Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 05:35 am GMT

PDB ID	:	4V5F
Title	:	The structure of the ribosome with elongation factor G trapped in the post-translocational state
Authors	:	Gao, Y.-G.; Selmer, M.; Dunham, C.M.; Weixlbaumer, A.; Kelley, A.C.; Ramakrishnan, V.
Deposited on	:	2009-09-01
Resolution	:	3.60 Å(reported)

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

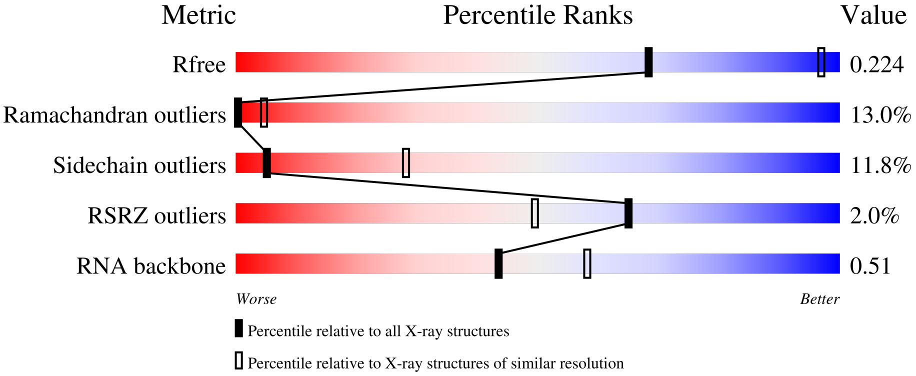
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

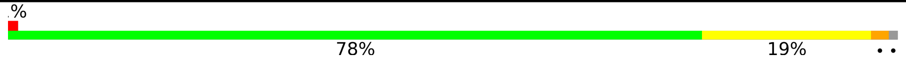
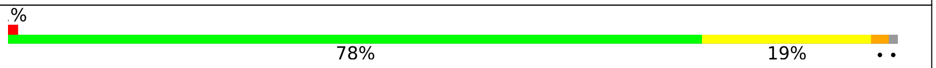
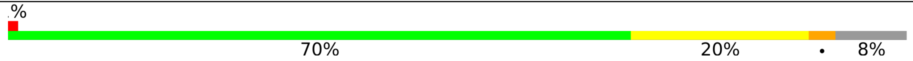
The reported resolution of this entry is 3.60 Å.

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	1257 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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	1522	
1	CA	1522	
2	AB	256	
2	CB	256	

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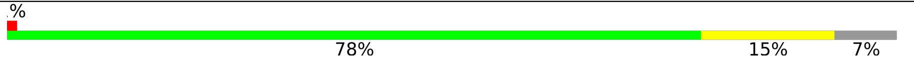
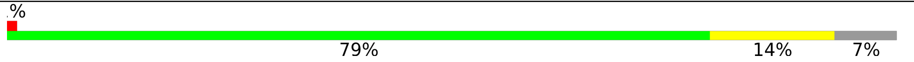
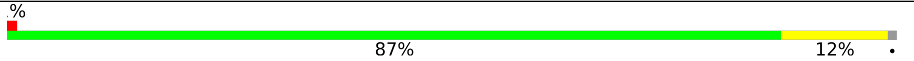
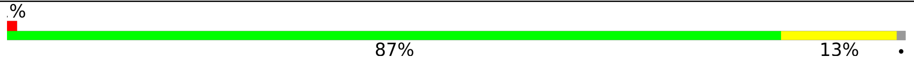
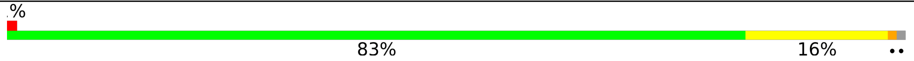
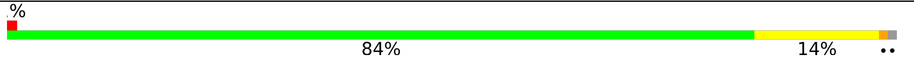
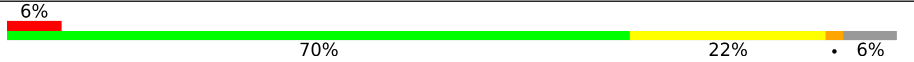
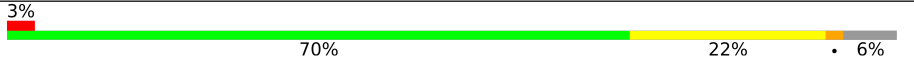
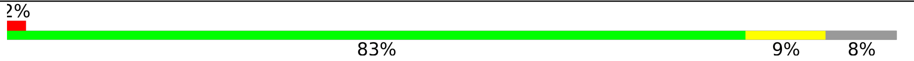
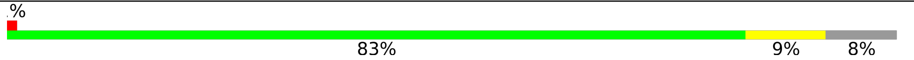
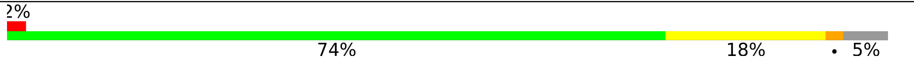
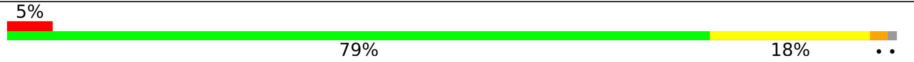
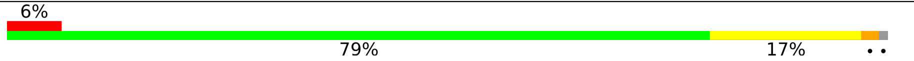
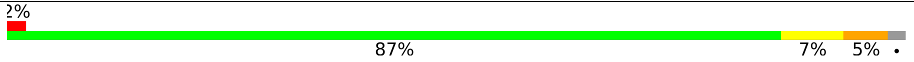
Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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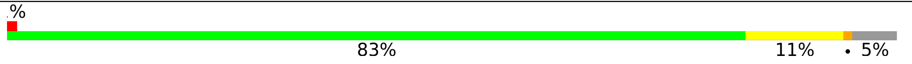
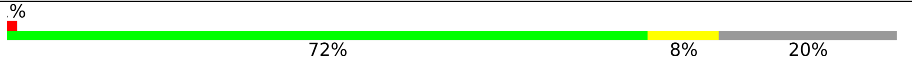
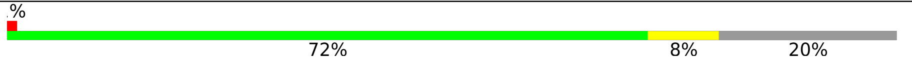
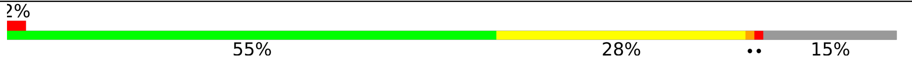
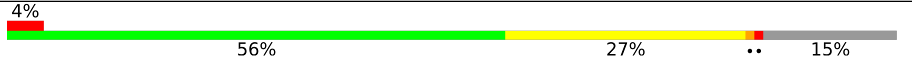
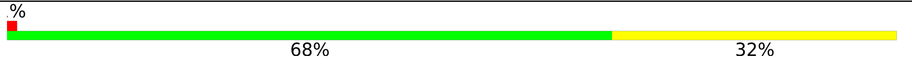
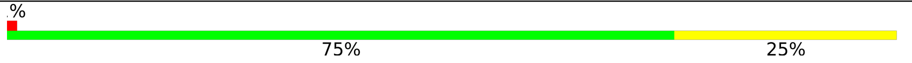
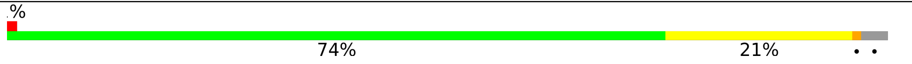
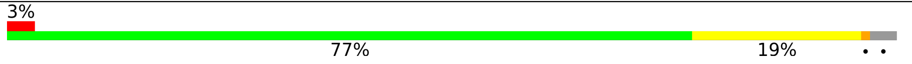
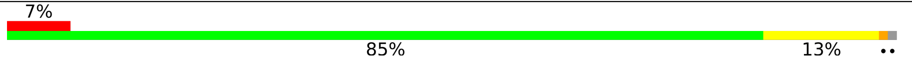
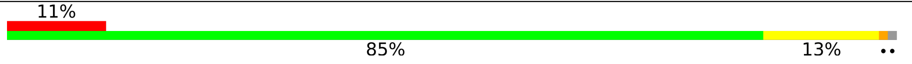
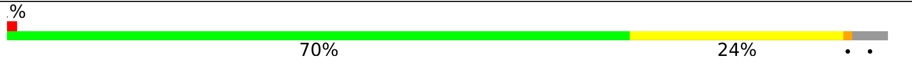
Mol	Chain	Length	Quality of chain
15	CO	89	 80% 19% •
16	AP	88	 83% 11% • 5%
16	CP	88	 % 83% 11% • 5%
17	AQ	105	 84% 11% 5%
17	CQ	105	 85% 10% 5%
18	AR	88	 % 72% 8% 20%
18	CR	88	 % 72% 8% 20%
19	AS	93	 2% 55% 28% •• 15%
19	CS	93	 4% 56% 27% •• 15%
20	AT	106	 74% 19% • 7%
20	CT	106	 74% 19% • 7%
21	AU	27	 81% 11% 7%
21	CU	27	 78% 15% 7%
22	AV	77	 79% 18% •
22	AW	77	 % 68% 32%
22	CV	77	 82% 17% •
22	CW	77	 % 75% 25%
23	AX	25	 20% 20% • 56%
23	CX	25	 24% 16% • 56%
24	AY	691	 % 74% 21% • •
24	CY	691	 3% 77% 19% • •
25	B0	85	 7% 85% 13% ••
25	D0	85	 11% 85% 13% ••
26	B1	98	 % 70% 24% • •
26	D1	98	 77% 18% • •

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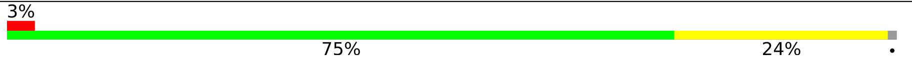
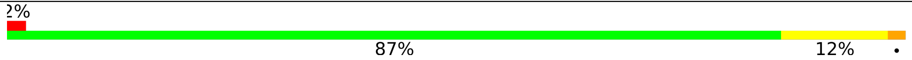
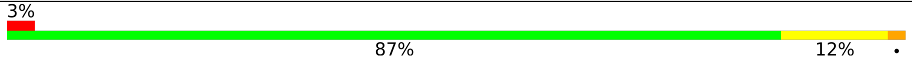
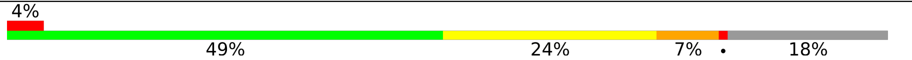
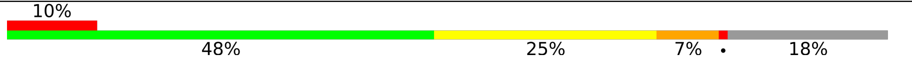
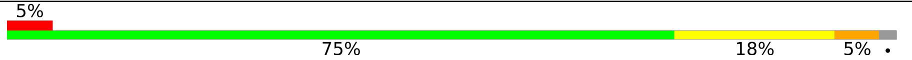
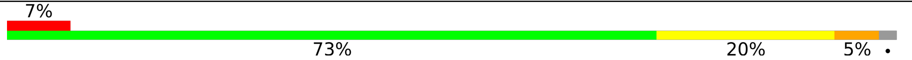
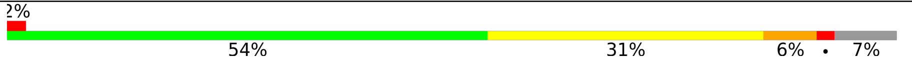
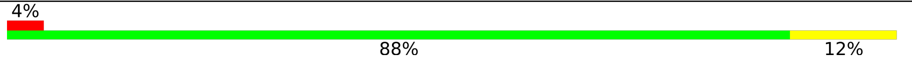
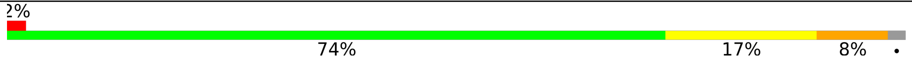
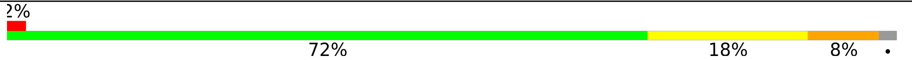
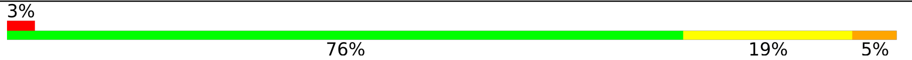
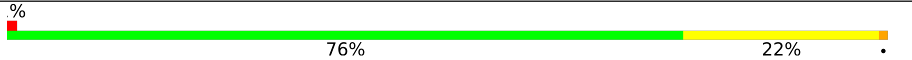
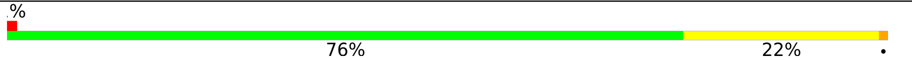
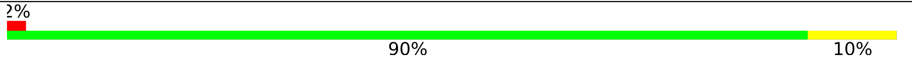
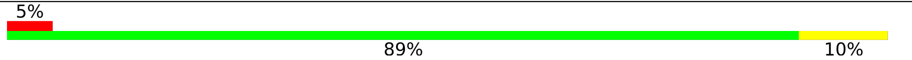
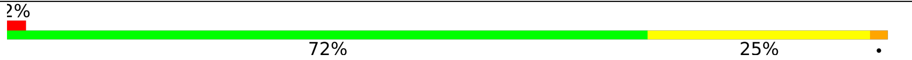
Mol	Chain	Length	Quality of chain
27	B2	72	
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2915	
35	DA	2915	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	

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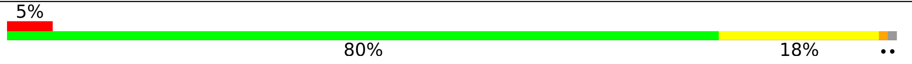
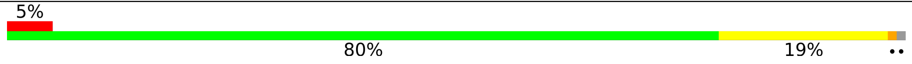
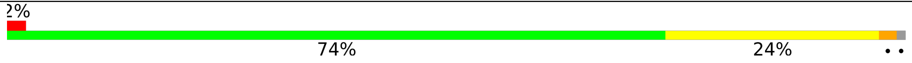
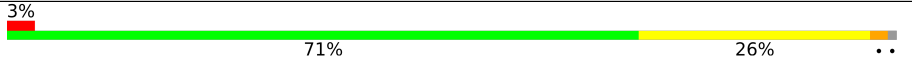
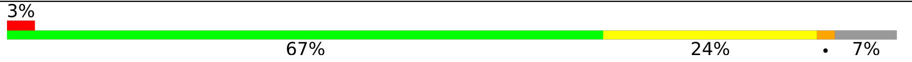
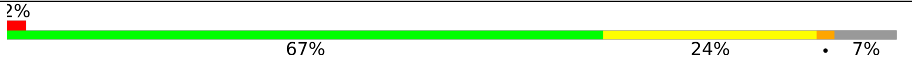
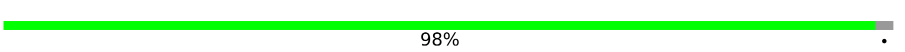
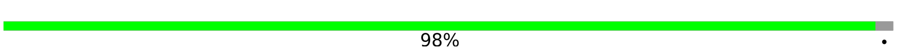
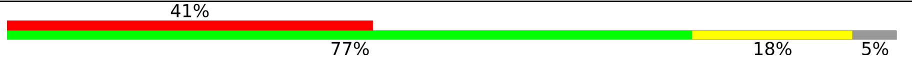
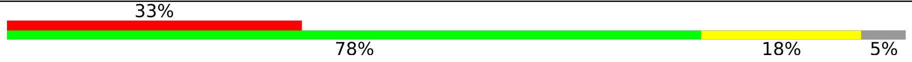
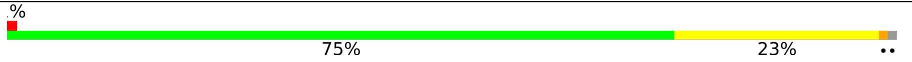
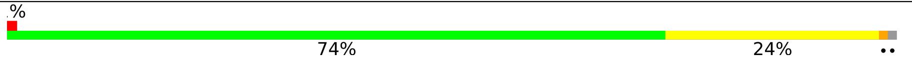
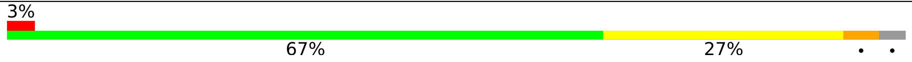
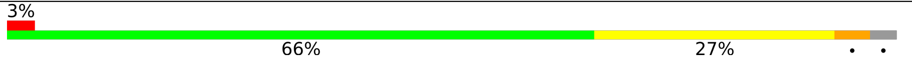
Mol	Chain	Length	Quality of chain
39	DE	206	
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BJ	173	
43	DJ	173	
44	BK	147	
44	DK	147	
45	BL	125	
45	BM	125	
45	Bl	125	
45	Bm	125	
45	DL	125	
45	DM	125	
45	Dl	125	
45	Dm	125	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	

