	CA	1533	C	2.0
39	CL	51	LYS	2.0
19	BS	81	ARG	2.0
1	BA	842	U	2.0
1	BA	259	G	2.0
1	BA	1475	G	2.0
31	CA	1867	G	2.0
14	AN	22	ALA	2.0
19	BS	32	ARG	2.0
31	CA	1213	A	2.0
50	CW	9	ARG	2.0
31	CA	334	C	2.0
34	CF	2	ALA	2.0
53	DZ	3	ALA	2.0
1	BA	177	G	2.0
2	AB	124	GLY	2.0
31	CA	1456	G	2.0
31	CA	2409	G	2.0
36	CH	13	GLY	2.0
1	BA	109	A	2.0
8	AH	3	MET	2.0
13	AM	104	THR	2.0
27	C0	41	THR	2.0
28	CB	52	A	2.0
31	CA	626	A	2.0
31	CA	2602	A	2.0
40	CM	38	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
3	BC	76	VAL	2.0
37	DJ	70	VAL	2.0
49	CV	22	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
31	PSU	CA	1917	20/21	0.89	0.24	120,123,132,132	0
31	2MA	CA	2503	23/24	0.89	0.20	90,100,103,104	0
1	2MG	BA	1207	24/25	0.90	0.20	140,147,149,151	0
12	D2T	BL	89	10/11	0.90	0.30	92,99,108,108	0
31	3TD	CA	1915	21/22	0.92	0.21	142,145,154,156	0
1	5MC	BA	967	21/22	0.93	0.24	115,124,127,128	0
31	2MG	CA	1835	24/25	0.93	0.18	76,80,83,83	0
31	PSU	CA	1911	20/21	0.93	0.21	104,121,124,125	0
1	2MG	BA	966	24/25	0.93	0.19	119,123,135,135	0
1	5MC	BA	1407	21/22	0.93	0.18	86,95,98,102	0
31	6MZ	CA	2030	23/24	0.93	0.18	81,86,89,90	0
31	2MG	CA	2445	24/25	0.93	0.27	74,80,84,85	0
1	2MG	BA	1516	24/25	0.93	0.16	66,73,79,81	0
55	3TD	DA	1915	21/22	0.93	0.17	91,98,111,112	0
12	D2T	AL	89	10/11	0.94	0.20	59,64,75,78	0
1	PSU	BA	516	20/21	0.94	0.17	100,101,104,104	0
31	1MG	CA	745	24/25	0.94	0.22	90,92,94,96	0
31	PSU	CA	2504	20/21	0.94	0.17	76,87,89,93	0
31	PSU	CA	2605	20/21	0.94	0.18	82,84,87,88	0
31	6MZ	CA	1618	23/24	0.94	0.22	109,114,116,117	0
41	4D4	CN	81	12/13	0.94	0.22	90,96,114,114	0
31	G7M	CA	2069	24/25	0.95	0.18	80,84,87,88	0
1	MA6	BA	1519	24/25	0.95	0.22	76,78,81,82	0
31	PSU	CA	2457	20/21	0.95	0.18	87,89,92,92	0
1	2MG	AA	1207	24/25	0.95	0.13	89,100,106,109	0
1	MA6	BA	1518	24/25	0.95	0.20	74,80,82,83	0
31	PSU	CA	746	20/21	0.95	0.13	86,98,100,101	0
31	5MU	CA	747	21/22	0.95	0.17	97,103,106,106	0
31	PSU	CA	955	20/21	0.95	0.17	85,87,92,92	0
1	2MG	AA	966	24/25	0.96	0.15	76,84,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	OMC	CA	2498	21/22	0.96	0.22	84,87,93,97	0
31	5MC	CA	1962	21/22	0.96	0.25	81,88,89,92	0
1	G7M	BA	527	24/25	0.96	0.19	93,95,98,99	0
31	OMU	CA	2552	21/22	0.96	0.33	83,84,98,101	0
31	PSU	CA	2580	20/21	0.96	0.16	83,91,93,93	0
1	4OC	BA	1402	22/23	0.96	0.16	78,79,81,82	0
31	OMG	CA	2251	24/25	0.96	0.22	82,83,85,86	0
1	5MC	AA	967	21/22	0.96	0.17	80,86,94,96	0
1	G7M	AA	527	24/25	0.97	0.14	58,70,72,74	0
1	5MC	AA	1407	21/22	0.97	0.14	50,55,58,61	0
1	UR3	AA	1498	21/22	0.97	0.16	55,59,62,66	0
31	5MU	CA	1939	21/22	0.97	0.15	74,76,85,88	0
55	2MG	DA	1835	24/25	0.97	0.19	43,49,53,53	0
55	PSU	DA	1911	20/21	0.97	0.14	66,80,82,83	0
1	2MG	AA	1516	24/25	0.97	0.16	50,54,57,58	0
55	PSU	DA	1917	20/21	0.97	0.15	77,81,87,88	0
1	UR3	BA	1498	21/22	0.97	0.11	80,82,84,88	0
1	4OC	AA	1402	22/23	0.98	0.15	60,61,63,64	0
1	PSU	AA	516	20/21	0.98	0.13	75,79,82,82	0
1	MA6	AA	1518	24/25	0.98	0.17	41,46,49,51	0
55	5MC	DA	1962	21/22	0.98	0.18	33,44,47,50	0
55	PSU	DA	2604	20/21	0.98	0.17	33,39,50,51	0
1	MA6	AA	1519	24/25	0.98	0.17	44,48,49,50	0
41	4D4	DN	81[A]	12/13	0.98	0.19	29,40,50,51	9
41	4D4	DN	81[B]	12/13	0.98	0.19	21,29,35,36	9
55	1MG	DA	745	24/25	0.99	0.17	18,25,33,38	0
55	PSU	DA	746	20/21	0.99	0.16	18,24,29,33	0
55	5MU	DA	1939	21/22	0.99	0.21	31,36,39,44	0
55	5MU	DA	747	21/22	0.99	0.16	24,31,35,40	0
55	6MZ	DA	2030	23/24	0.99	0.19	13,20,24,33	0
55	G7M	DA	2069	24/25	0.99	0.17	30,33,35,38	0
55	OMG	DA	2251	24/25	0.99	0.17	22,27,45,51	0
55	2MG	DA	2445	24/25	0.99	0.18	17,23,27,29	0
55	H2U	DA	2449	20/21	0.99	0.18	25,28,29,32	0
55	PSU	DA	2457	20/21	0.99	0.16	23,26,31,32	0