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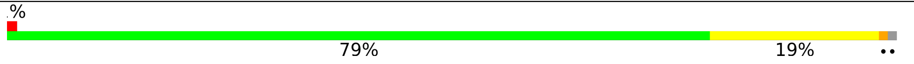
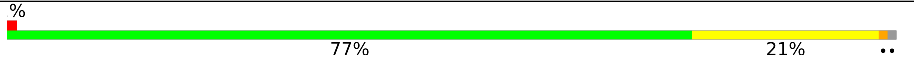
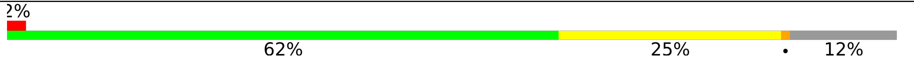
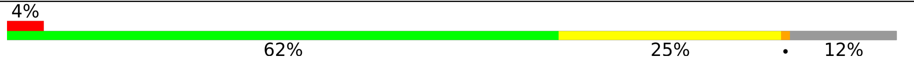
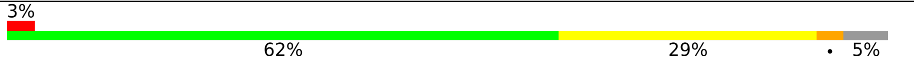
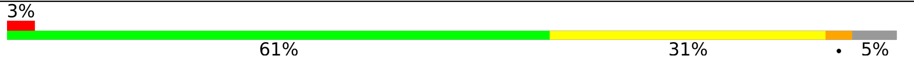
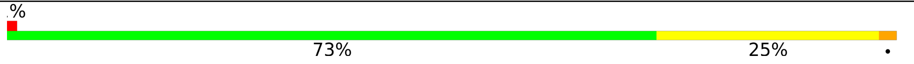
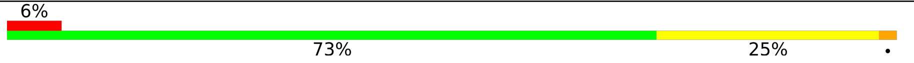
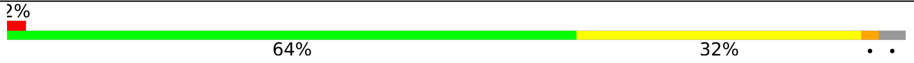
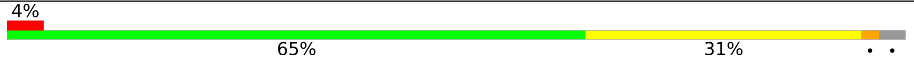
Mol	Chain	Length	Quality of chain
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	
52	BT	146	
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 311552 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	AE	151	Total C N O S 1147 724 218 201 4	0	0	1
5	CE	151	Total C N O S 1147 724 218 201 4	0	0	1

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	AF	101	Total C N O S 843 531 155 154 3	0	0	0
6	CF	101	Total C N O S 843 531 155 154 3	0	0	0

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	AG	155	Total C N O S 1257 781 252 218 6	0	0	0
7	CG	155	Total C N O S 1257 781 252 218 6	0	0	0

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	AH	138	Total C N O S 1116 705 215 193 3	0	0	0
8	CH	138	Total C N O S 1116 705 215 193 3	0	0	0

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	AI	127	Total C N O 1010 639 197 174	0	0	0
9	CI	127	Total C N O 1010 639 197 174	0	0	0

- 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 795 499 157 138 1	0	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total 795	C 499	N 157	O 138	S 1	0	0	1

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total 885	C 549	N 168	O 165	S 3	0	0	0
11	CK	119	Total 885	C 549	N 168	O 165	S 3	0	0	0

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total 971	C 611	N 196	O 163	S 1	0	0	1
12	CL	125	Total 971	C 611	N 196	O 163	S 1	0	0	1

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total 988	C 611	N 206	O 169	S 2	0	0	1
13	CM	125	Total 988	C 611	N 206	O 169	S 2	0	0	1

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total 492	C 312	N 104	O 72	S 4	0	0	0
14	CN	60	Total 492	C 312	N 104	O 72	S 4	0	0	0

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total 734	C 459	N 147	O 126	S 2	0	0	0
15	CO	88	Total 734	C 459	N 147	O 126	S 2	0	0	0

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	AP	84	Total C N O S 701 443 140 117 1	0	0	1
16	CP	84	Total C N O S 701 443 140 117 1	0	0	1

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	AQ	100	Total C N O S 824 528 152 142 2	0	0	1
17	CQ	100	Total C N O S 824 528 152 142 2	0	0	1

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	AR	70	Total C N O 574 367 112 95	0	0	0
18	CR	70	Total C N O 574 367 112 95	0	0	0

- 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 630 403 115 110 2	0	0	1
19	CS	79	Total C N O S 630 403 115 110 2	0	0	1

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	AT	99	Total C N O S 763 470 162 129 2	0	0	0
20	CT	99	Total C N O S 763 470 162 129 2	0	0	0

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	AU	25	Total C N O 209 128 51 30	0	0	1
21	CU	25	Total C N O 209 128 51 30	0	0	1

- Molecule 22 is a RNA chain called E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	AV	77	Total C N O P 1640 732 297 535 76	0	0	0
22	AW	77	Total C N O P 1640 732 297 535 76	0	0	0
22	CV	77	Total C N O P 1640 732 297 535 76	0	0	0
22	CW	77	Total C N O P 1640 732 297 535 76	0	0	0

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	AX	11	Total C N O P 230 105 41 74 10	0	0	0
23	CX	11	Total C N O P 230 105 41 74 10	0	0	0

- Molecule 24 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	AY	667	Total C N O S 5215 3316 893 988 18	0	0	1
24	CY	667	Total C N O S 5215 3316 893 988 18	0	0	1

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	B0	84	Total C N O S 662 410 140 111 1	0	0	0
25	D0	84	Total C N O S 662 410 140 111 1	0	0	0

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	B1	94	Total C N O S 732 460 146 125 1	0	0	1
26	D1	94	Total C N O S 732 460 146 125 1	0	0	1

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	B2	71	Total C N O S 598 370 121 106 1	0	0	0
27	D2	71	Total C N O S 598 370 121 106 1	0	0	0

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	B3	60	Total C N O S 468 298 91 78 1	0	0	1
28	D3	60	Total C N O S 468 298 91 78 1	0	0	1

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	B4	58	Total C N O S 451 285 78 83 5	0	0	1
29	D4	58	Total C N O S 451 285 78 83 5	0	0	1

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	B5	59	Total C N O S 459 288 90 76 5	0	0	0
30	D5	59	Total C N O S 459 288 90 76 5	0	0	0

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	B6	50	Total C N O S 433 270 88 71 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	D6	50	433	270	88	71	4	0	0	0

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	B7	49	419	257	105	55	2	0	0	1
32	D7	49	419	257	105	55	2	0	0	1

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	B8	64	508	326	102	78	2	0	0	1
33	D8	64	508	326	102	78	2	0	0	1

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	B9	37	307	188	68	47	4	0	0	0
34	D9	37	307	188	68	47	4	0	0	0

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
35	BA	2901	62474	27806	11681	20087	2900	0	0	0
35	DA	2901	62474	27806	11681	20087	2900	0	0	0

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
36	BB	119	2551	1136	471	826	118	0	0	0
36	DB	119	2551	1136	471	826	118	0	0	0

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
37	BC	228	Total C N O S 1742 1101 319 319 3	0	0	0
37	DC	228	Total C N O S 1742 1101 319 319 3	0	0	0

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
38	BD	275	Total C N O S 2145 1353 428 361 3	0	0	0
38	DD	275	Total C N O S 2145 1353 428 361 3	0	0	0

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
39	BE	205	Total C N O S 1564 988 300 270 6	0	0	1
39	DE	205	Total C N O S 1564 988 300 270 6	0	0	1

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
40	BF	208	Total C N O S 1624 1035 304 282 3	0	0	1
40	DF	208	Total C N O S 1624 1035 304 282 3	0	0	1

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
41	BG	181	Total C N O S 1474 942 268 260 4	0	0	0
41	DG	181	Total C N O S 1474 942 268 260 4	0	0	0

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	BH	167	1269	803	238	227	1	0	0	1
42	DH	167	1269	803	238	227	1	0	0	1

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
43	BJ	170	851	510	170	171	0	0	0
43	DJ	170	851	510	170	171	0	0	0

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	BK	140	1026	653	182	186	5	0	0	1
44	DK	140	1026	653	182	186	5	0	0	1

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
45	BL	102	506	303	102	101	0	0	1
45	BM	31	151	90	31	30	0	0	1
45	Bl	31	151	90	31	30	0	0	1
45	Bm	30	146	87	30	29	0	0	1
45	DL	102	506	303	102	101	0	0	1
45	DM	31	151	90	31	30	0	0	1
45	Dl	31	151	90	31	30	0	0	1
45	Dm	30	146	87	30	29	0	0	1

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	139	Total 1105	C 712	N 207	O 182	S 4	0	0	1
46	DN	139	Total 1105	C 712	N 207	O 182	S 4	0	0	1

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	122	Total 933	C 588	N 171	O 170	S 4	0	0	0
47	DO	122	Total 933	C 588	N 171	O 170	S 4	0	0	0

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	146	Total 1114	C 692	N 227	O 193	S 2	0	0	0
48	DP	146	Total 1114	C 692	N 227	O 193	S 2	0	0	0

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	141	Total 1122	C 715	N 212	O 188	S 7	0	0	0
49	DQ	141	Total 1122	C 715	N 212	O 188	S 7	0	0	0

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BR	117	Total 960	C 599	N 202	O 159	0	0	0
50	DR	117	Total 960	C 599	N 202	O 159	0	0	0

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BS	99	Total 771	C 486	N 155	O 130	0	0	1

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
51	DS	99	771	486	155	130	0	0	1

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	BT	138	1142	710	235	196	1	0	0	1
52	DT	138	1142	710	235	196	1	0	0	1

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	BU	117	958	604	202	151	1	0	0	0
53	DU	117	958	604	202	151	1	0	0	0

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	BV	101	779	501	142	135	1	0	0	0
54	DV	101	779	501	142	135	1	0	0	0

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	BW	113	896	563	176	155	2	0	0	0
55	DW	113	896	563	176	155	2	0	0	0

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
56	BX	93	726	471	132	123	0	0	1
56	DX	93	726	471	132	123	0	0	1

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	107	Total 811	C 520	N 155	O 131	S 5	0	0	1
57	DY	107	Total 811	C 520	N 155	O 131	S 5	0	0	1

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	185	Total 1468	C 936	N 262	O 268	S 2	0	0	1
58	DZ	185	Total 1468	C 936	N 262	O 268	S 2	0	0	1

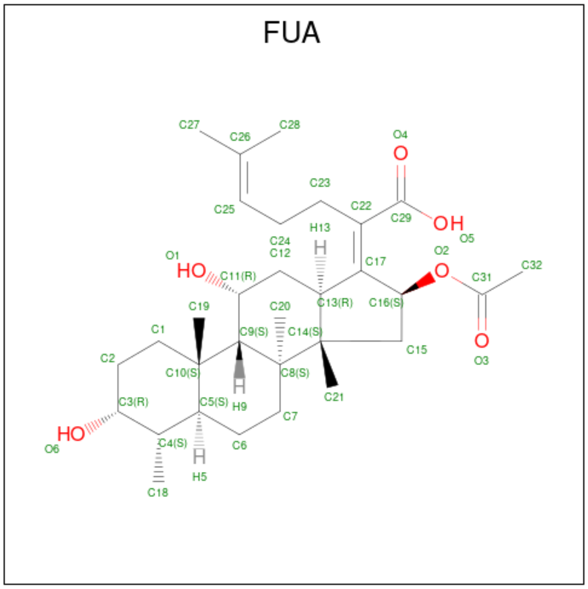
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	1	Total 1	Zn 1	0	0
59	AN	1	Total 1	Zn 1	0	0
59	B4	1	Total 1	Zn 1	0	0
59	B9	1	Total 1	Zn 1	0	0
59	CD	1	Total 1	Zn 1	0	0
59	CN	1	Total 1	Zn 1	0	0
59	D4	1	Total 1	Zn 1	0	0
59	D9	1	Total 1	Zn 1	0	0

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

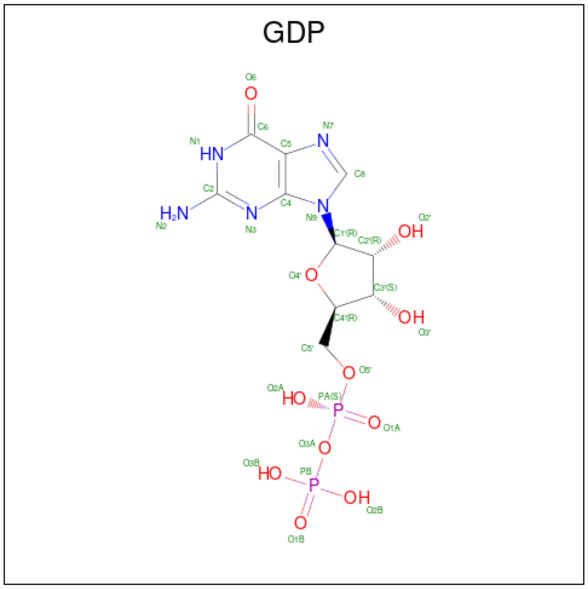
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AY	1	Total 1	Mg 1	0	0
60	CY	1	Total 1	Mg 1	0	0

- Molecule 61 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AY	1	Total C O 37 31 6	0	0
61	CY	1	Total C O 37 31 6	0	0

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

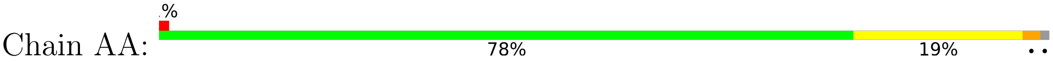


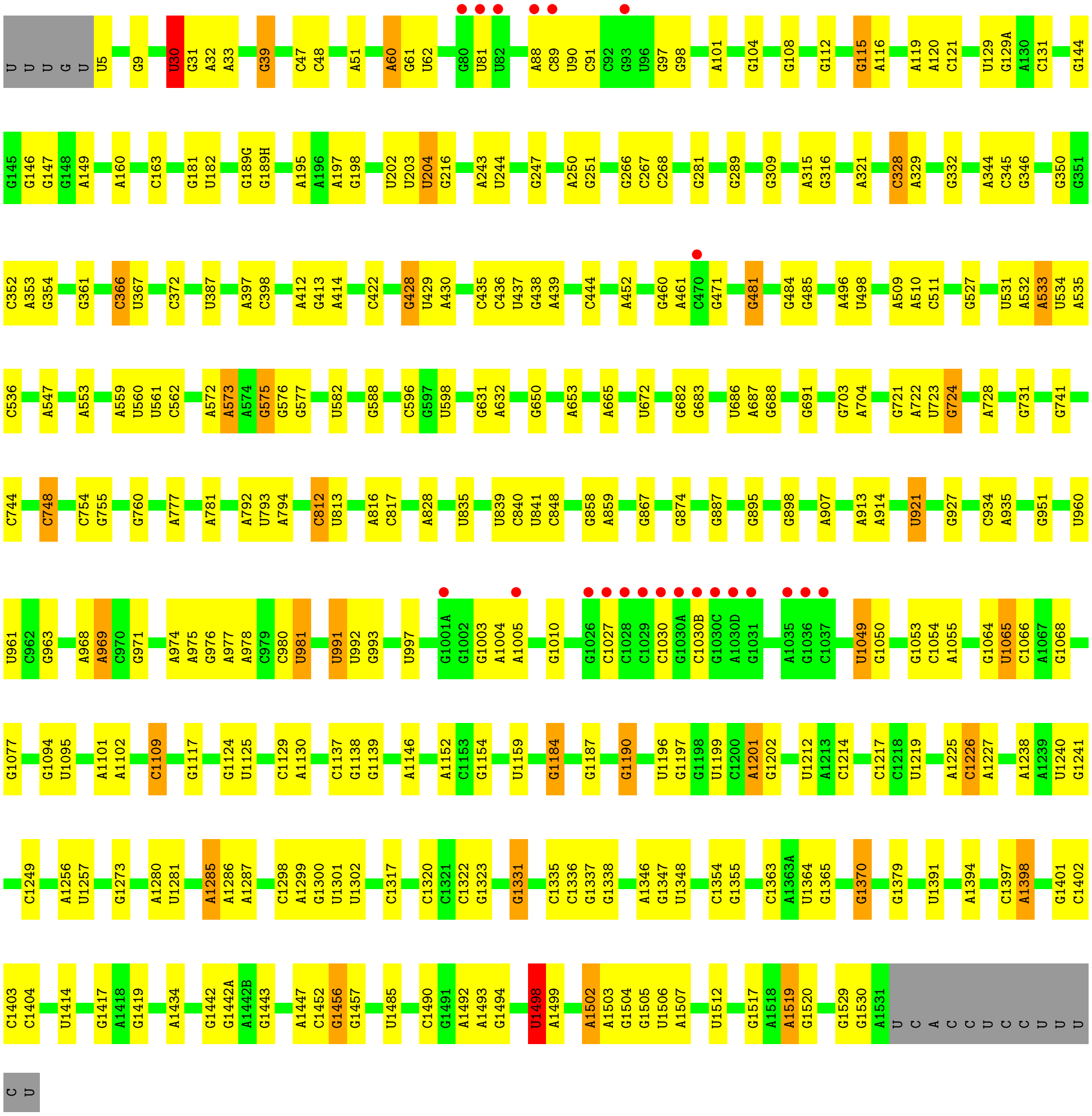
<table>
<tr><th>Mol</th><th>Chain</th><th>Residues</th><th colspan="5">Atoms</th><th>ZeroOcc</th><th>AltConf</th></tr>
<tr><td rowspan="2">62</td><td rowspan="2">AY</td><td rowspan="2">1</td><td>Total</td><td>C</td><td>N</td><td>O</td><td>P</td><td rowspan="2">0</td><td rowspan="2">0</td></tr>
<tr><td>28</td><td>10</td><td>5</td><td>11</td><td>2</td></tr>
<tr><td rowspan="2">62</td><td rowspan="2">CY</td><td rowspan="2">1</td><td>Total</td><td>C</td><td>N</td><td>O</td><td>P</td><td rowspan="2">0</td><td rowspan="2">0</td></tr>
<tr><td>28</td><td>10</td><td>5</td><td>11</td><td>2</td></tr>
</table>

3 Residue-property plots ⓘ

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.