55	OMC	DA	2498	21/22	0.99	0.18	15,24,25,29	0
55	2MA	DA	2503	23/24	0.99	0.20	17,29,37,40	0
55	PSU	DA	2504	20/21	0.99	0.18	33,36,37,40	0
55	OMU	DA	2552	21/22	0.99	0.18	30,32,35,44	0
55	PSU	DA	2580	20/21	0.99	0.17	20,24,29,32	0
55	PSU	DA	955	20/21	0.99	0.18	24,25,28,28	0
55	PSU	DA	2605	20/21	0.99	0.16	30,35,41,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	6MZ	DA	1618	23/24	0.99	0.15	24,29,32,37	0
32	MEQ	DD	150[A]	10/11	0.99	0.19	7,12,22,24	10
32	MEQ	DD	150[B]	10/11	0.99	0.19	18,24,29,30	10

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	3154	1/1	0.16	0.70	152,152,152,152	0
56	MG	CA	3139	1/1	0.21	0.72	114,114,114,114	0
56	MG	CA	3060	1/1	0.24	0.40	194,194,194,194	0
56	MG	DA	3183	1/1	0.28	2.52	97,97,97,97	0
56	MG	DA	3179	1/1	0.36	0.62	102,102,102,102	0
56	MG	CA	3126	1/1	0.38	0.39	107,107,107,107	0
56	MG	CA	3038	1/1	0.41	0.13	234,234,234,234	0
56	MG	BA	1630	1/1	0.42	0.15	271,271,271,271	0
56	MG	AA	1606	1/1	0.46	0.84	125,125,125,125	0
56	MG	CA	3134	1/1	0.50	0.61	107,107,107,107	0
56	MG	AA	1603	1/1	0.51	0.50	108,108,108,108	0
56	MG	CA	3140	1/1	0.53	0.46	88,88,88,88	0
56	MG	CA	3110	1/1	0.54	0.24	92,92,92,92	0
56	MG	CA	3075	1/1	0.54	2.38	238,238,238,238	0
56	MG	BA	1604	1/1	0.55	0.51	272,272,272,272	0
56	MG	CA	3113	1/1	0.58	0.56	90,90,90,90	0
56	MG	DA	3166	1/1	0.58	0.27	81,81,81,81	0
56	MG	AA	1614	1/1	0.59	0.85	117,117,117,117	0
56	MG	CA	3132	1/1	0.59	0.50	102,102,102,102	0
56	MG	CA	3105	1/1	0.59	1.37	250,250,250,250	0
56	MG	CA	3055	1/1	0.60	0.16	260,260,260,260	0
56	MG	AA	1626	1/1	0.61	0.94	111,111,111,111	0
56	MG	AA	1625	1/1	0.62	0.66	90,90,90,90	0
56	MG	AA	1619	1/1	0.63	0.61	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	PUT	AA	1675	6/6	0.63	0.70	101,102,103,103	0
56	MG	CA	3021	1/1	0.64	0.79	260,260,260,260	0
56	MG	BA	1609	1/1	0.64	0.22	270,270,270,270	0
56	MG	CA	3014	1/1	0.64	0.16	161,161,161,161	0
56	MG	BA	1638	1/1	0.65	0.70	109,109,109,109	0
58	MPD	DE	301	8/8	0.65	0.84	153,155,156,156	0
56	MG	CA	3047	1/1	0.65	0.69	272,272,272,272	0
63	PGE	D3	101	10/10	0.65	0.81	105,111,114,114	0
56	MG	CA	3129	1/1	0.67	0.40	125,125,125,125	0
56	MG	CA	3152	1/1	0.67	0.39	158,158,158,158	0
56	MG	CA	3007	1/1	0.67	0.31	216,216,216,216	0
56	MG	AA	1617	1/1	0.68	0.39	101,101,101,101	0
56	MG	CA	3135	1/1	0.68	0.29	81,81,81,81	0
59	PUT	AA	1674	6/6	0.69	0.63	112,117,121,123	0
56	MG	CA	3124	1/1	0.69	0.31	156,156,156,156	0
56	MG	CA	3106	1/1	0.69	0.28	84,84,84,84	0
56	MG	CA	3001	1/1	0.70	0.22	291,291,291,291	0
56	MG	BA	1616	1/1	0.70	0.27	185,185,185,185	0
61	PEG	D3	102	7/7	0.70	1.26	88,94,99,99	0
63	PGE	D1	102	10/10	0.70	0.68	113,119,122,122	0
56	MG	BA	1641	1/1	0.70	0.14	94,94,94,94	0
56	MG	CA	3022	1/1	0.71	0.41	170,170,170,170	0
59	PUT	DA	3198	6/6	0.71	0.61	102,102,104,105	0
56	MG	DA	3154	1/1	0.71	0.17	80,80,80,80	0
56	MG	CA	3111	1/1	0.71	0.39	83,83,83,83	0
56	MG	DA	3171	1/1	0.71	0.68	111,111,111,111	0
56	MG	CA	3116	1/1	0.72	0.51	79,79,79,79	0
56	MG	DA	3170	1/1	0.72	0.53	106,106,106,106	0
58	MPD	DN	201	8/8	0.72	0.45	91,96,102,102	0
68	TRS	DA	3222	8/8	0.72	0.68	107,112,117,117	0
56	MG	CA	3028	1/1	0.73	0.21	277,277,277,277	0
56	MG	DA	3158	1/1	0.73	0.61	75,75,75,75	0
56	MG	CA	3023	1/1	0.73	0.18	245,245,245,245	0
59	PUT	DA	3207	6/6	0.73	0.45	95,100,104,105	0
56	MG	CA	3131	1/1	0.74	0.31	56,56,56,56	0
56	MG	DB	206	1/1	0.74	0.33	129,129,129,129	0
61	PEG	DP	201	7/7	0.74	0.72	108,109,109,110	0
61	PEG	DQ	201	7/7	0.75	0.78	92,94,96,97	0
56	MG	CA	3061	1/1	0.75	0.16	250,250,250,250	0
56	MG	CA	3133	1/1	0.75	0.30	88,88,88,88	0
56	MG	DA	3168	1/1	0.75	0.49	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3031	1/1	0.76	0.09	87,87,87,87	0
61	PEG	D1	103	7/7	0.76	0.45	81,87,93,95	0
56	MG	AA	1623	1/1	0.76	0.41	77,77,77,77	0
66	ACY	DA	3199	4/4	0.76	0.41	108,109,109,109	0
56	MG	AA	1622	1/1	0.76	1.23	112,112,112,112	0
56	MG	CA	3136	1/1	0.77	0.34	82,82,82,82	0
56	MG	AA	1604	1/1	0.77	0.35	66,66,66,66	0
56	MG	CA	3122	1/1	0.77	1.02	100,100,100,100	0
56	MG	CA	3127	1/1	0.77	0.14	87,87,87,87	0
56	MG	DA	3181	1/1	0.78	0.44	85,85,85,85	0
59	PUT	DA	3224	6/6	0.78	0.37	50,53,55,56	0
56	MG	DA	3175	1/1	0.78	0.42	97,97,97,97	0
57	PG4	DR	202	13/13	0.78	0.40	98,111,116,116	0
56	MG	AA	1602	1/1	0.78	0.39	81,81,81,81	0
56	MG	CA	3130	1/1	0.79	0.23	72,72,72,72	0
58	MPD	DT	201	8/8	0.79	0.39	111,114,115,115	0
59	PUT	DA	3215	6/6	0.79	0.42	83,90,96,98	0
58	MPD	DA	3004	8/8	0.79	0.37	106,109,119,121	0
63	PGE	DS	201	10/10	0.79	0.46	87,98,101,102	0
56	MG	AA	1664	1/1	0.79	0.45	225,225,225,225	0
56	MG	AA	1660	1/1	0.79	0.22	277,277,277,277	0
56	MG	CA	3076	1/1	0.80	0.15	163,163,163,163	0
56	MG	BA	1614	1/1	0.80	0.11	136,136,136,136	0
56	MG	AA	1621	1/1	0.80	0.34	69,69,69,69	0
61	PEG	DA	3220	7/7	0.80	0.35	136,137,139,139	0
62	EDO	DA	3003	4/4	0.80	0.51	97,98,98,98	0
56	MG	CA	3039	1/1	0.80	1.17	252,252,252,252	0
56	MG	DA	3133	1/1	0.80	0.29	68,68,68,68	0
59	PUT	DA	3223	6/6	0.80	0.66	118,122,122,123	0
56	MG	DA	3148	1/1	0.80	0.30	84,84,84,84	0
56	MG	CA	3006	1/1	0.80	0.10	144,144,144,144	0
56	MG	DA	3156	1/1	0.81	0.44	83,83,83,83	0
56	MG	BA	1602	1/1	0.81	0.07	90,90,90,90	0
56	MG	BA	1637	1/1	0.81	0.77	87,87,87,87	0
56	MG	CA	3149	1/1	0.81	0.46	76,76,76,76	0
61	PEG	DA	3202	7/7	0.81	0.56	87,88,91,91	0
56	MG	AA	1628	1/1	0.81	0.38	118,118,118,118	0
56	MG	AA	1609	1/1	0.81	0.30	84,84,84,84	0
56	MG	BA	1612	1/1	0.81	0.45	201,201,201,201	0
56	MG	DA	3132	1/1	0.81	0.24	78,78,78,78	0
56	MG	CA	3002	1/1	0.81	0.31	265,265,265,265	0
56	MG	AA	1627	1/1	0.81	0.40	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1678	1/1	0.81	0.14	59,59,59,59	0
59	PUT	AA	1672	6/6	0.82	0.36	79,82,85,85	0
56	MG	BA	1639	1/1	0.82	0.28	103,103,103,103	0
56	MG	CA	3114	1/1	0.82	0.29	51,51,51,51	0
56	MG	AA	1612	1/1	0.82	0.33	78,78,78,78	0
57	PG4	DS	202	13/13	0.82	0.43	67,78,83,83	0
56	MG	CB	201	1/1	0.83	0.07	157,157,157,157	0
61	PEG	DA	3203	7/7	0.83	0.62	84,88,95,96	0
56	MG	DA	3173	1/1	0.83	0.26	69,69,69,69	0
56	MG	DA	3157	1/1	0.83	0.15	69,69,69,69	0
62	EDO	DA	3005	4/4	0.83	0.30	104,105,107,110	0
62	EDO	DA	3217	4/4	0.83	0.28	84,85,86,87	0
56	MG	CA	3077	1/1	0.83	0.32	206,206,206,206	0
56	MG	CA	3092	1/1	0.83	0.14	195,195,195,195	0
56	MG	CA	3123	1/1	0.83	0.26	104,104,104,104	0
56	MG	DA	3169	1/1	0.83	0.94	95,95,95,95	0
56	MG	BA	1603	1/1	0.83	0.64	276,276,276,276	0
56	MG	BA	1640	1/1	0.84	0.32	118,118,118,118	0
56	MG	AA	1616	1/1	0.84	0.53	75,75,75,75	0
58	MPD	DA	3206	8/8	0.84	0.64	85,88,99,101	0
56	MG	CA	3019	1/1	0.84	0.16	62,62,62,62	0
59	PUT	AA	1673	6/6	0.84	0.50	110,110,112,112	0
56	MG	CA	3026	1/1	0.84	0.67	129,129,129,129	0
56	MG	DA	3185	1/1	0.84	0.33	70,70,70,70	0
57	PG4	AA	1670	13/13	0.84	0.32	74,86,104,104	0
56	MG	DA	3139	1/1	0.84	0.27	86,86,86,86	0
59	PUT	DA	3214	6/6	0.84	0.30	71,79,82,85	0
56	MG	CA	3063	1/1	0.84	0.13	103,103,103,103	0
56	MG	CA	3068	1/1	0.84	0.24	185,185,185,185	0
64	SPD	DA	3208	10/10	0.84	0.23	112,117,118,119	0
58	MPD	DE	302	8/8	0.84	0.68	91,94,97,97	0
56	MG	CA	3070	1/1	0.84	0.08	79,79,79,79	0
61	PEG	DA	3228	7/7	0.85	0.28	64,78,90,90	0
62	EDO	DB	210	4/4	0.85	0.29	95,95,96,97	0
56	MG	CA	3119	1/1	0.85	0.22	76,76,76,76	0
56	MG	CA	3120	1/1	0.85	0.41	168,168,168,168	0
62	EDO	DA	3211	4/4	0.85	0.39	103,104,104,106	0
56	MG	CA	3005	1/1	0.85	1.22	235,235,235,235	0
56	MG	CA	3057	1/1	0.85	0.16	121,121,121,121	0