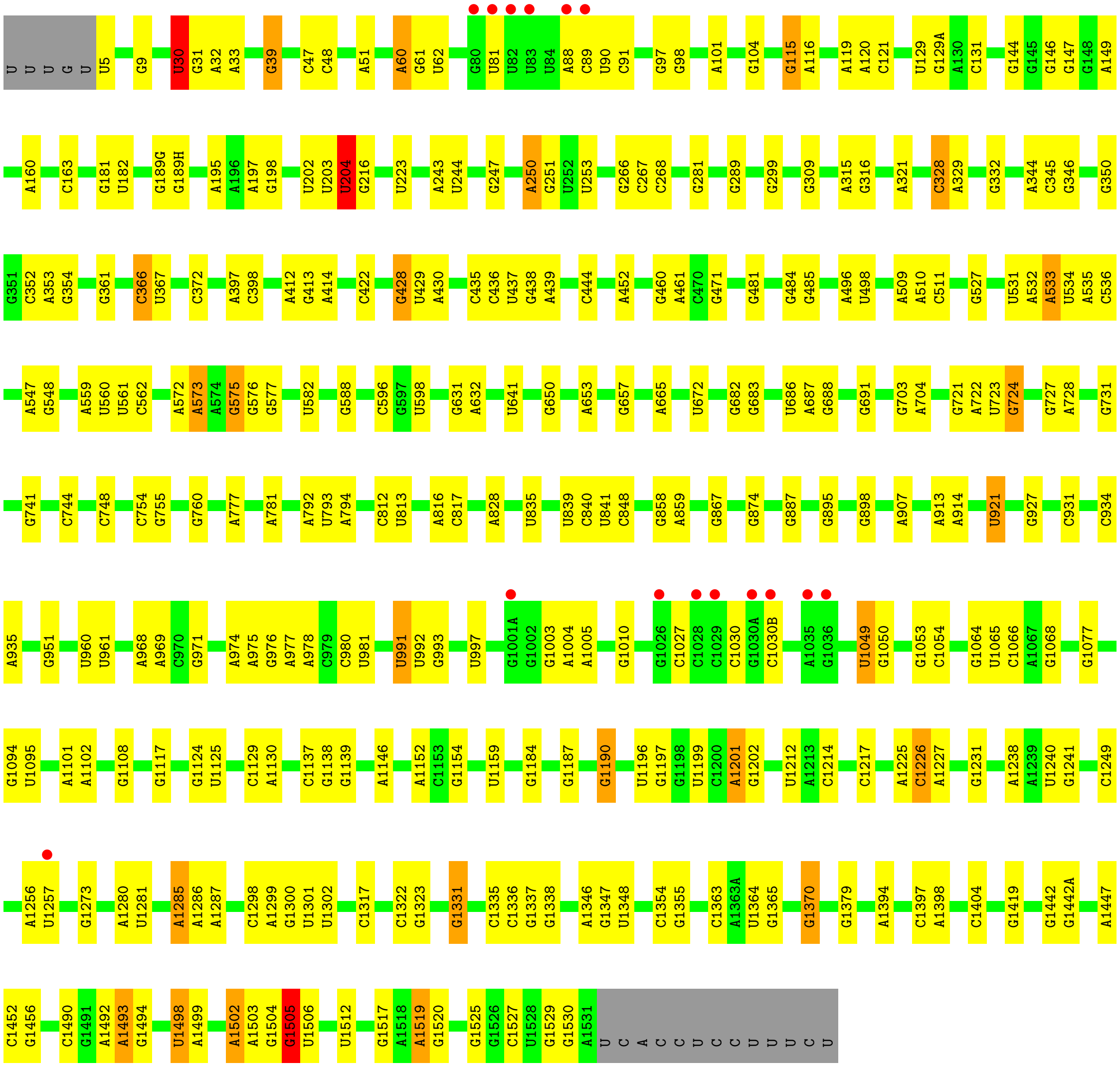
- Molecule 1: 16S ribosomal RNA





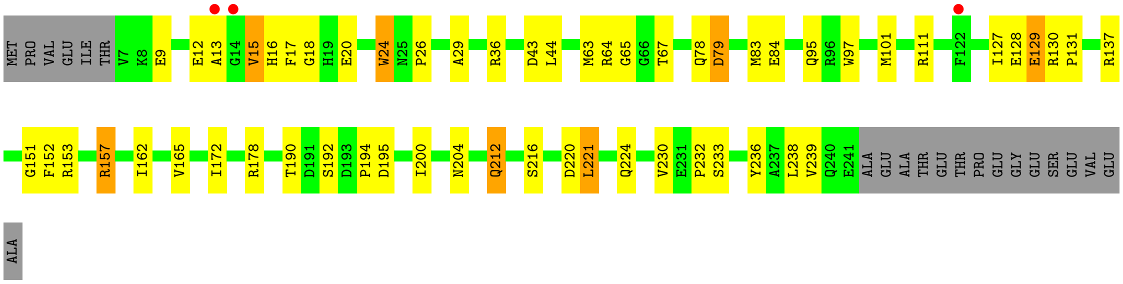
- Molecule 1: 16S ribosomal RNA

Chain CA:



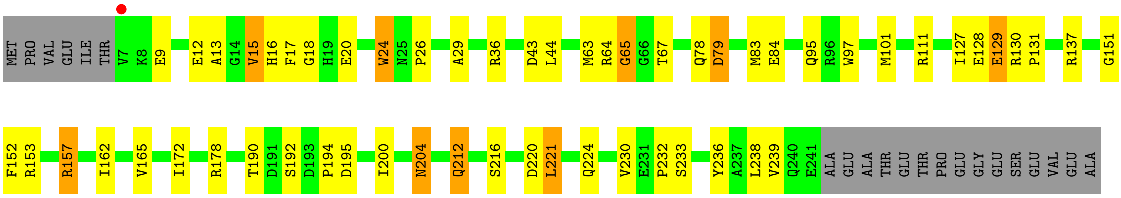
- Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB:



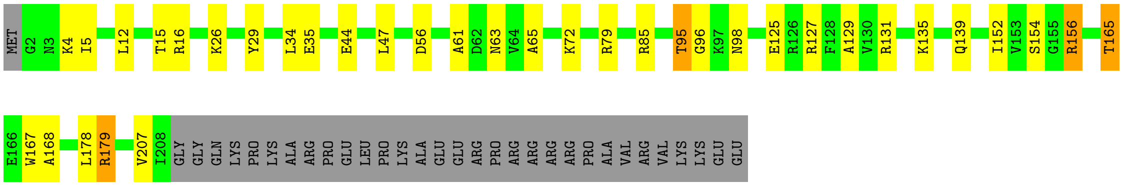
- Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain CB:



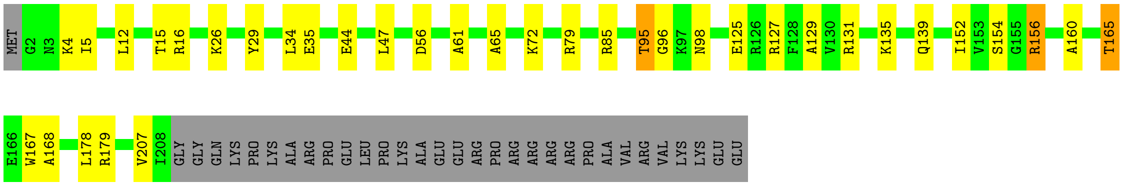
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:



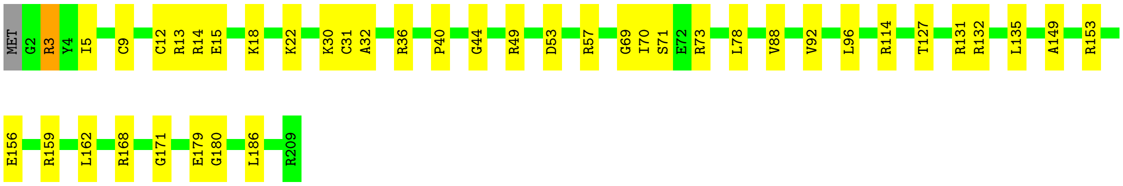
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC:



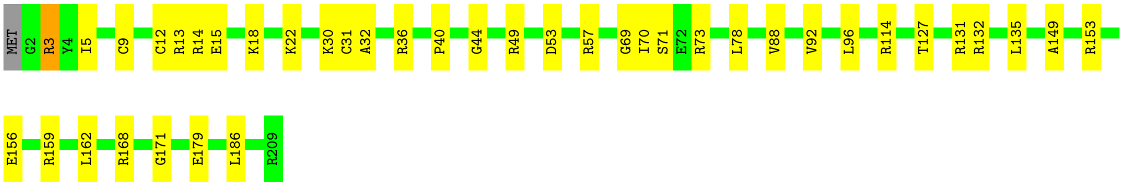
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



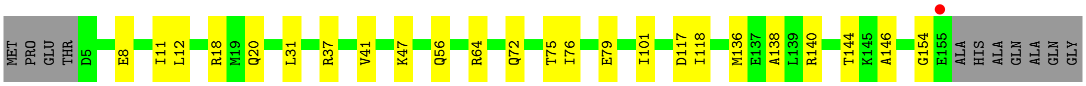
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CD:



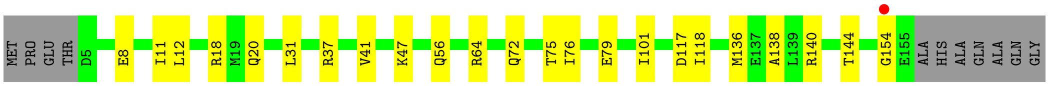
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:



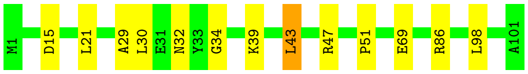
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:



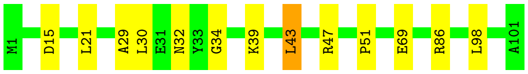
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



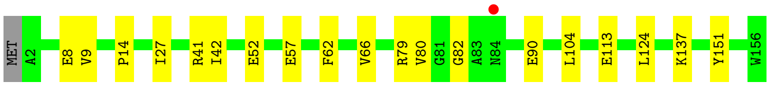
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CF:



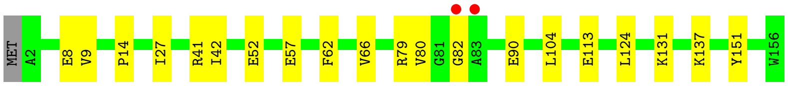
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:



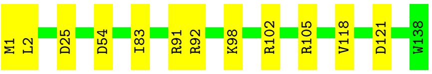
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG:



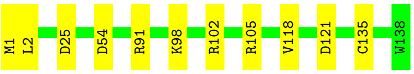
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



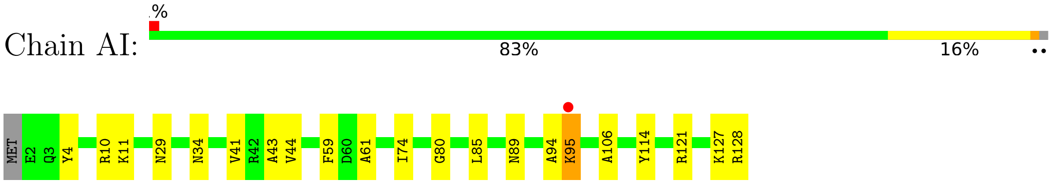
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH:



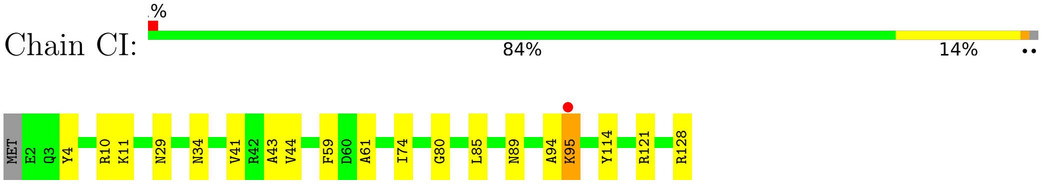
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



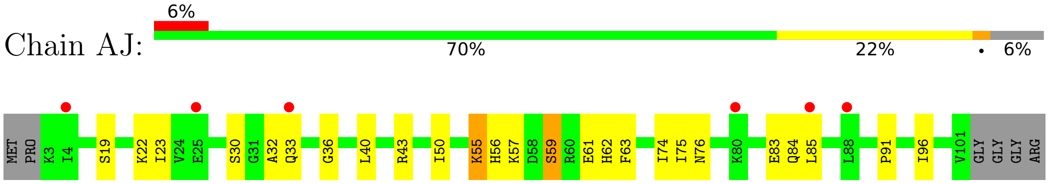
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



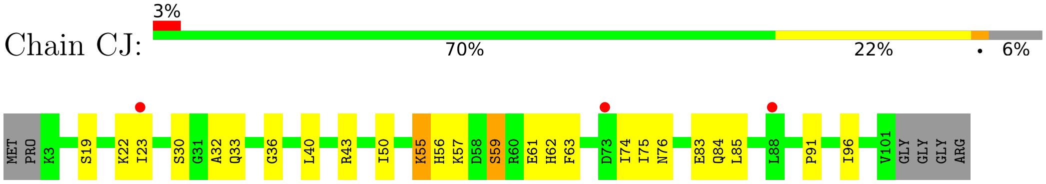
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



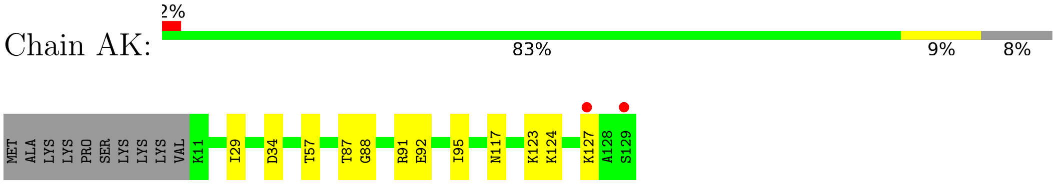
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:



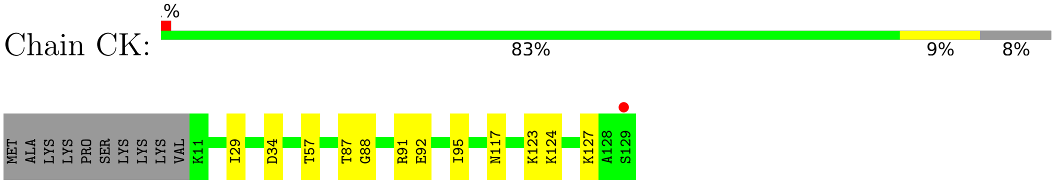
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



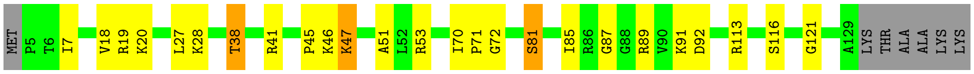
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



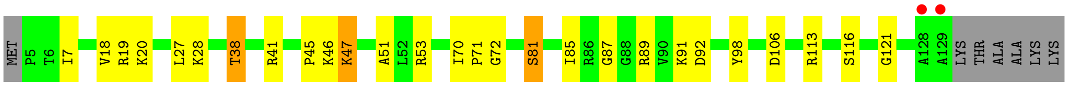
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



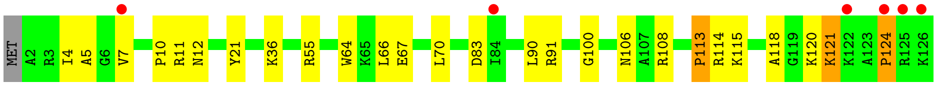
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL:



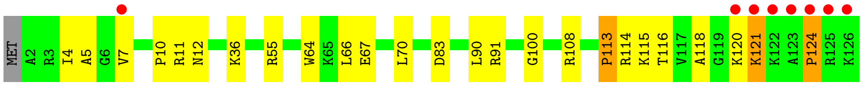
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



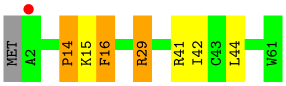
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



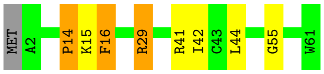
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:



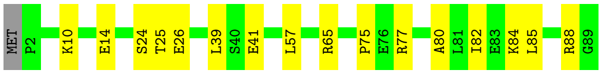
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN:



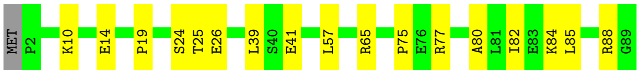
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



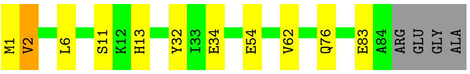
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



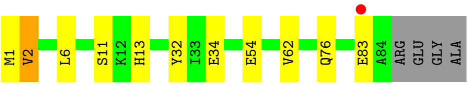
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



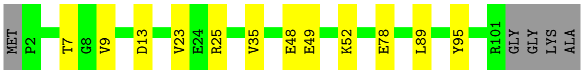
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