56	MG	CA	3069	1/1	0.85	0.18	135,135,135,135	0
56	MG	BA	1606	1/1	0.85	0.22	273,273,273,273	0
64	SPD	DA	3186	10/10	0.85	0.49	84,87,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3048	1/1	0.85	0.09	97,97,97,97	0
56	MG	DA	3124	1/1	0.85	1.08	49,49,49,49	0
67	GUN	DA	3213	11/11	0.85	0.58	119,121,122,122	0
56	MG	DA	3125	1/1	0.85	0.45	81,81,81,81	0
56	MG	CA	3043	1/1	0.86	0.07	90,90,90,90	0
56	MG	DA	3136	1/1	0.86	0.33	87,87,87,87	0
56	MG	DA	3178	1/1	0.86	0.69	89,89,89,89	0
56	MG	CA	3137	1/1	0.86	0.48	117,117,117,117	0
56	MG	CA	3067	1/1	0.86	0.77	278,278,278,278	0
56	MG	CA	3045	1/1	0.86	0.12	110,110,110,110	0
62	EDO	DA	3210	4/4	0.86	0.27	88,88,89,89	0
56	MG	AA	1642	1/1	0.86	0.31	126,126,126,126	0
56	MG	CA	3150	1/1	0.86	0.97	89,89,89,89	0
57	PG4	BA	1642	13/13	0.86	0.42	77,87,100,100	0
56	MG	BA	1607	1/1	0.86	0.38	195,195,195,195	0
56	MG	CA	3054	1/1	0.86	0.09	105,105,105,105	0
56	MG	DA	3167	1/1	0.86	0.41	63,63,63,63	0
56	MG	BA	1634	1/1	0.86	0.07	199,199,199,199	0
56	MG	AA	1658	1/1	0.86	0.10	65,65,65,65	0
56	MG	AA	1620	1/1	0.86	0.30	67,67,67,67	0
56	MG	AA	1601	1/1	0.86	1.10	86,86,86,86	0
56	MG	AA	1608	1/1	0.87	0.48	87,87,87,87	0
57	PG4	DA	3196	13/13	0.87	0.93	90,94,96,97	0
65	1PE	DA	3205	16/16	0.87	0.33	77,84,87,88	0
56	MG	CA	3151	1/1	0.87	0.31	72,72,72,72	0
56	MG	DA	3174	1/1	0.87	0.49	90,90,90,90	0
56	MG	CA	3009	1/1	0.87	0.17	222,222,222,222	0
56	MG	DB	205	1/1	0.88	0.47	73,73,73,73	0
62	EDO	DB	211	4/4	0.88	0.31	98,99,99,100	0
56	MG	CA	3065	1/1	0.88	0.09	107,107,107,107	0
59	PUT	DA	3221	6/6	0.88	0.38	65,71,74,75	0
62	EDO	DA	3201	4/4	0.88	0.23	91,92,93,94	0
58	MPD	DA	3195	8/8	0.88	0.55	92,97,98,98	0
56	MG	CA	3128	1/1	0.88	0.23	81,81,81,81	0
58	MPD	DA	3209	8/8	0.88	0.42	90,94,98,98	0
58	MPD	DA	3212	8/8	0.88	0.28	83,85,86,90	0
61	PEG	DL	201	7/7	0.88	0.25	73,79,80,80	0
56	MG	CA	3062	1/1	0.88	0.28	232,232,232,232	0
63	PGE	DU	101	10/10	0.88	0.36	71,82,92,93	0
58	MPD	AA	1671	8/8	0.88	0.61	109,110,113,114	0
56	MG	CA	3115	1/1	0.88	0.23	77,77,77,77	0
56	MG	BA	1626	1/1	0.88	0.06	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MPD	DK	201	8/8	0.88	0.29	104,107,110,111	0
56	MG	CA	3104	1/1	0.88	0.10	196,196,196,196	0
61	PEG	DA	3229	7/7	0.88	0.33	79,83,88,88	0
56	MG	CA	3032	1/1	0.89	0.15	236,236,236,236	0
56	MG	DA	3127	1/1	0.89	0.24	60,60,60,60	0
56	MG	CA	3156	1/1	0.89	0.22	210,210,210,210	0
61	PEG	AL	201	7/7	0.89	0.29	87,91,98,100	0
56	MG	AA	1636	1/1	0.89	0.17	110,110,110,110	0
56	MG	AA	1655	1/1	0.89	0.20	214,214,214,214	0
56	MG	DB	209	1/1	0.89	0.53	71,71,71,71	0
56	MG	CA	3141	1/1	0.89	0.14	53,53,53,53	0
56	MG	AA	1624	1/1	0.90	0.61	107,107,107,107	0
56	MG	CA	3147	1/1	0.90	0.39	25,25,25,25	1
56	MG	AA	1666	1/1	0.90	0.06	97,97,97,97	0
58	MPD	DA	3193	8/8	0.90	0.33	89,91,93,93	0
56	MG	CA	3093	1/1	0.90	0.09	72,72,72,72	0
56	MG	AA	1613	1/1	0.90	0.90	64,64,64,64	0
56	MG	DA	3177	1/1	0.90	0.47	80,80,80,80	0
57	PG4	DA	3218	13/13	0.90	0.35	90,94,98,99	0
56	MG	CA	3073	1/1	0.90	0.21	175,175,175,175	0
56	MG	BA	1625	1/1	0.90	0.07	235,235,235,235	0
56	MG	CA	3108	1/1	0.90	0.18	65,65,65,65	0
56	MG	CA	3034	1/1	0.90	0.10	235,235,235,235	0
62	EDO	D1	101	4/4	0.91	0.18	61,62,64,66	0
56	MG	DA	3165	1/1	0.91	0.14	72,72,72,72	0
56	MG	DA	3143	1/1	0.91	0.39	51,51,51,51	0
62	EDO	DA	3002	4/4	0.91	0.30	78,79,79,79	0
63	PGE	DA	3219	10/10	0.91	0.35	85,88,91,91	0
56	MG	DA	3130	1/1	0.91	1.05	68,68,68,68	0
56	MG	DA	3149	1/1	0.91	0.09	123,123,123,123	0
56	MG	CA	3010	1/1	0.91	0.84	270,270,270,270	0
56	MG	CA	3145	1/1	0.91	0.18	60,60,60,60	0
56	MG	DA	3126	1/1	0.91	0.22	83,83,83,83	0
56	MG	AA	1654	1/1	0.91	0.20	244,244,244,244	0
56	MG	DA	3135	1/1	0.92	0.21	56,56,56,56	0
56	MG	AA	1605	1/1	0.92	0.73	91,91,91,91	0
56	MG	DA	3138	1/1	0.92	0.21	72,72,72,72	0
56	MG	CA	3112	1/1	0.92	0.24	65,65,65,65	0
56	MG	AA	1615	1/1	0.92	0.45	81,81,81,81	0
56	MG	DA	3145	1/1	0.92	0.22	63,63,63,63	0
56	MG	DA	3184	1/1	0.92	0.26	74,74,74,74	0
56	MG	CA	3044	1/1	0.92	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	PUT	DA	3191	6/6	0.92	0.24	48,54,57,59	0
59	PUT	DA	3192	6/6	0.92	0.26	44,49,50,50	0
56	MG	CA	3079	1/1	0.92	0.11	110,110,110,110	0
56	MG	CA	3080	1/1	0.92	0.27	143,143,143,143	0
56	MG	AA	1633	1/1	0.92	0.15	225,225,225,225	0
56	MG	CA	3046	1/1	0.92	0.13	116,116,116,116	0
56	MG	DB	208	1/1	0.92	0.29	56,56,56,56	0
56	MG	CA	3099	1/1	0.92	0.25	129,129,129,129	0
63	PGE	DD	301	10/10	0.92	0.24	86,89,95,96	0
56	MG	DA	3064	1/1	0.92	0.20	243,243,243,243	0
60	ZN	C5	101	1/1	0.92	0.09	155,155,155,155	0
63	PGE	DA	3216	10/10	0.92	0.41	68,72,83,84	0
56	MG	BA	1633	1/1	0.92	0.38	163,163,163,163	0
56	MG	BA	1605	1/1	0.92	0.08	206,206,206,206	0
56	MG	CB	203	1/1	0.92	0.06	125,125,125,125	0
56	MG	CA	3142	1/1	0.92	0.14	69,69,69,69	0
56	MG	BA	1636	1/1	0.92	0.44	97,97,97,97	0
56	MG	CA	3146	1/1	0.92	0.24	149,149,149,149	0
56	MG	AA	1610	1/1	0.92	0.28	85,85,85,85	0
56	MG	DR	201	1/1	0.93	0.30	30,30,30,30	0
56	MG	DA	3146	1/1	0.93	0.80	80,80,80,80	0
56	MG	CA	3121	1/1	0.93	0.15	60,60,60,60	0
56	MG	CA	3008	1/1	0.93	0.07	131,131,131,131	0
56	MG	AA	1640	1/1	0.93	0.10	60,60,60,60	0
59	PUT	DA	3187	6/6	0.93	0.22	49,51,53,54	0
56	MG	AA	1632	1/1	0.93	0.06	94,94,94,94	0
56	MG	CA	3125	1/1	0.93	0.23	97,97,97,97	0
56	MG	CA	3109	1/1	0.93	0.24	63,63,63,63	0
57	PG4	DQ	202	13/13	0.93	0.29	66,71,76,78	0
56	MG	DA	3161	1/1	0.93	0.16	119,119,119,119	0
56	MG	DA	3163	1/1	0.93	0.44	78,78,78,78	0
56	MG	DA	3164	1/1	0.93	0.24	62,62,62,62	0
56	MG	CA	3143	1/1	0.93	0.22	104,104,104,104	0
56	MG	AA	1611	1/1	0.93	0.12	91,91,91,91	0
56	MG	AA	1618	1/1	0.93	0.82	83,83,83,83	0
56	MG	CA	3049	1/1	0.93	0.13	56,56,56,56	0
56	MG	AA	1638	1/1	0.93	0.06	100,100,100,100	0
56	MG	BA	1631	1/1	0.93	0.07	63,63,63,63	0
56	MG	CA	3094	1/1	0.93	0.08	68,68,68,68	0
56	MG	AA	1659	1/1	0.93	0.09	61,61,61,61	0
56	MG	CA	3102	1/1	0.93	0.14	107,107,107,107	0
56	MG	CA	3155	1/1	0.93	0.23	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3176	1/1	0.93	0.41	92,92,92,92	0
56	MG	CA	3071	1/1	0.93	0.21	146,146,146,146	0
56	MG	CA	3148	1/1	0.94	0.44	50,50,50,50	1
56	MG	CA	3012	1/1	0.94	0.10	89,89,89,89	0
56	MG	DA	3087	1/1	0.94	0.14	49,49,49,49	0
56	MG	AA	1669	1/1	0.94	0.13	89,89,89,89	0
56	MG	BA	1627	1/1	0.94	0.39	142,142,142,142	0
56	MG	BA	1617	1/1	0.94	0.12	130,130,130,130	0
56	MG	BA	1610	1/1	0.94	0.08	130,130,130,130	0
58	MPD	AA	1676	8/8	0.94	0.42	87,90,96,97	0
56	MG	CA	3036	1/1	0.94	0.09	102,102,102,102	0
63	PGE	DA	3189	10/10	0.94	0.18	42,45,49,49	0
56	MG	CA	3064	1/1	0.94	0.48	274,274,274,274	0
56	MG	DA	3160	1/1	0.94	0.55	57,57,57,57	0
63	PGE	DA	3227	10/10	0.94	0.28	81,90,107,109	0
56	MG	BA	1644	1/1	0.94	0.13	64,64,64,64	0
56	MG	DA	3134	1/1	0.94	0.15	68,68,68,68	0
64	SPD	DA	3226	10/10	0.94	0.23	37,46,63,65	0
56	MG	DB	204	1/1	0.94	0.11	48,48,48,48	0
66	ACY	DA	3194	4/4	0.94	0.20	92,93,94,94	0
56	MG	CA	3066	1/1	0.94	0.09	129,129,129,129	0
56	MG	CA	3024	1/1	0.94	0.07	75,75,75,75	0
56	MG	CA	3090	1/1	0.94	0.15	118,118,118,118	0
62	EDO	DA	3197	4/4	0.95	0.27	52,57,59,60	0
62	EDO	DA	3200	4/4	0.95	0.20	53,54,54,55	0
56	MG	DA	3150	1/1	0.95	0.34	63,63,63,63	0
56	MG	CA	3072	1/1	0.95	0.66	274,274,274,274	0
59	PUT	DA	3225	6/6	0.95	0.21	61,62,70,72	0
56	MG	CA	3095	1/1	0.95	0.11	68,68,68,68	0
56	MG	BA	1611	1/1	0.95	0.09	80,80,80,80	0
56	MG	DA	3128	1/1	0.95	0.35	54,54,54,54	0
56	MG	CA	3074	1/1	0.95	0.24	131,131,131,131	0
56	MG	BA	1618	1/1	0.95	0.10	106,106,106,106	0
56	MG	BA	1623	1/1	0.95	0.14	166,166,166,166	0
56	MG	BA	1643	1/1	0.95	0.21	105,105,105,105	0
56	MG	BA	1624	1/1	0.95	0.14	157,157,157,157	0
56	MG	AA	1665	1/1	0.95	0.27	123,123,123,123	0
56	MG	DA	3054	1/1	0.95	0.18	190,190,190,190	0
56	MG	AA	1639	1/1	0.95	0.13	122,122,122,122	0
56	MG	DA	3072	1/1	0.95	0.08	86,86,86,86	0
56	MG	CA	3011	1/1	0.95	0.15	72,72,72,72	0
65	1PE	DA	3188	16/16	0.95	0.18	47,60,87,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3100	1/1	0.95	0.22	207,207,207,207	0
56	MG	DA	3172	1/1	0.95	0.22	57,57,57,57	0
56	MG	DA	3147	1/1	0.95	0.25	95,95,95,95	0
66	ACY	DA	3204	4/4	0.95	0.24	75,76,77,77	0
56	MG	DA	3122	1/1	0.95	0.29	76,76,76,76	0
56	MG	AA	1644	1/1	0.95	0.20	115,115,115,115	0
56	MG	DA	3113	1/1	0.96	0.16	280,280,280,280	0
56	MG	AA	1663	1/1	0.96	0.17	99,99,99,99	0
56	MG	DA	3123	1/1	0.96	0.13	78,78,78,78	0
56	MG	CA	3025	1/1	0.96	0.08	88,88,88,88	0
56	MG	AA	1645	1/1	0.96	0.11	61,61,61,61	0
56	MG	BA	1632	1/1	0.96	0.10	85,85,85,85	0
56	MG	CA	3003	1/1	0.96	0.85	258,258,258,258	0
56	MG	CA	3082	1/1	0.96	0.14	90,90,90,90	0
56	MG	CA	3153	1/1	0.96	0.21	58,58,58,58	0
56	MG	DA	3131	1/1	0.96	0.23	79,79,79,79	0
56	MG	CA	3084	1/1	0.96	0.24	181,181,181,181	0
56	MG	CA	3087	1/1	0.96	0.08	65,65,65,65	0
56	MG	CA	3089	1/1	0.96	0.19	54,54,54,54	0
56	MG	CA	3004	1/1	0.96	0.07	83,83,83,83	0
59	PUT	DM	201	6/6	0.96	0.24	49,50,53,56	0
56	MG	CA	3091	1/1	0.96	0.11	71,71,71,71	0
56	MG	CA	3017	1/1	0.96	0.08	97,97,97,97	0
56	MG	CA	3138	1/1	0.96	0.05	74,74,74,74	0
56	MG	DA	3140	1/1	0.96	0.33	43,43,43,43	1
56	MG	DA	3180	1/1	0.96	0.51	54,54,54,54	0
56	MG	DB	207	1/1	0.96	0.66	84,84,84,84	0
56	MG	BA	1613	1/1	0.96	0.21	112,112,112,112	0
56	MG	CA	3037	1/1	0.96	0.15	107,107,107,107	0
56	MG	DA	3014	1/1	0.96	0.17	122,122,122,122	0
56	MG	DA	3017	1/1	0.96	0.12	60,60,60,60	0
56	MG	AA	1641	1/1	0.96	0.07	65,65,65,65	0
60	ZN	AB	301	1/1	0.96	0.07	141,141,141,141	0
56	MG	AA	1661	1/1	0.96	0.17	178,178,178,178	0
56	MG	CA	3100	1/1	0.96	0.17	90,90,90,90	0
56	MG	DA	3155	1/1	0.96	0.43	73,73,73,73	0
56	MG	AA	1667	1/1	0.96	0.09	42,42,42,42	0
56	MG	DA	3094	1/1	0.96	0.14	36,36,36,36	0
56	MG	DA	3099	1/1	0.96	0.09	31,31,31,31	0
56	MG	DA	3159	1/1	0.96	0.14	70,70,70,70	0
56	MG	CA	3103	1/1	0.96	0.11	82,82,82,82	0
56	MG	DA	3065	1/1	0.97	0.12	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3067	1/1	0.97	0.16	26,26,26,26	0
56	MG	AA	1656	1/1	0.97	0.12	95,95,95,95	0
56	MG	DA	3076	1/1	0.97	0.09	39,39,39,39	0
56	MG	DA	3082	1/1	0.97	0.13	173,173,173,173	0
56	MG	DA	3083	1/1	0.97	0.10	46,46,46,46	0
56	MG	DA	3084	1/1	0.97	0.04	75,75,75,75	0
56	MG	CA	3097	1/1	0.97	0.09	109,109,109,109	0
56	MG	CA	3056	1/1	0.97	0.13	66,66,66,66	0
56	MG	DA	3096	1/1	0.97	0.13	19,19,19,19	0
56	MG	BA	1608	1/1	0.97	0.17	114,114,114,114	0
56	MG	AA	1647	1/1	0.97	0.12	157,157,157,157	0
56	MG	DA	3109	1/1	0.97	0.17	34,34,34,34	0
56	MG	AA	1630	1/1	0.97	0.11	102,102,102,102	0
56	MG	DA	3121	1/1	0.97	0.30	64,64,64,64	0
56	MG	CA	3078	1/1	0.97	0.08	133,133,133,133	0
56	MG	CA	3040	1/1	0.97	0.07	85,85,85,85	0
56	MG	CA	3015	1/1	0.97	0.17	48,48,48,48	0
56	MG	CA	3107	1/1	0.97	0.29	65,65,65,65	0
56	MG	CA	3016	1/1	0.97	0.54	150,150,150,150	0
56	MG	CA	3083	1/1	0.97	0.09	136,136,136,136	0
56	MG	DD	302	1/1	0.97	0.22	41,41,41,41	0
56	MG	DA	3129	1/1	0.97	0.28	64,64,64,64	0
56	MG	CA	3029	1/1	0.97	0.14	166,166,166,166	0
56	MG	DB	201	1/1	0.97	0.10	56,56,56,56	0
56	MG	CA	3085	1/1	0.97	0.07	56,56,56,56	0
56	MG	AA	1634	1/1	0.97	0.22	163,163,163,163	0
56	MG	BA	1621	1/1	0.97	0.18	29,29,29,29	0
56	MG	CA	3033	1/1	0.97	0.07	79,79,79,79	0
56	MG	BA	1601	1/1	0.97	0.24	158,158,158,158	0
56	MG	DA	3137	1/1	0.97	0.06	96,96,96,96	0
56	MG	CA	3052	1/1	0.97	0.11	60,60,60,60	0
56	MG	CA	3117	1/1	0.97	0.35	76,76,76,76	0
56	MG	CA	3118	1/1	0.97	0.23	47,47,47,47	0
56	MG	DA	3032	1/1	0.97	0.20	47,47,47,47	0
56	MG	DA	3144	1/1	0.97	0.26	72,72,72,72	0
56	MG	CA	3053	1/1	0.97	0.12	58,58,58,58	0
56	MG	CA	3035	1/1	0.97	0.17	83,83,83,83	0
56	MG	DA	3070	1/1	0.98	0.17	37,37,37,37	0
56	MG	DA	3153	1/1	0.98	0.19	33,33,33,33	0
56	MG	AA	1635	1/1	0.98	0.14	119,119,119,119	0
56	MG	DA	3074	1/1	0.98	0.25	53,53,53,53	0
56	MG	AA	1657	1/1	0.98	0.18	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3078	1/1	0.98	0.11	32,32,32,32	0
56	MG	DA	3081	1/1	0.98	0.25	130,130,130,130	0
56	MG	AA	1629	1/1	0.98	0.17	99,99,99,99	0
56	MG	CA	3096	1/1	0.98	0.05	97,97,97,97	0
56	MG	BA	1619	1/1	0.98	0.12	70,70,70,70	0
56	MG	DA	3162	1/1	0.98	0.11	67,67,67,67	0
56	MG	CA	3098	1/1	0.98	0.07	91,91,91,91	0
56	MG	DA	3089	1/1	0.98	0.17	32,32,32,32	0
56	MG	DA	3091	1/1	0.98	0.20	30,30,30,30	0
56	MG	BA	1620	1/1	0.98	0.10	115,115,115,115	0
56	MG	CA	3027	1/1	0.98	0.15	61,61,61,61	0
56	MG	DA	3097	1/1	0.98	0.15	106,106,106,106	0
56	MG	CA	3101	1/1	0.98	0.09	71,71,71,71	0
56	MG	CA	3050	1/1	0.98	0.07	51,51,51,51	0
56	MG	DA	3102	1/1	0.98	0.16	29,29,29,29	0
56	MG	DA	3103	1/1	0.98	0.15	50,50,50,50	0
56	MG	AA	1648	1/1	0.98	0.05	77,77,77,77	0
56	MG	AA	1677	1/1	0.98	0.08	155,155,155,155	0
56	MG	DA	3116	1/1	0.98	0.09	40,40,40,40	0
56	MG	DA	3119	1/1	0.98	0.14	82,82,82,82	0
56	MG	DA	3120	1/1	0.98	0.10	48,48,48,48	0
56	MG	CA	3030	1/1	0.98	0.07	84,84,84,84	0
56	MG	AA	1650	1/1	0.98	0.10	87,87,87,87	0
56	MG	AA	1651	1/1	0.98	0.05	68,68,68,68	0
56	MG	AA	1662	1/1	0.98	0.20	89,89,89,89	0
56	MG	DA	3182	1/1	0.98	0.46	109,109,109,109	0
56	MG	CA	3058	1/1	0.98	0.09	87,87,87,87	0
56	MG	CA	3013	1/1	0.98	0.17	123,123,123,123	0
56	MG	AA	1607	1/1	0.98	0.63	90,90,90,90	0
56	MG	DA	3232	1/1	0.98	0.23	30,30,30,30	0
56	MG	BA	1628	1/1	0.98	0.06	70,70,70,70	0
56	MG	DA	3007	1/1	0.98	0.13	77,77,77,77	0
56	MG	DA	3009	1/1	0.98	0.07	82,82,82,82	0
56	MG	CA	3086	1/1	0.98	0.05	74,74,74,74	0
56	MG	CB	202	1/1	0.98	0.05	100,100,100,100	0
56	MG	DA	3025	1/1	0.98	0.19	26,26,26,26	0
56	MG	DA	3028	1/1	0.98	0.07	83,83,83,83	0
56	MG	BA	1629	1/1	0.98	0.55	144,144,144,144	0
56	MG	DA	3035	1/1	0.98	0.14	22,22,22,22	0
56	MG	DA	3039	1/1	0.98	0.23	21,21,21,21	0
56	MG	DA	3045	1/1	0.98	0.14	41,41,41,41	0
56	MG	DA	3046	1/1	0.98	0.04	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3049	1/1	0.98	0.12	48,48,48,48	0
58	MPD	DS	203	8/8	0.98	0.23	55,56,58,61	0
64	SPD	DA	3190	10/10	0.98	0.22	38,46,49,53	0
56	MG	DA	3141	1/1	0.98	0.19	57,57,57,57	0
56	MG	DA	3142	1/1	0.98	0.21	74,74,74,74	0
56	MG	DA	3051	1/1	0.98	0.14	46,46,46,46	0
56	MG	CA	3018	1/1	0.98	0.11	125,125,125,125	0
56	MG	DA	3056	1/1	0.98	0.13	151,151,151,151	0
56	MG	AA	1631	1/1	0.98	0.06	43,43,43,43	0
56	MG	CA	3144	1/1	0.98	0.05	60,60,60,60	0
56	MG	BA	1615	1/1	0.98	0.10	65,65,65,65	0
56	MG	DA	3069	1/1	0.98	0.15	42,42,42,42	0
56	MG	AA	1646	1/1	0.99	0.06	57,57,57,57	0
56	MG	DM	202	1/1	0.99	0.05	43,43,43,43	0
56	MG	DA	3040	1/1	0.99	0.11	20,20,20,20	0
56	MG	DA	3042	1/1	0.99	0.06	56,56,56,56	0
56	MG	DA	3043	1/1	0.99	0.18	13,13,13,13	0
56	MG	DA	3044	1/1	0.99	0.13	29,29,29,29	0
56	MG	AA	1637	1/1	0.99	0.08	43,43,43,43	0
56	MG	CA	3051	1/1	0.99	0.08	52,52,52,52	0
56	MG	DA	3047	1/1	0.99	0.07	61,61,61,61	0
56	MG	DA	3048	1/1	0.99	0.12	36,36,36,36	0
56	MG	DB	203	1/1	0.99	0.12	34,34,34,34	0
56	MG	AA	1652	1/1	0.99	0.22	30,30,30,30	0
56	MG	DA	3052	1/1	0.99	0.14	29,29,29,29	0
56	MG	DA	3053	1/1	0.99	0.13	22,22,22,22	0
56	MG	CA	3081	1/1	0.99	0.12	82,82,82,82	0
56	MG	DA	3055	1/1	0.99	0.09	40,40,40,40	0
56	MG	CA	3020	1/1	0.99	0.16	60,60,60,60	0
56	MG	DA	3057	1/1	0.99	0.23	30,30,30,30	0
56	MG	DA	3058	1/1	0.99	0.14	38,38,38,38	0
56	MG	DA	3059	1/1	0.99	0.13	27,27,27,27	0
56	MG	DA	3060	1/1	0.99	0.10	31,31,31,31	0
56	MG	DA	3061	1/1	0.99	0.08	33,33,33,33	0
56	MG	DA	3063	1/1	0.99	0.16	36,36,36,36	0
56	MG	CA	3041	1/1	0.99	0.08	62,62,62,62	0
56	MG	CA	3042	1/1	0.99	0.12	87,87,87,87	0
56	MG	DA	3066	1/1	0.99	0.08	44,44,44,44	0
56	MG	BA	1622	1/1	0.99	0.07	104,104,104,104	0
56	MG	DA	3068	1/1	0.99	0.16	37,37,37,37	0
56	MG	DA	3001	1/1	0.99	0.13	25,25,25,25	0
56	MG	DA	3006	1/1	0.99	0.09	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	1653	1/1	0.99	0.08	67,67,67,67	0
56	MG	DA	3151	1/1	0.99	0.09	41,41,41,41	0
60	ZN	D5	101	1/1	0.99	0.15	56,56,56,56	0
56	MG	DA	3073	1/1	0.99	0.06	49,49,49,49	0
56	MG	DA	3008	1/1	0.99	0.10	77,77,77,77	0
56	MG	DA	3075	1/1	0.99	0.10	23,23,23,23	0
56	MG	AA	1643	1/1	0.99	0.17	69,69,69,69	0
56	MG	DA	3010	1/1	0.99	0.05	74,74,74,74	0
56	MG	DA	3079	1/1	0.99	0.06	31,31,31,31	0
56	MG	DA	3080	1/1	0.99	0.06	50,50,50,50	0
56	MG	DA	3011	1/1	0.99	0.12	20,20,20,20	0
56	MG	DA	3013	1/1	0.99	0.09	33,33,33,33	0
56	MG	CA	3088	1/1	0.99	0.06	78,78,78,78	0
56	MG	CA	3059	1/1	0.99	0.09	70,70,70,70	0
56	MG	DA	3085	1/1	0.99	0.06	52,52,52,52	0
56	MG	DA	3018	1/1	0.99	0.10	69,69,69,69	0
56	MG	DA	3088	1/1	0.99	0.11	36,36,36,36	0
56	MG	DA	3020	1/1	0.99	0.10	42,42,42,42	0
56	MG	DA	3090	1/1	0.99	0.06	52,52,52,52	0
56	MG	DA	3021	1/1	0.99	0.24	9,9,9,9	0
56	MG	DA	3092	1/1	0.99	0.13	23,23,23,23	0
56	MG	DA	3093	1/1	0.99	0.15	23,23,23,23	0
56	MG	DA	3022	1/1	0.99	0.10	43,43,43,43	0
56	MG	DA	3095	1/1	0.99	0.19	26,26,26,26	0
56	MG	DA	3023	1/1	0.99	0.13	22,22,22,22	0
56	MG	DA	3024	1/1	0.99	0.14	28,28,28,28	0
56	MG	AA	1649	1/1	0.99	0.05	57,57,57,57	0
56	MG	DA	3026	1/1	0.99	0.20	33,33,33,33	0
56	MG	DA	3101	1/1	0.99	0.16	22,22,22,22	0
56	MG	AA	1668	1/1	0.99	0.11	58,58,58,58	0
56	MG	DA	3029	1/1	0.99	0.20	48,48,48,48	0
56	MG	DA	3104	1/1	0.99	0.10	37,37,37,37	0
56	MG	DA	3105	1/1	0.99	0.13	38,38,38,38	0
56	MG	DA	3107	1/1	0.99	0.17	25,25,25,25	0
56	MG	DA	3108	1/1	0.99	0.17	37,37,37,37	0
56	MG	DA	3030	1/1	0.99	0.10	55,55,55,55	0
56	MG	DA	3230	1/1	0.99	0.05	53,53,53,53	0
56	MG	DA	3231	1/1	0.99	0.06	46,46,46,46	0
56	MG	DA	3110	1/1	0.99	0.09	32,32,32,32	0
56	MG	DA	3111	1/1	0.99	0.14	32,32,32,32	0
56	MG	DA	3112	1/1	0.99	0.15	35,35,35,35	0
56	MG	DA	3031	1/1	0.99	0.16	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3115	1/1	0.99	0.10	81,81,81,81	0
56	MG	BA	1635	1/1	0.99	0.09	106,106,106,106	0
56	MG	DA	3117	1/1	0.99	0.17	36,36,36,36	0
56	MG	DA	3034	1/1	0.99	0.16	22,22,22,22	0
56	MG	DA	3106	1/1	1.00	0.17	25,25,25,25	0
56	MG	DA	3036	1/1	1.00	0.12	28,28,28,28	0
56	MG	DA	3037	1/1	1.00	0.17	29,29,29,29	0
56	MG	DA	3038	1/1	1.00	0.17	20,20,20,20	0
56	MG	DA	3062	1/1	1.00	0.14	28,28,28,28	0
56	MG	DA	3077	1/1	1.00	0.15	42,42,42,42	0
56	MG	DA	3152	1/1	1.00	0.12	53,53,53,53	0
56	MG	DA	3050	1/1	1.00	0.12	25,25,25,25	0
56	MG	DA	3012	1/1	1.00	0.14	31,31,31,31	0
56	MG	DA	3114	1/1	1.00	0.17	27,27,27,27	0
56	MG	DA	3019	1/1	1.00	0.17	17,17,17,17	0
56	MG	DA	3041	1/1	1.00	0.12	23,23,23,23	0
56	MG	DA	3098	1/1	1.00	0.13	32,32,32,32	0
56	MG	DA	3118	1/1	1.00	0.12	45,45,45,45	0
56	MG	DA	3015	1/1	1.00	0.21	22,22,22,22	0
56	MG	DA	3016	1/1	1.00	0.13	13,13,13,13	0
56	MG	DA	3033	1/1	1.00	0.17	26,26,26,26	0
56	MG	DA	3027	1/1	1.00	0.10	43,43,43,43	0
56	MG	DA	3086	1/1	1.00	0.11	30,30,30,30	0
56	MG	DA	3071	1/1	1.00	0.11	50,50,50,50	0
56	MG	DB	202	1/1	1.00	0.08	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.