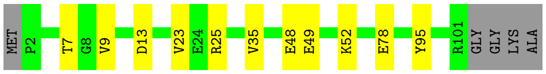
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



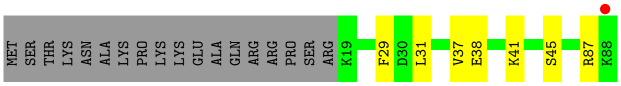
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



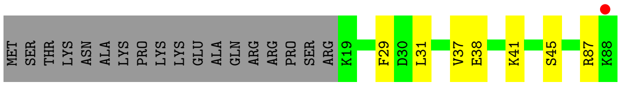
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



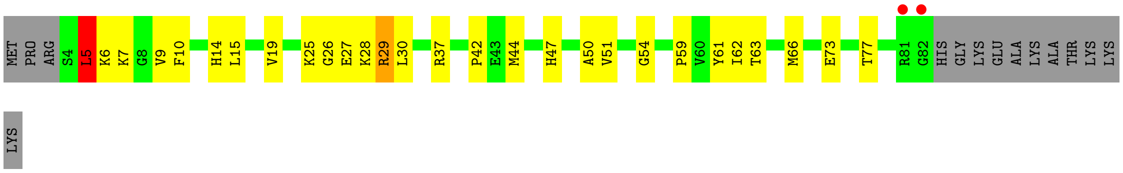
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:

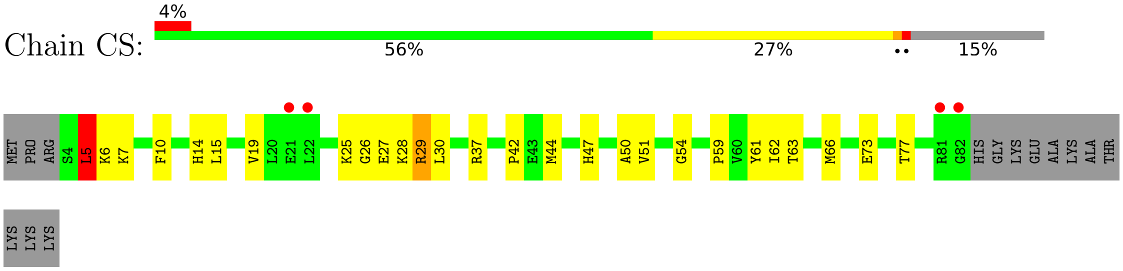


- Molecule 19: 30S RIBOSOMAL PROTEIN S19

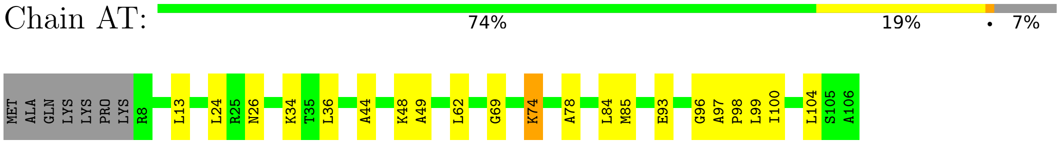
Chain AS:



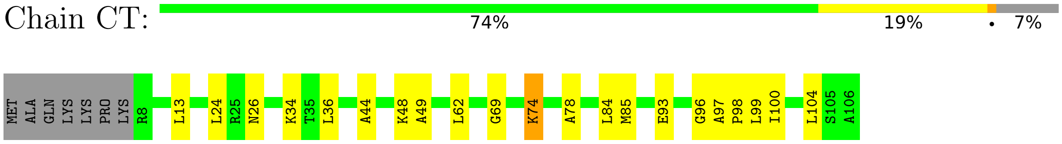
- Molecule 19: 30S RIBOSOMAL PROTEIN S19



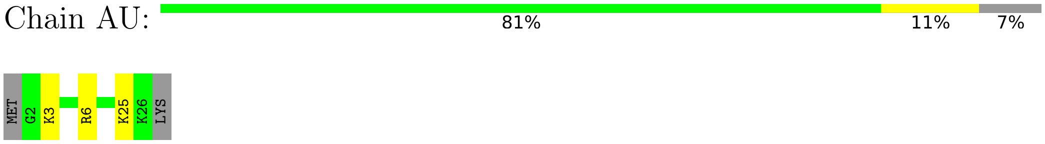
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



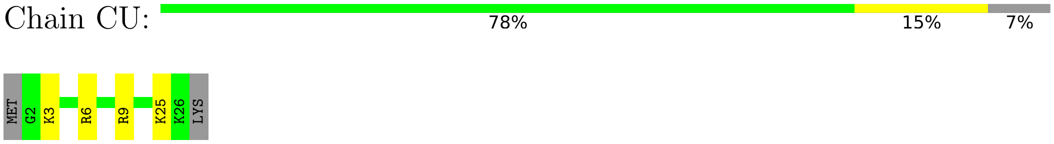
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



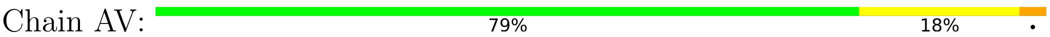
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

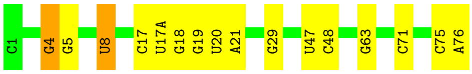


- Molecule 21: 30S RIBOSOMAL PROTEIN THX



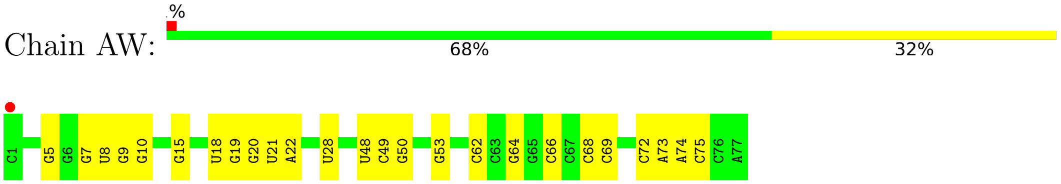
- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)





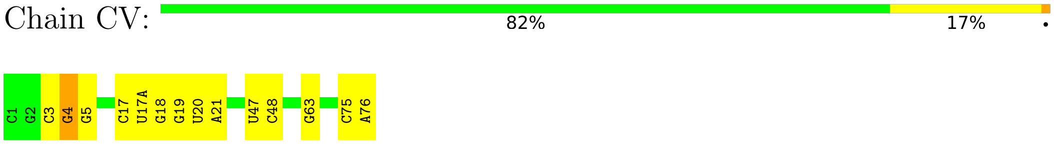
- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)

Chain AW:



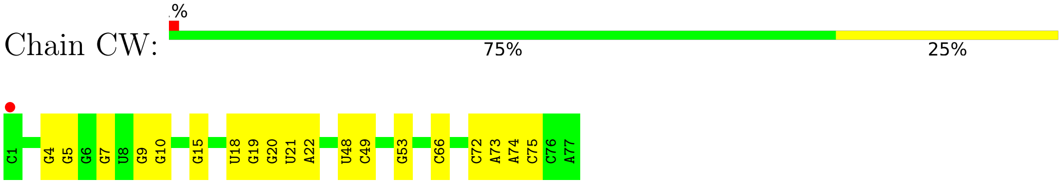
- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)

Chain CV:



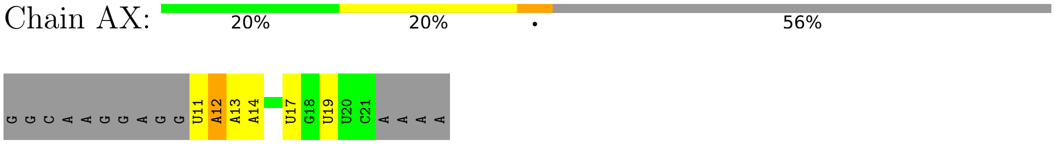
- Molecule 22: E-SITE TRNA FMET OR P-SITE TRNA FMET (UNMODIFIED BASES EXCEPT FOR THYMINE 54)

Chain CW:



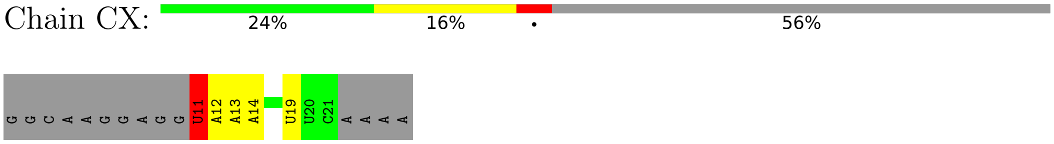
- Molecule 23: MRNA

Chain AX:



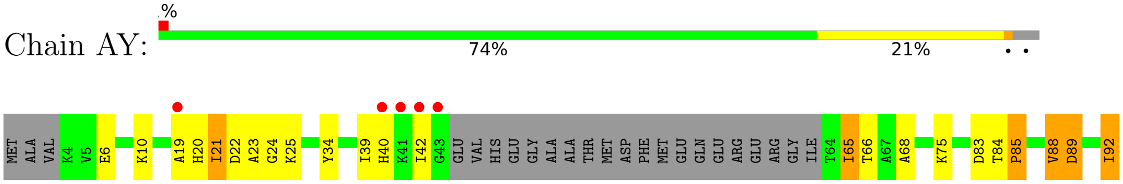
- Molecule 23: MRNA

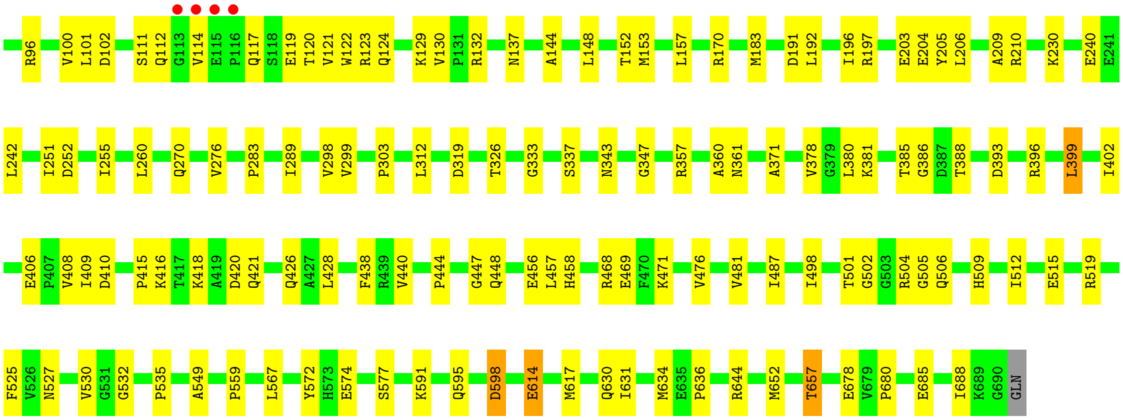
Chain CX:



- Molecule 24: ELONGATION FACTOR G

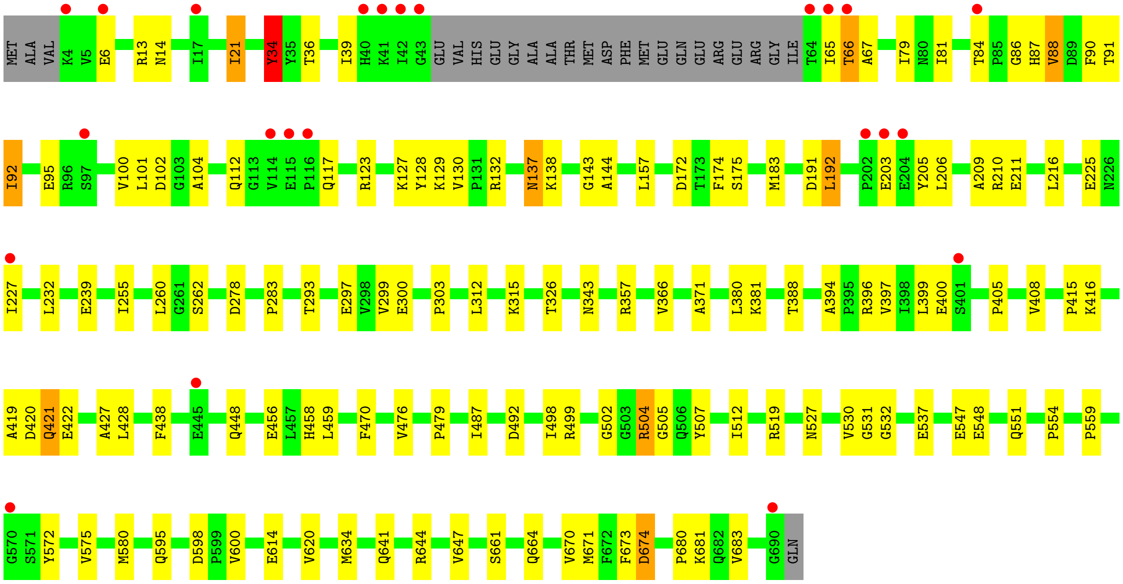
Chain AY:





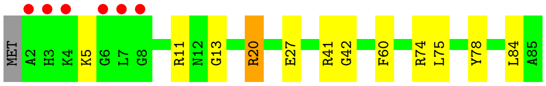
- Molecule 24: ELONGATION FACTOR G

Chain CY:



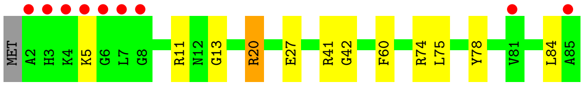
- Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain B0:



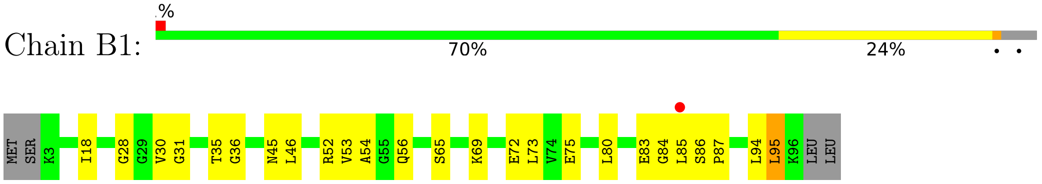
- Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain D0:



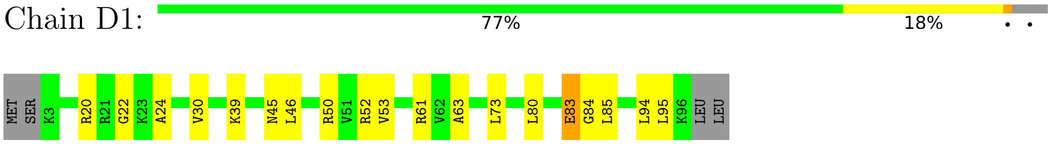
- Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain B1:



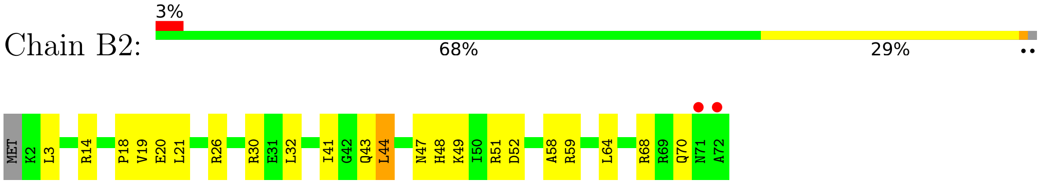
• Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain D1:



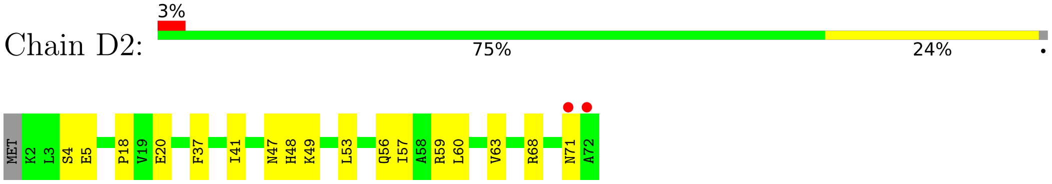
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain B2:



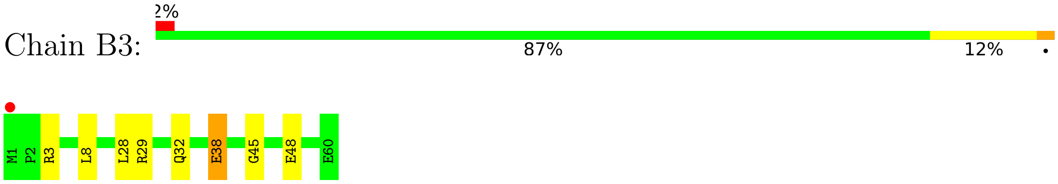
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain D2:



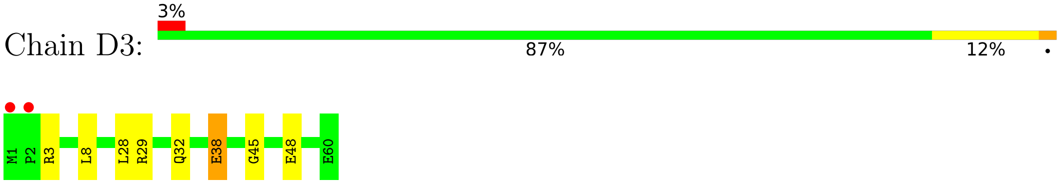
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain B3:



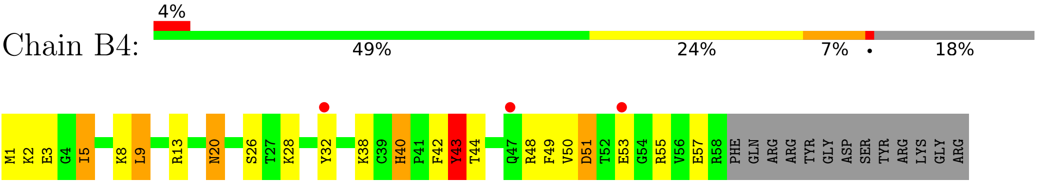
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain D3:

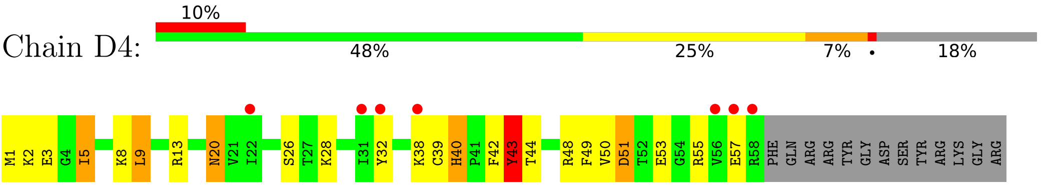


• Molecule 29: 50S RIBOSOMAL PROTEIN L31

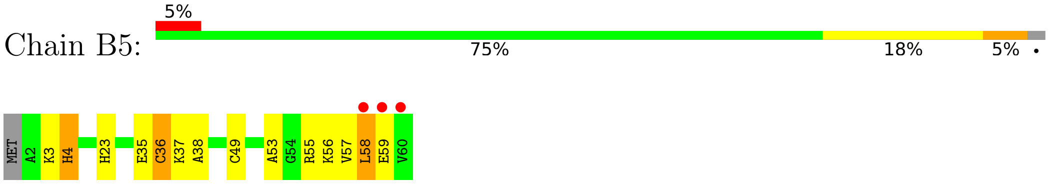
Chain B4:



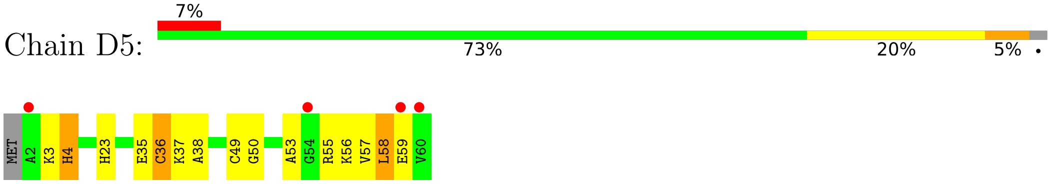
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



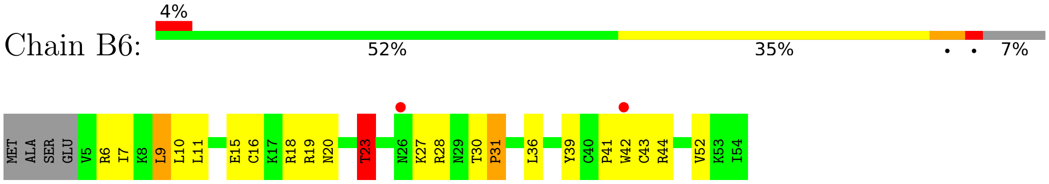
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



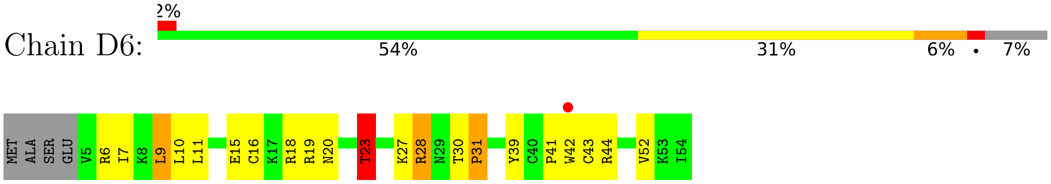
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



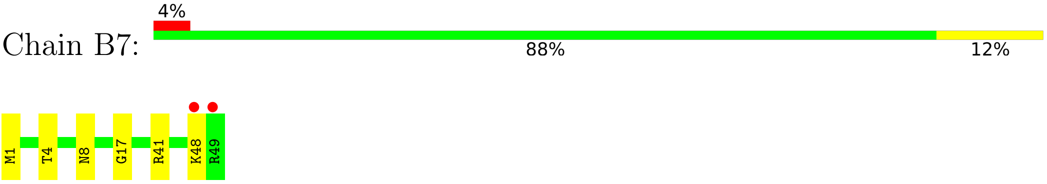
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



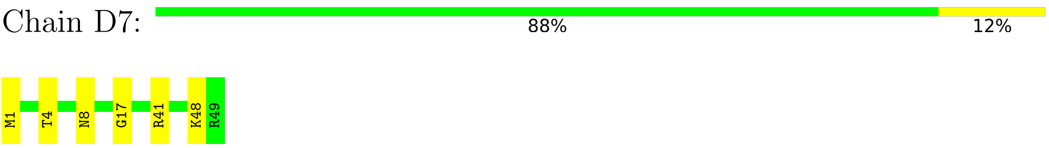
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



• Molecule 32: 50S RIBOSOMAL PROTEIN L34

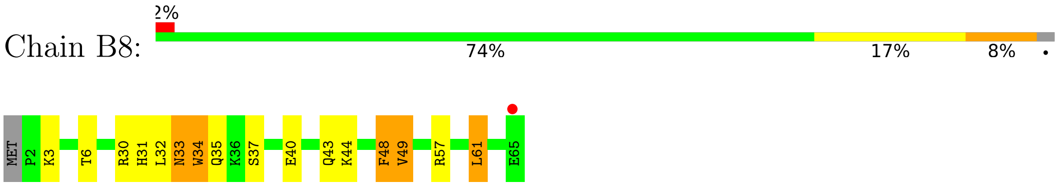


• Molecule 32: 50S RIBOSOMAL PROTEIN L34



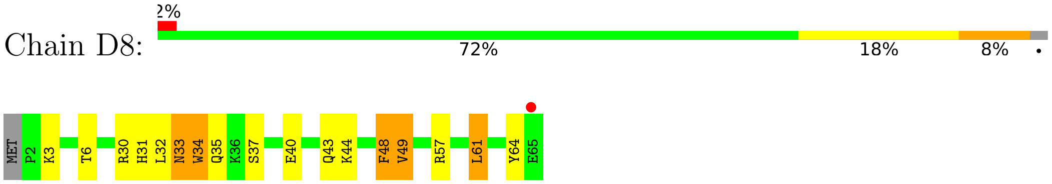
• Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain B8:



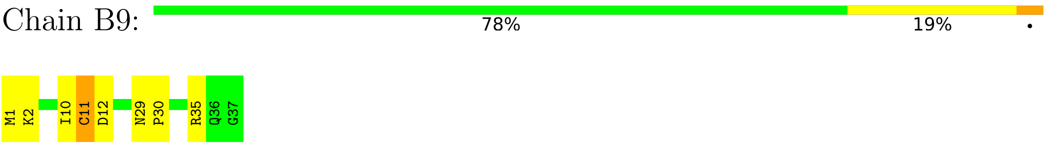
- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain D8:



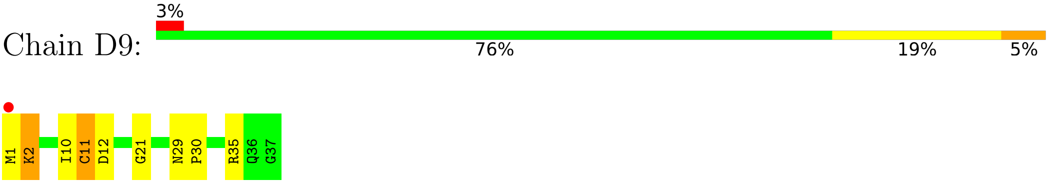
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain B9:



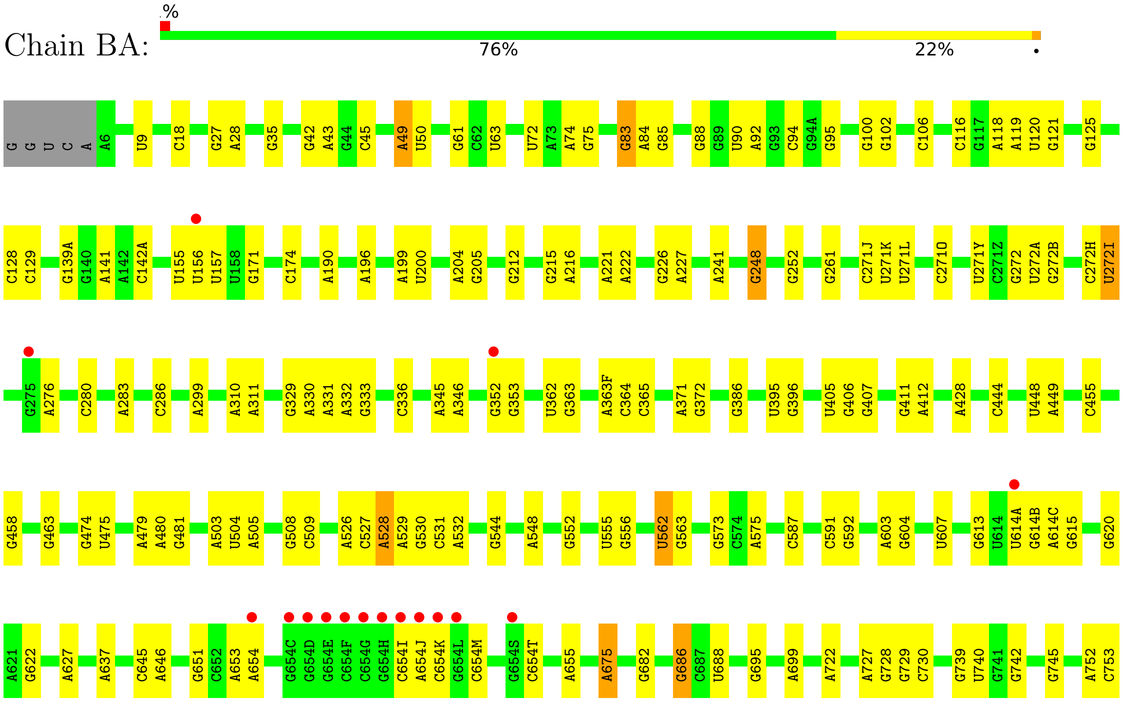
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

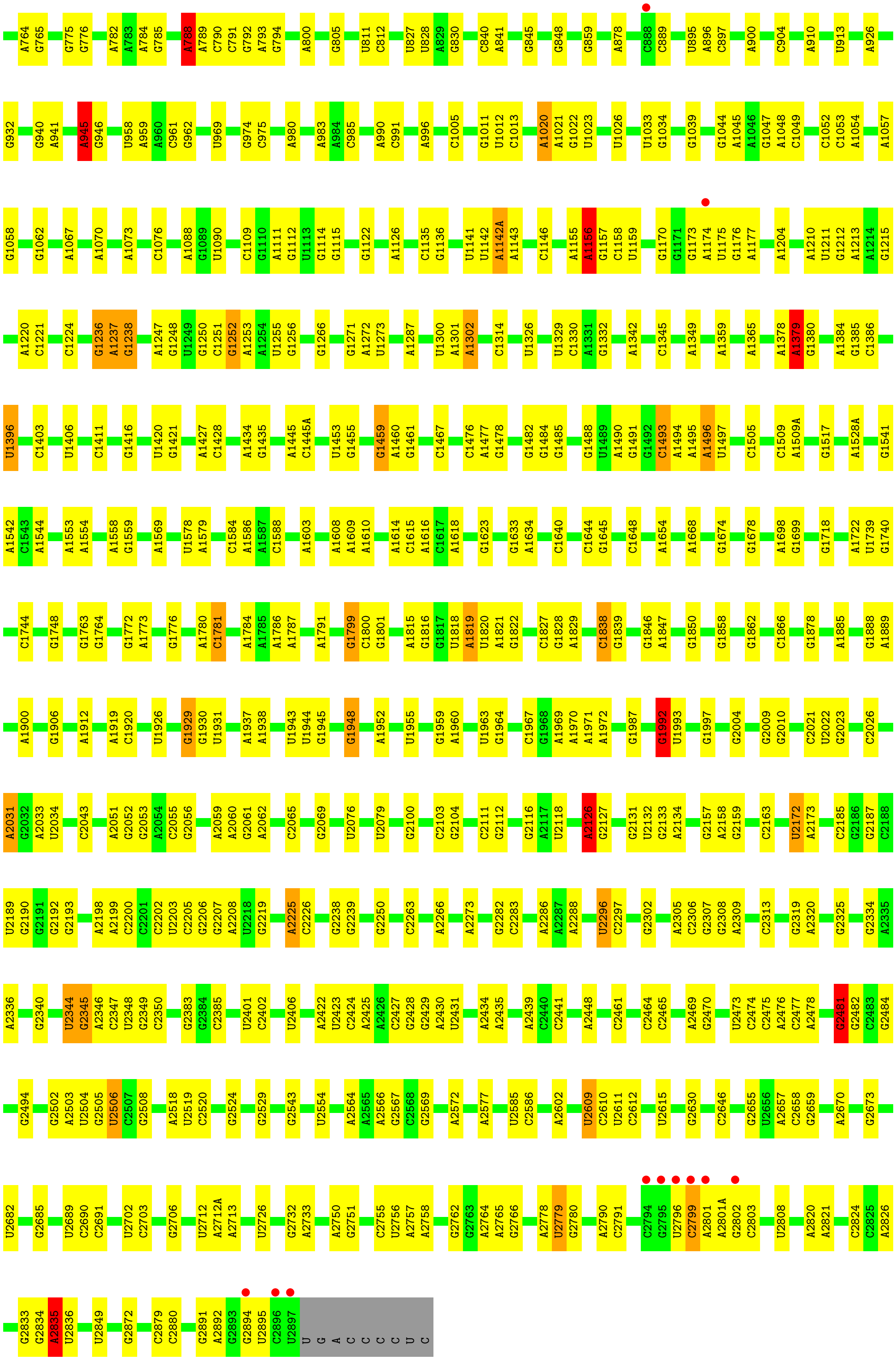
Chain D9:



- Molecule 35: 23S RIBOSOMAL RNA

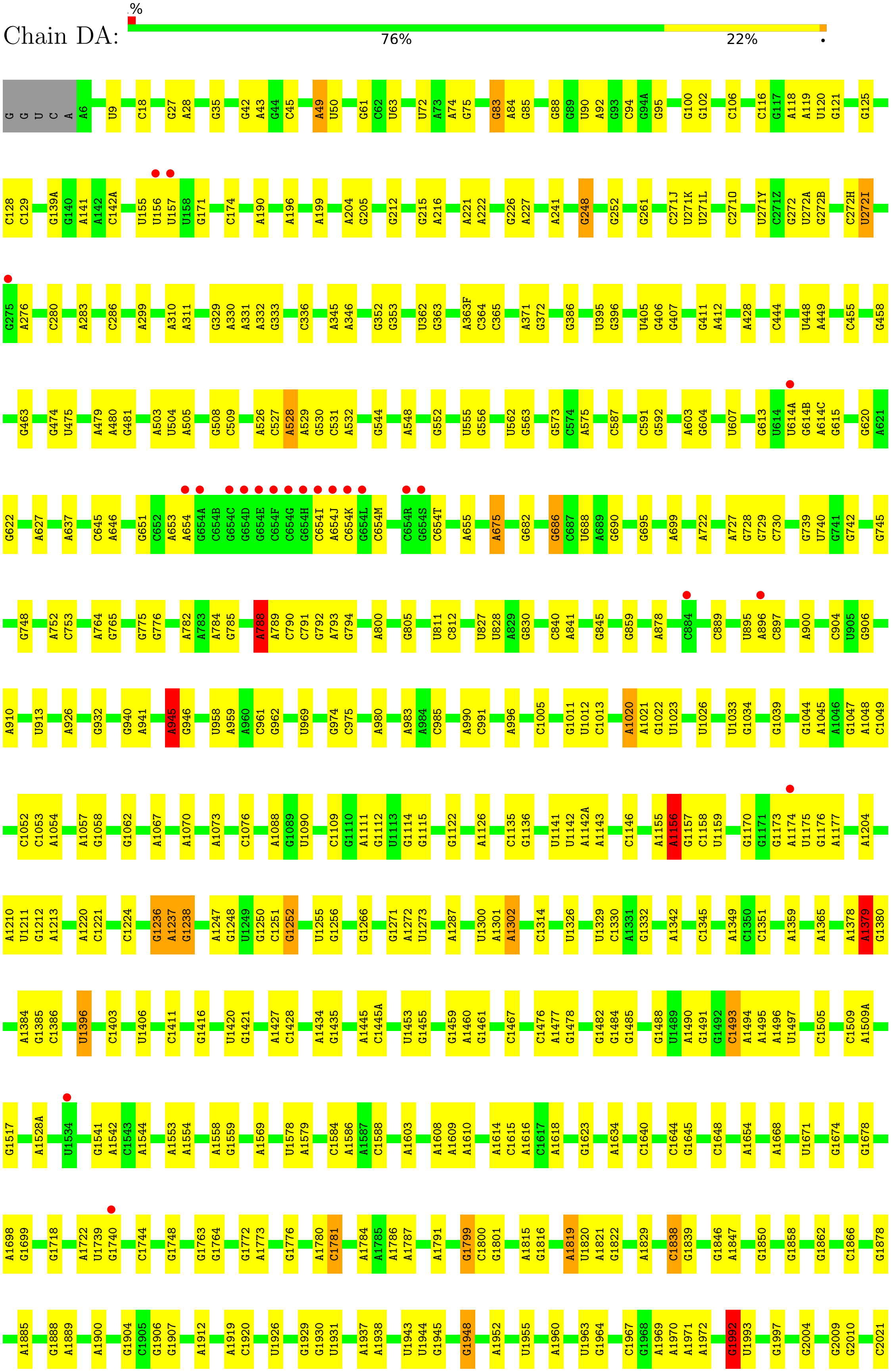
Chain BA:





- Molecule 35: 23S RIBOSOMAL RNA

Chain DA:


.%
76%
22%
•
G G U C A A6 U9 C18 G27 A28 G35 G42 A43 G44 C45 A49 U50 G61 C62 U63 U72 A73 A74 G75 G83 A84 G85 G88 G89 U90 A92 G93 C94 G94A G95 G100 G102 C106 C116 G117 A118 A119 U120 G121 G125
C128 C129 G139A G140 A141 A142 C142A U155 U156 U157 U158 G171 C174 A190 A196 A199 A204 G205 G212 G215 A216 A221 A222 G226 A227 A241 G248 G252 G261 C271J U271K U271L C271O U271Y C271Z G272 U272A G272B C272H U272I
G275 A276 C280 A283 C286 A299 A310 A311 G329 A330 A331 A332 G333 C336 A345 A346 G352 G353 U362 G363 A363F C364 C365 A371 G372 G386 U395 G396 U405 G406 G407 G411 A412 A428 C444 U448 A449 C455 G458
G463 G474 U475 A479 A480 G481 A503 U504 A505 G508 C509 A526 C527 A528 A529 G530 C531 A532 G544 A548 G552 U555 G556 U562 G563 G573 C574 A575 C587 C591 G592 A603 G604 U607 G613 U614 U614A G614B A614C G615 G620 A621
G622 A627 A637 C645 A646 G651 C652 A653 A654 G654A C654B G654C G654D G654E C654F C654G G654H C654I A654J C654K G654L C654M C654R G654S C654T A655 A675 G682 G686 C687 U688 A689 G690 G695 A699 A722 A727 G728 A729 C730 G739 U740 G741 G742 G745
G748 A752 C753 A764 G765 G775 G776 A782 A783 A784 G785 A788 A789 C790 C791 G792 A793 G794 A800 G805 U811 C812 U827 U828 A829 G830 C840 A841 G845 G859 A878 C884 C889 U895 A896 C897 A900 C904 U905 G906
A910 U913 A926 G932 G940 A941 A945 G946 U958 A959 A960 C961 G962 U969 G974 C975 A980 A983 A984 C985 A990 C991 A996 C1005 G1011 U1012 C1013 A1020 A1021 G1022 U1023 U1026 U1033 G1034 G1039 G1044 A1045 A1046 G1047 A1048 C1049
C1052 C1053 A1054 A1057 G1058 G1062 A1067 A1070 A1073 C1076 A1088 G1089 U1090 C1109 G1110 A1111 G1112 U1113 G1114 G1115 G1122 A1126 C1135 G1136 U1141 U1142 A1142A A1143 C1146 A1155 A1156 G1157 C1158 U1159 G1170 G1171 G1173 A1174 U1175 G1176 A1177 A1204
A1210 U1211 G1212 A1213 A1220 C1221 C1224 G1236 A1237 G1238 A1247 G1248 U1249 G1250 C1251 G1252 U1255 G1256 G1266 G1271 A1272 U1273 A1287 U1300 A1301 A1302 C1314 U1326 U1329 C1330 A1331 G1332 A1342 C1345 A1349 C1350 C1351 A1359 A1365 A1378 A1379 G1380
A1384 G1385 C1386 U1396 C1403 U1406 C1411 G1416 U1420 G1421 A1427 C1428 A1434 G1435 A1445 C1445A U1453 G1455 G1459 A1460 G1461 C1467 C1476 A1477 G1478 G1482 G1484 G1485 G1488 U1489 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1505 C1509 A1509A
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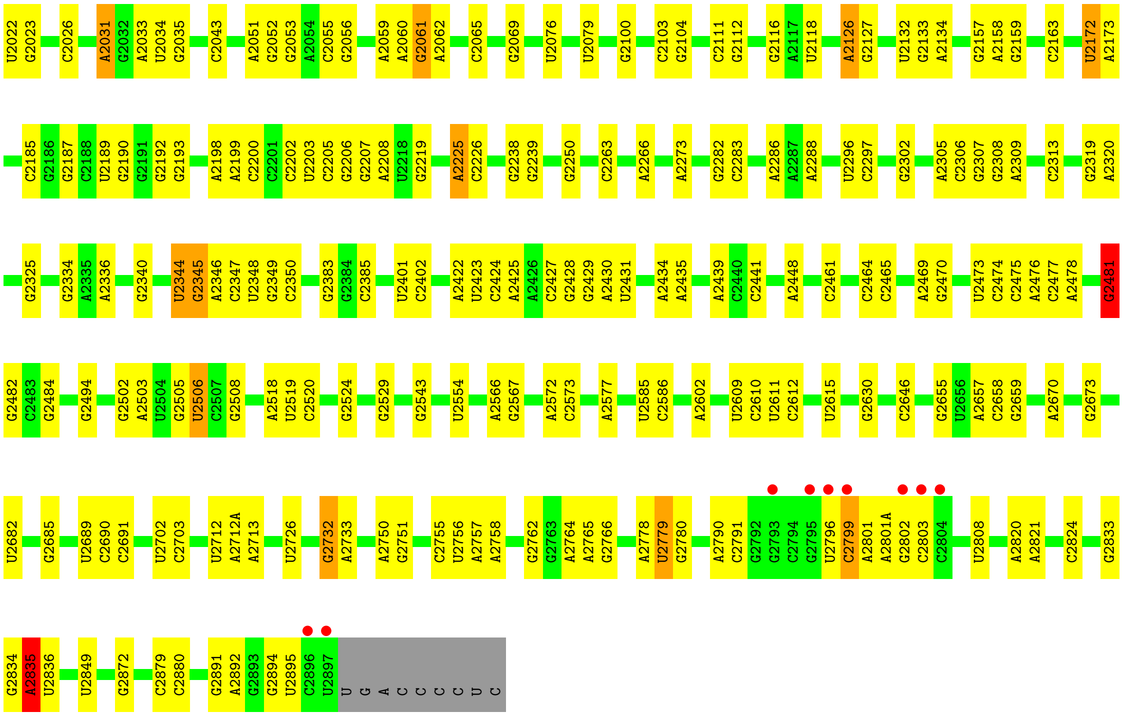
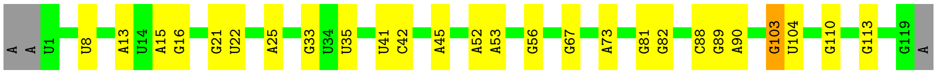
A1698 G1699 G1718 A1722 U1739 G1740 C1744 G1748 G1763 G1764 G1772 A1773 G1776 A1780 C1781 A1784 A1785 A1786 A1787 A1791 G1799 C1800 G1801 A1815 G1816 A1819 U1820 A1821 G1822 A1829 C1838 G1839 G1846 A1847 G1850 G1858 G1862 C1866 G1878
A1885 G1888 A1889 A1900 G1904 C1905 G1906 G1907 A1912 A1919 C1920 U1926 G1929 G1930 U1931 A1937 A1938 U1943 U1944 G1945 G1948 A1952 U1955 A1960 U1963 G1964 C1967 G1968 A1969 A1970 A1971 A1972 G1992 U1993 G1997 G2004 G2009 G2010 C2021



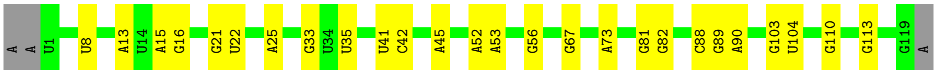
- Molecule 36: 5S RIBOSOMAL RNA

Chain BB:



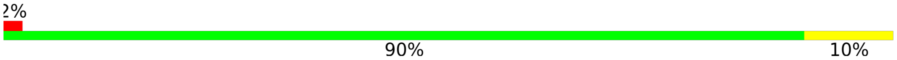
- Molecule 36: 5S RIBOSOMAL RNA

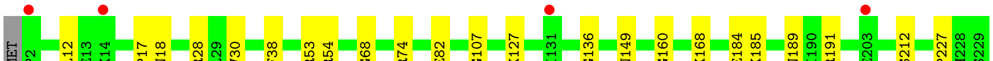
Chain DB:



- Molecule 37: 50S RIBOSOMAL PROTEIN L1

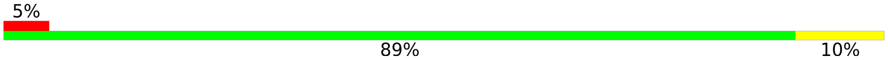
Chain BC:

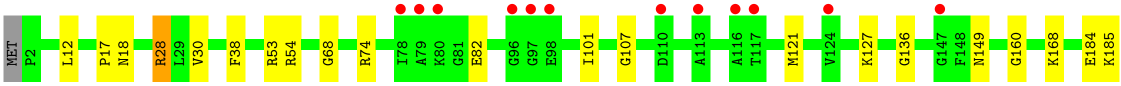


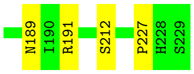


- Molecule 37: 50S RIBOSOMAL PROTEIN L1

Chain DC:

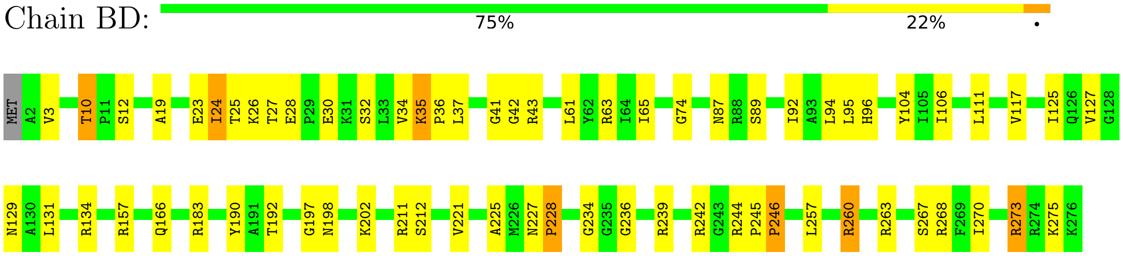






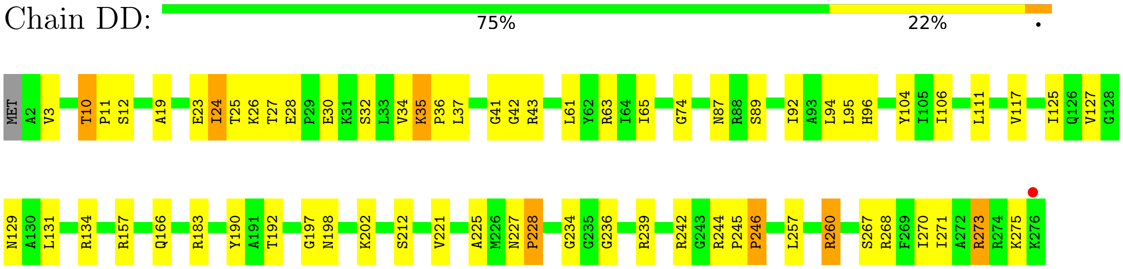
- Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain BD:



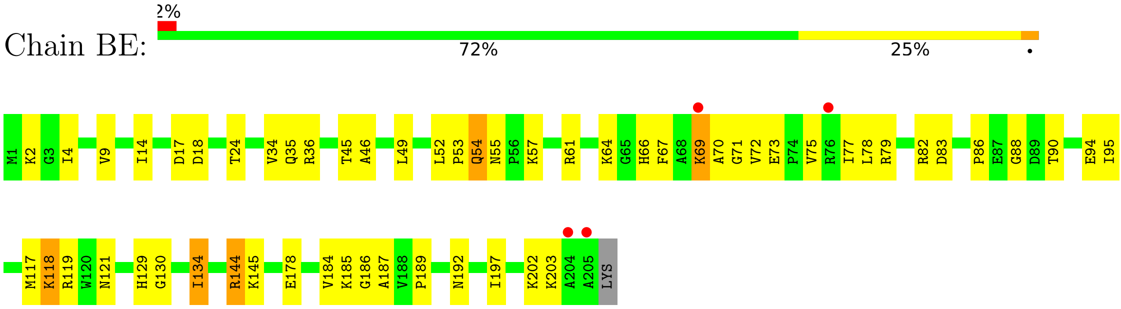
- Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain DD:



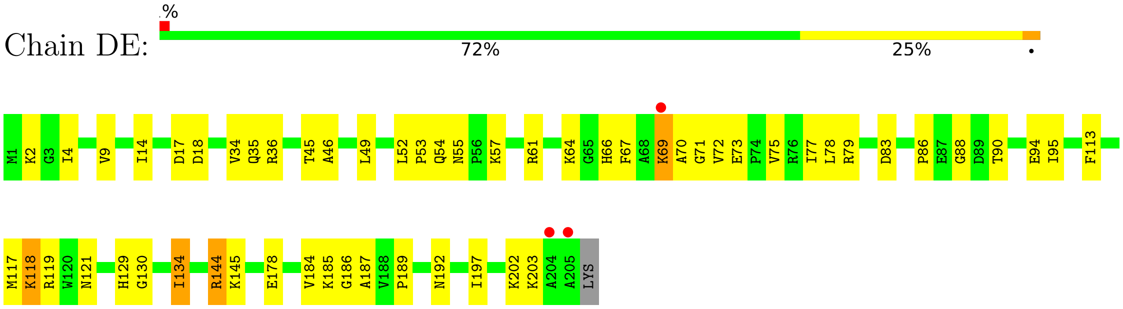
- Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain BE:



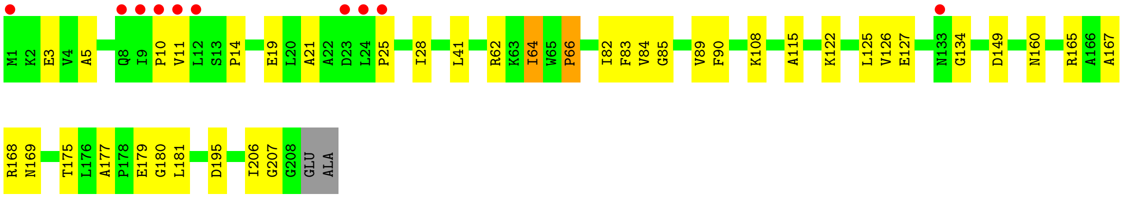
- Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain DE:



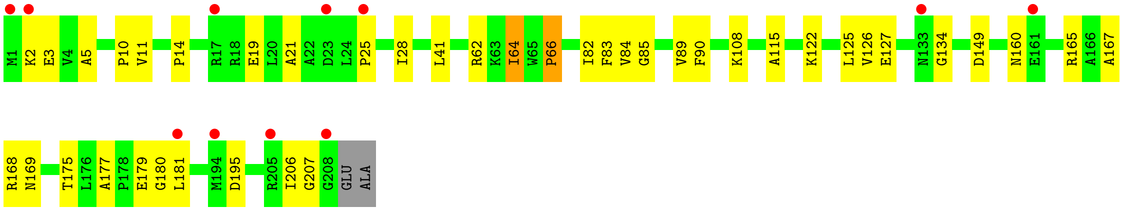
- Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain BF:



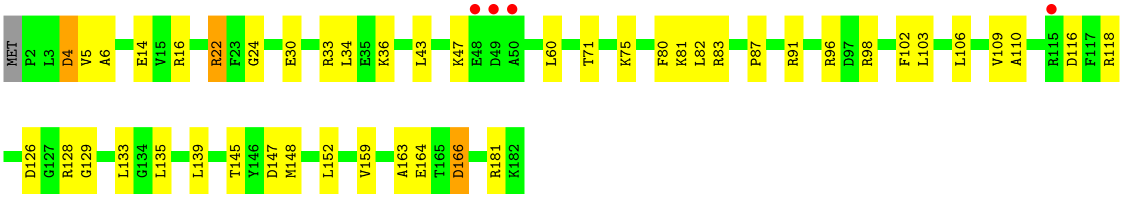
- Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain DF:



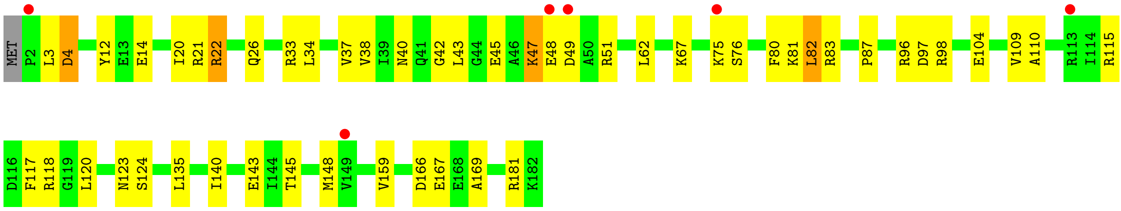
- Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain BG:



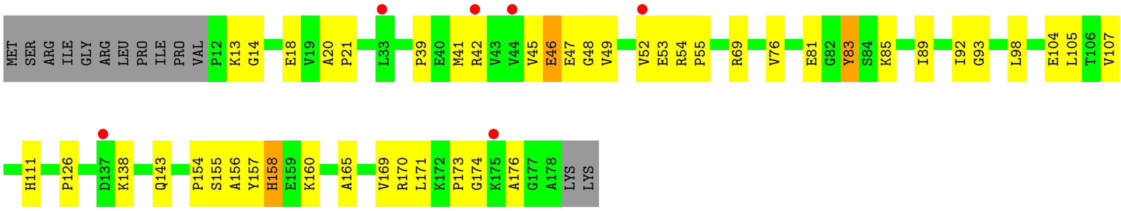
- Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain DG:



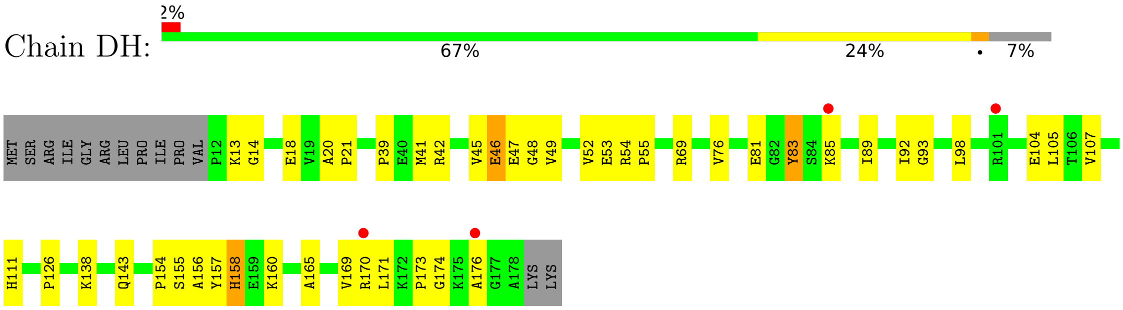
- Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain BH:



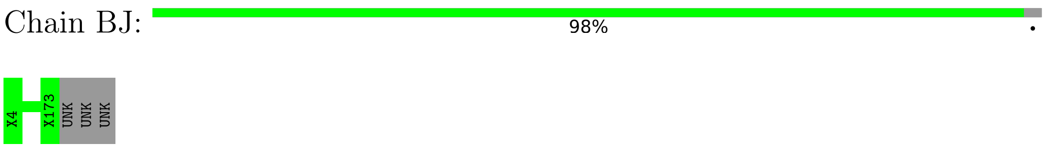
- Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain DH:



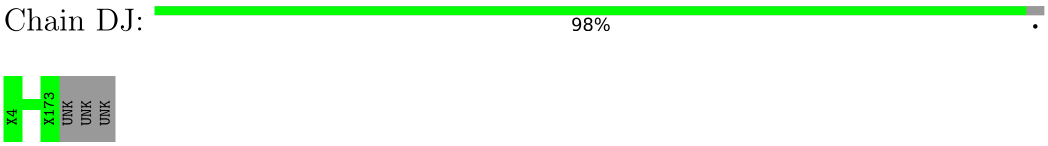
- Molecule 43: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



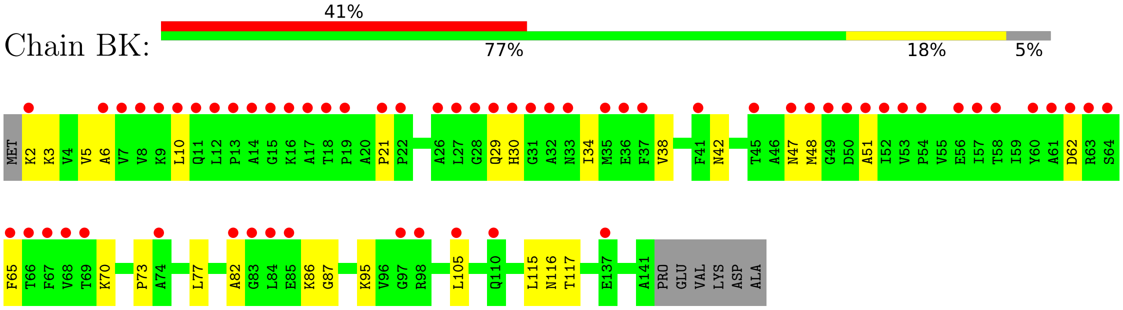
- Molecule 43: 50S RIBOSOMAL PROTEIN L10

Chain DJ:



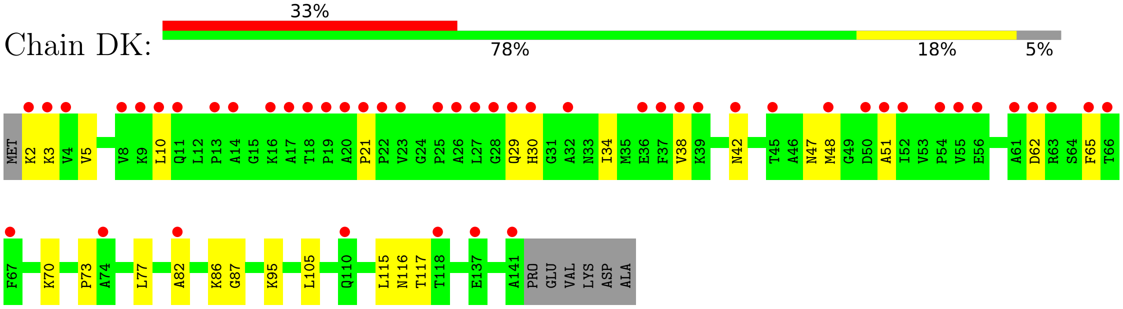
- Molecule 44: 50S RIBOSOMAL PROTEIN L11

Chain BK:



- Molecule 44: 50S RIBOSOMAL PROTEIN L11

Chain DK:

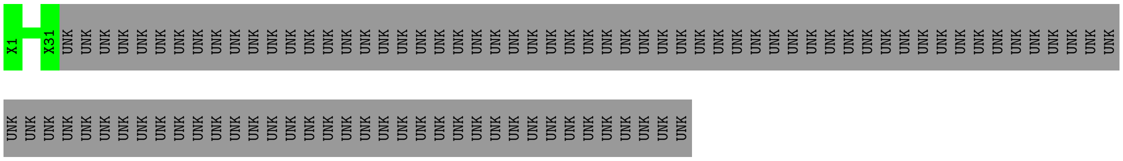


- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain BL:

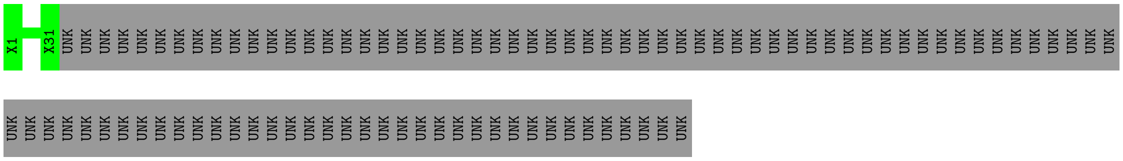
- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain BM:



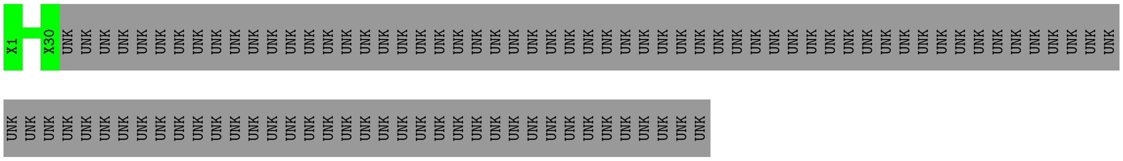
- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain Bl:



- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain Bm:

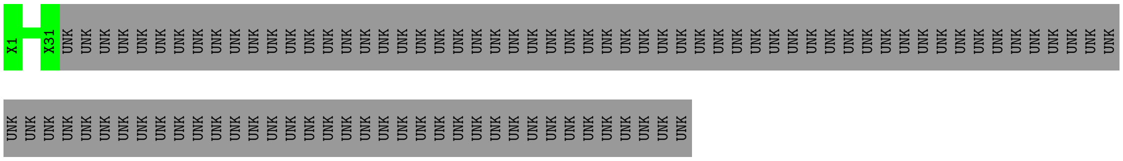


- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain DL:

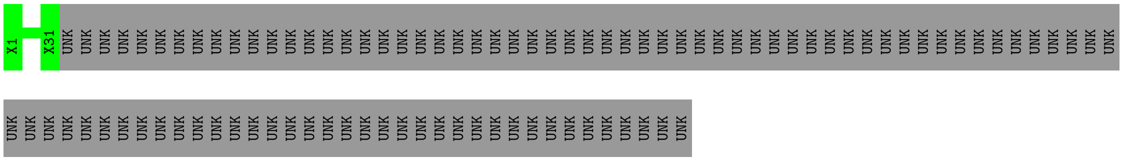
- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain DM:



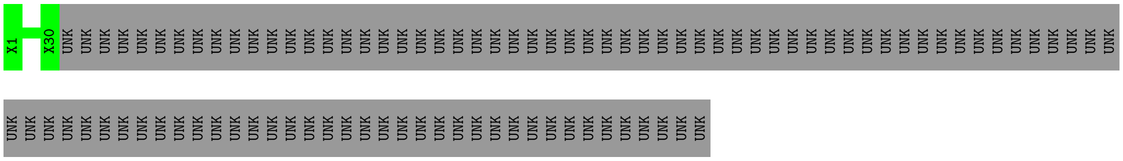
- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain Dl:



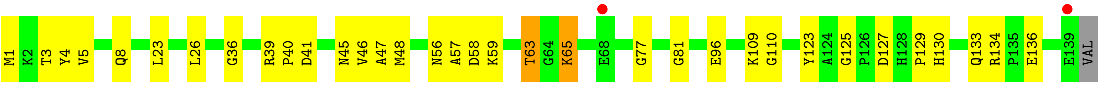
- Molecule 45: 50S RIBOSOMAL PROTEIN L12

Chain Dm:



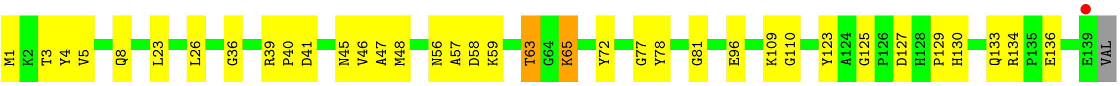
- Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:



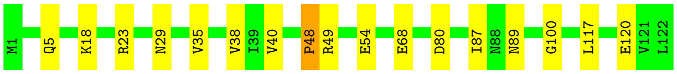
- Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN:



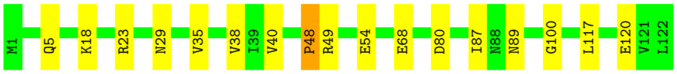
- Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:



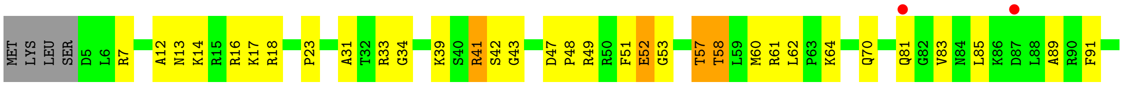
- Molecule 47: 50S RIBOSOMAL PROTEIN L14

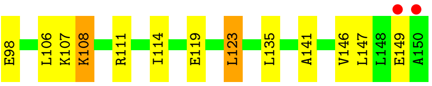
Chain DO:



- Molecule 48: 50S RIBOSOMAL PROTEIN L15

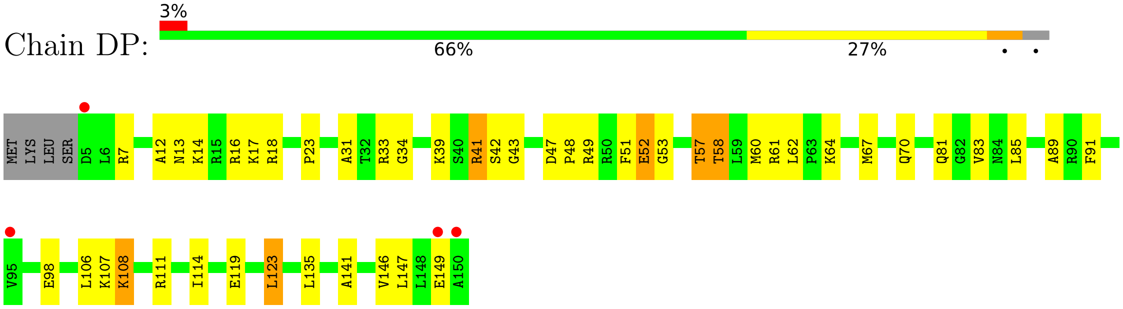
Chain BP:





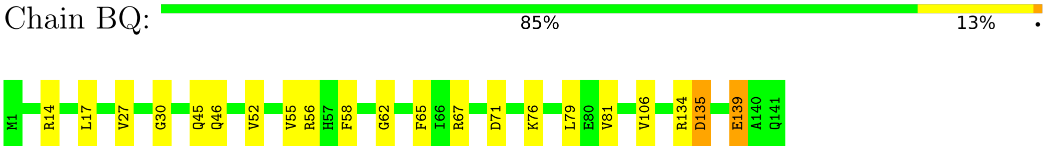
- Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP:



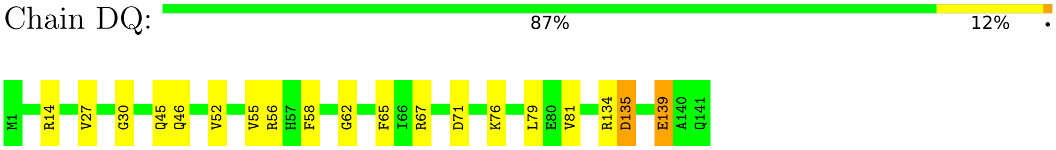
- Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



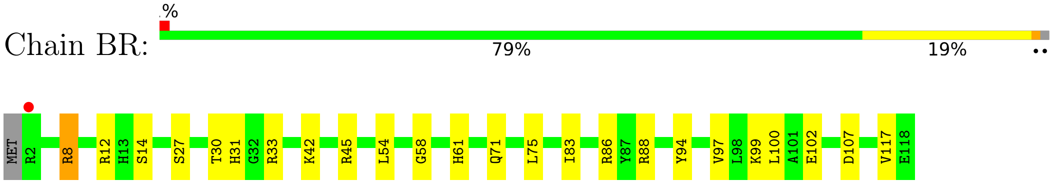
- Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain DQ:



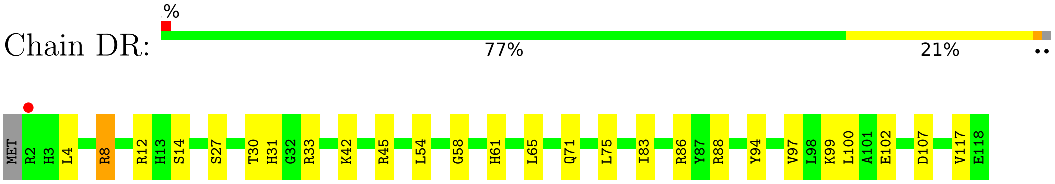
- Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain BR:



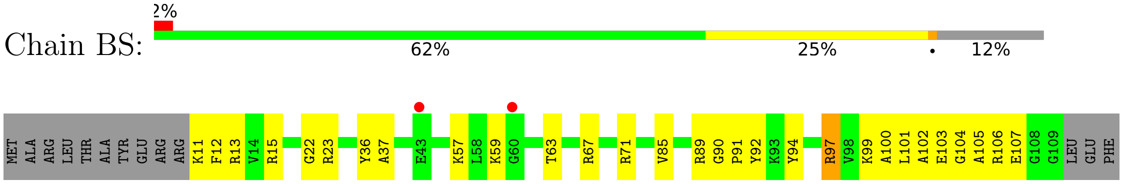
- Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain DR:



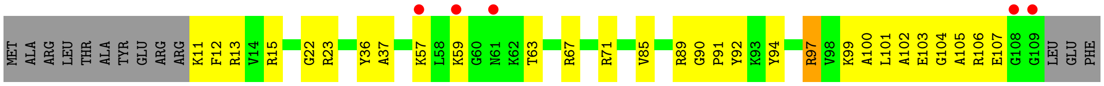
- Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS:



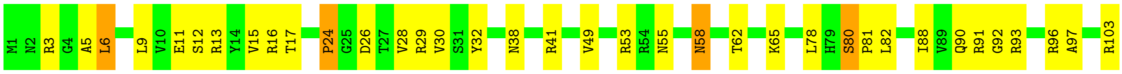
- Molecule 51: 50S RIBOSOMAL PROTEIN L18

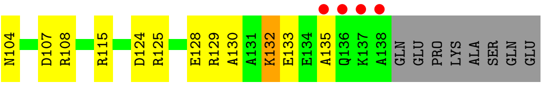
Chain DS:



- Molecule 52: 50S RIBOSOMAL PROTEIN L19

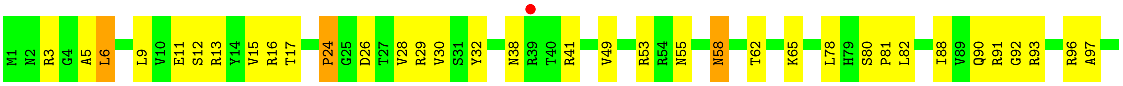
Chain BT:

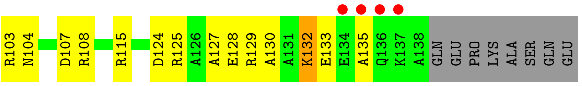




- Molecule 52: 50S RIBOSOMAL PROTEIN L19

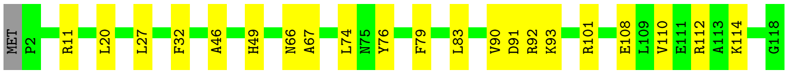
Chain DT:





- Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU:

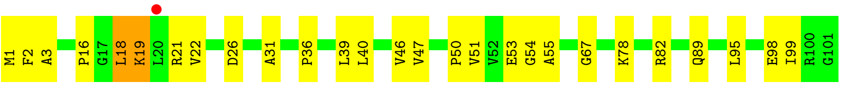


- Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain DU:

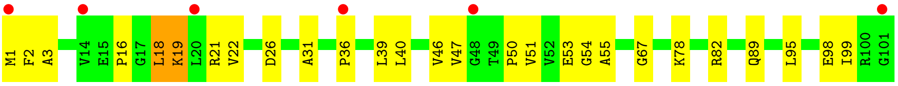
- Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain BV:



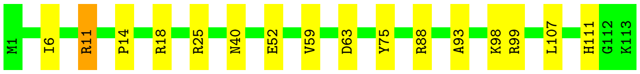
- Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain DV:



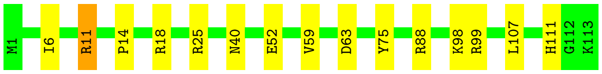
- Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain BW:



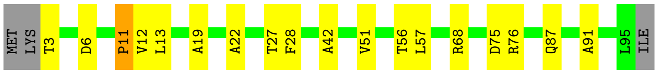
- Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain DW:



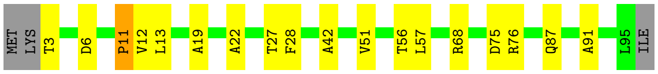
- Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



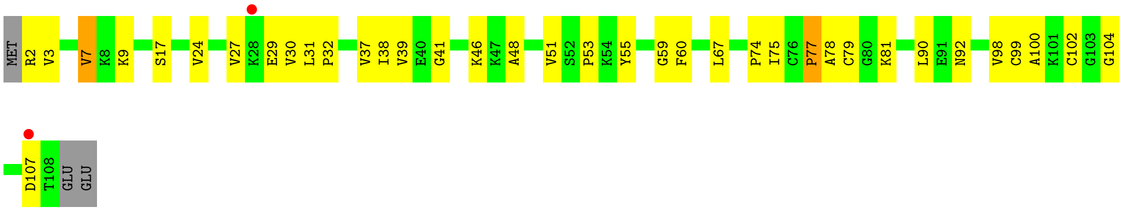
- Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain DX:



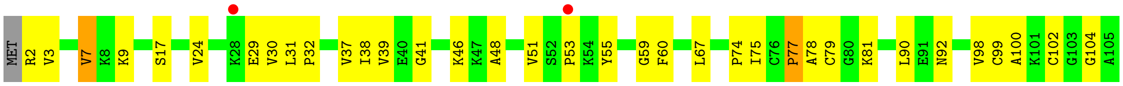
- Molecule 57: 50S RIBOSOMAL PROTEIN L24

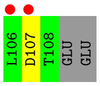
Chain BY:



- Molecule 57: 50S RIBOSOMAL PROTEIN L24

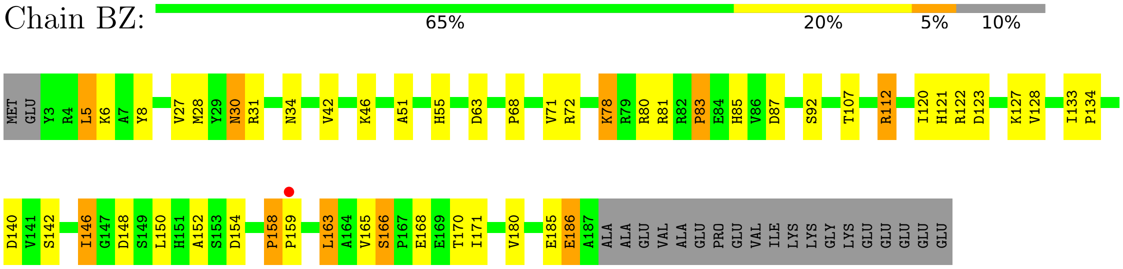
Chain DY:





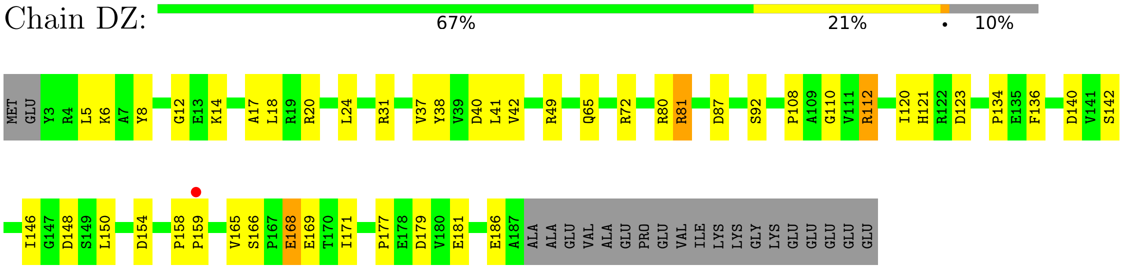
- Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain BZ:



- Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain DZ:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	291.84Å 270.36Å 402.36Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 49.57 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-3.60) 95.0 (49.57-3.40)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.227 , 0.260 0.225 , 0.224	Depositor DCC
R_{free} test set	40387 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	78.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 34.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	311552	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 5MU, GDP, FUA, ZN, MG

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	0.61	1/36190 (0.0%)	0.76	26/56486 (0.0%)
1	CA	0.60	2/36190 (0.0%)	0.76	20/56486 (0.0%)
2	AB	0.46	0/1936	0.70	0/2611
2	CB	0.44	0/1936	0.70	0/2611
3	AC	0.52	0/1637	0.69	0/2207
3	CC	0.46	0/1637	0.69	0/2207
4	AD	0.42	0/1733	0.66	0/2318
4	CD	0.41	0/1733	0.66	0/2318
5	AE	0.59	0/1163	0.72	0/1566
5	CE	0.55	0/1163	0.71	0/1566
6	AF	0.44	0/856	0.67	0/1154
6	CF	0.40	0/856	0.66	0/1154
7	AG	0.45	0/1276	0.65	0/1709
7	CG	0.45	0/1276	0.65	0/1709
8	AH	0.51	0/1136	0.74	0/1527
8	CH	0.46	0/1136	0.74	0/1527
9	AI	0.44	0/1027	0.68	0/1373
9	CI	0.41	0/1027	0.67	0/1373
10	AJ	0.47	0/808	0.72	0/1087
10	CJ	0.42	0/808	0.71	0/1087
11	AK	0.50	0/900	0.70	0/1213
11	CK	0.47	0/900	0.70	0/1213
12	AL	0.52	0/987	0.75	0/1322
12	CL	0.48	0/987	0.74	0/1322
13	AM	0.41	0/999	0.69	0/1338
13	CM	0.39	0/999	0.69	0/1338
14	AN	0.49	0/501	0.69	0/664
14	CN	0.47	0/501	0.69	0/664
15	AO	0.45	0/745	0.67	0/992
15	CO	0.43	0/745	0.66	0/992
16	AP	0.45	0/717	0.68	0/965
16	CP	0.43	0/717	0.68	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.51	0/837	0.69	0/1119
17	CQ	0.49	0/837	0.69	0/1119
18	AR	0.47	0/579	0.72	0/768
18	CR	0.45	0/579	0.73	0/768
19	AS	0.46	0/643	0.68	1/867 (0.1%)
19	CS	0.44	0/643	0.67	1/867 (0.1%)
20	AT	0.40	0/765	0.66	0/1007
20	CT	0.39	0/765	0.66	0/1007
21	AU	0.52	0/213	0.65	0/279
21	CU	0.50	0/213	0.65	0/279
22	AV	0.57	0/1810	0.73	0/2821
22	AW	0.41	0/1810	0.72	0/2821
22	CV	0.54	0/1810	0.70	0/2821
22	CW	0.38	0/1810	0.69	0/2821
23	AX	0.82	0/257	0.86	0/398
23	CX	0.79	0/257	0.84	1/398 (0.3%)
24	AY	0.40	0/5313	0.69	0/7195
24	CY	0.42	0/5313	0.69	1/7195 (0.0%)
25	B0	0.43	0/671	0.66	0/892
25	D0	0.42	0/671	0.67	0/892
26	B1	0.48	0/739	0.78	0/983
26	D1	0.45	0/739	0.69	0/983
27	B2	0.36	0/600	0.66	0/793
27	D2	0.37	0/600	0.62	0/793
28	B3	0.43	0/473	0.63	0/636
28	D3	0.43	0/473	0.64	0/636
29	B4	0.68	0/461	0.92	2/623 (0.3%)
29	D4	0.74	0/461	0.93	2/623 (0.3%)
30	B5	0.43	0/473	0.75	0/639
30	D5	0.44	0/473	0.74	0/639
31	B6	0.64	0/440	0.96	1/586 (0.2%)
31	D6	0.64	0/440	0.96	1/586 (0.2%)
32	B7	0.45	0/427	0.71	0/563
32	D7	0.45	0/427	0.71	0/563
33	B8	0.54	0/516	0.83	0/681
33	D8	0.54	0/516	0.83	0/681
34	B9	0.47	0/310	0.69	0/407
34	D9	0.46	0/310	0.70	0/407
35	BA	0.56	3/69972 (0.0%)	0.75	35/109237 (0.0%)
35	DA	0.55	4/69972 (0.0%)	0.75	36/109237 (0.0%)
36	BB	0.44	0/2853	0.72	1/4451 (0.0%)
36	DB	0.44	0/2853	0.72	0/4451
37	BC	0.35	0/1774	0.61	0/2391

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	DC	0.34	0/1774	0.61	0/2391
38	BD	0.54	0/2195	0.83	0/2955
38	DD	0.53	0/2195	0.82	0/2955
39	BE	0.48	0/1597	0.74	0/2155
39	DE	0.46	0/1597	0.74	0/2155
40	BF	0.39	0/1659	0.66	0/2246
40	DF	0.38	0/1659	0.66	0/2246
41	BG	0.42	0/1498	0.78	1/2013 (0.0%)
41	DG	0.43	0/1498	0.74	0/2013
42	BH	0.36	0/1293	0.71	0/1746
42	DH	0.35	0/1293	0.69	0/1746
44	BK	0.35	0/1045	0.60	0/1418
44	DK	0.36	0/1045	0.60	0/1418
46	BN	0.40	0/1132	0.73	1/1527 (0.1%)
46	DN	0.39	0/1132	0.73	1/1527 (0.1%)
47	BO	0.49	0/943	0.72	0/1269
47	DO	0.47	0/943	0.72	0/1269
48	BP	0.44	0/1131	0.93	4/1504 (0.3%)
48	DP	0.44	0/1131	0.91	4/1504 (0.3%)
49	BQ	0.49	0/1143	0.69	0/1527
49	DQ	0.48	0/1143	0.70	0/1527
50	BR	0.39	0/974	0.68	0/1302
50	DR	0.38	0/974	0.68	1/1302 (0.1%)
51	BS	0.41	0/779	0.69	0/1038
51	DS	0.40	0/779	0.70	0/1038
52	BT	0.47	0/1156	0.79	2/1544 (0.1%)
52	DT	0.49	0/1156	0.79	1/1544 (0.1%)
53	BU	0.43	0/975	0.68	0/1297
53	DU	0.44	0/975	0.69	0/1297
54	BV	0.39	0/790	0.70	0/1057
54	DV	0.39	0/790	0.70	0/1057
55	BW	0.37	0/907	0.65	0/1216
55	DW	0.39	0/907	0.65	0/1216
56	BX	0.42	0/740	0.66	0/995
56	DX	0.42	0/740	0.66	0/995
57	BY	0.41	0/824	0.67	0/1100
57	DY	0.42	0/824	0.68	0/1100
58	BZ	0.48	0/1500	0.74	0/2037
58	DZ	0.46	0/1500	0.73	0/2037
All	All	0.53	10/333656 (0.0%)	0.74	143/497270 (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	48
1	CA	0	43
22	AV	0	3
22	CV	0	1
23	AX	0	2
23	CX	0	1
35	BA	2	69
35	DA	2	58
36	BB	0	1
36	DB	0	1
37	BC	0	1
37	DC	0	1
44	BK	0	1
44	DK	0	1
46	DN	0	1
All	All	4	232

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	2506	U	N1-C2	7.05	1.44	1.38
35	DA	2506	U	N1-C2	6.48	1.44	1.38
35	BA	272(I)	U	C1'-N1	5.69	1.57	1.48
1	AA	1417	G	C6-O6	5.55	1.29	1.24
35	DA	272(I)	U	C1'-N1	5.49	1.56	1.48
35	DA	1786	A	C5-C6	-5.20	1.36	1.41
35	DA	1671	U	N3-C4	5.12	1.43	1.38
1	CA	1108	G	C5-C6	5.04	1.47	1.42
1	CA	299	G	C6-O6	5.03	1.28	1.24
35	BA	1828	G	P-OP2	5.02	1.57	1.49

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	BA	1992	G	C2'-C3'-O3'	10.77	133.19	109.50
35	DA	1992	G	C2'-C3'-O3'	10.61	132.85	109.50
1	CA	575	G	C2'-C3'-O3'	9.68	130.80	109.50
1	AA	575	G	C2'-C3'-O3'	9.65	130.72	109.50
35	BA	945	A	N9-C1'-C2'	9.34	126.14	114.00
35	DA	945	A	N9-C1'-C2'	9.33	126.13	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	DA	1799	G	C2'-C3'-O3'	9.18	129.70	109.50
35	BA	1799	G	C2'-C3'-O3'	9.10	129.52	109.50
1	CA	1498	U	C2'-C3'-O3'	9.09	129.49	109.50
1	AA	1498	U	C2'-C3'-O3'	8.88	129.05	109.50
1	AA	115	G	C2'-C3'-O3'	8.46	128.11	109.50
35	DA	1379	A	N9-C1'-C2'	8.43	124.96	114.00
1	CA	115	G	C2'-C3'-O3'	8.27	127.69	109.50
35	BA	1379	A	N9-C1'-C2'	8.20	124.66	114.00
35	DA	1786	A	N9-C1'-C2'	7.82	124.16	114.00
35	BA	1786	A	N9-C1'-C2'	7.61	123.89	114.00
1	AA	1502	A	N9-C1'-C2'	7.58	123.85	114.00
35	DA	2799	C	C2'-C3'-O3'	7.49	125.97	109.50
35	BA	2799	C	C2'-C3'-O3'	7.44	125.87	109.50
36	BB	103	G	C5'-C4'-C3'	-7.43	104.11	116.00
35	BA	1156	A	N9-C1'-C2'	7.15	123.29	114.00
35	DA	1156	A	N9-C1'-C2'	7.11	123.25	114.00
1	CA	60	A	C2'-C3'-O3'	7.11	125.14	109.50
48	BP	53	GLY	N-CA-C	-7.06	95.45	113.10
1	AA	60	A	C2'-C3'-O3'	7.04	124.99	109.50
48	DP	53	GLY	N-CA-C	-6.98	95.64	113.10
1	CA	921	U	C5'-C4'-C3'	-6.96	104.86	116.00
1	AA	921	U	C5'-C4'-C3'	-6.76	105.18	116.00
48	DP	52	GLU	N-CA-C	6.76	129.25	111.00
48	BP	52	GLU	N-CA-C	6.72	129.15	111.00
35	DA	1654	A	C5'-C4'-C3'	6.65	126.64	116.00
35	BA	788	A	N9-C1'-C2'	6.55	122.51	114.00
35	BA	1396	U	N1-C1'-C2'	6.51	122.46	114.00
35	BA	1654	A	C5'-C4'-C3'	6.48	126.37	116.00
1	AA	1285	A	C2'-C3'-O3'	6.45	124.02	113.70
1	CA	1505	G	O5'-P-OP1	-6.43	99.91	105.70
35	DA	1020	A	N9-C1'-C2'	6.43	122.36	114.00
1	CA	792	A	C5'-C4'-C3'	-6.36	105.83	116.00
35	DA	1396	U	N1-C1'-C2'	6.35	122.25	114.00
1	AA	1457	G	N9-C1'-C2'	-6.33	105.03	112.00
19	AS	5	LEU	CA-CB-CG	6.33	129.85	115.30
1	AA	792	A	C5'-C4'-C3'	-6.31	105.90	116.00
35	BA	1236	G	N9-C1'-C2'	6.30	122.20	114.00
31	D6	23	THR	N-CA-C	6.29	127.98	111.00
1	AA	328	C	C2'-C3'-O3'	6.28	123.75	113.70
35	BA	49	A	C2'-C3'-O3'	6.28	123.75	113.70
1	CA	533	A	C2'-C3'-O3'	6.27	123.73	113.70
29	B4	43	TYR	N-CA-C	6.26	127.92	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B6	23	THR	N-CA-C	6.24	127.86	111.00
29	D4	43	TYR	N-CA-C	6.23	127.82	111.00
1	AA	1190	G	N9-C1'-C2'	6.21	122.07	114.00
1	AA	1201	A	C2'-C3'-O3'	6.20	123.62	113.70
35	BA	1020	A	N9-C1'-C2'	6.17	122.03	114.00
35	DA	788	A	N9-C1'-C2'	6.15	122.00	114.00
35	BA	2732	G	N9-C1'-C2'	6.14	121.99	114.00
35	DA	945	A	O4'-C1'-N9	6.06	113.05	108.20
35	DA	1236	G	N9-C1'-C2'	6.06	121.87	114.00
48	DP	58	THR	N-CA-C	-6.03	94.73	111.00
1	CA	428	G	C2'-C3'-O3'	6.02	123.33	113.70
1	CA	1502	A	N9-C1'-C2'	6.02	121.82	114.00
35	BA	945	A	O4'-C1'-N9	6.00	113.00	108.20
35	BA	2225	A	C2'-C3'-O3'	6.00	123.29	113.70
1	CA	1190	G	N9-C1'-C2'	5.99	121.78	114.00
35	DA	1819	A	N9-C1'-C2'	5.99	121.79	114.00
1	AA	533	A	C2'-C3'-O3'	5.95	123.22	113.70
35	DA	49	A	C2'-C3'-O3'	5.95	123.22	113.70
1	CA	1493	A	C2'-C3'-O3'	5.95	123.22	113.70
1	CA	204	U	O4'-C1'-N1	5.94	112.95	108.20
35	BA	1493	C	N1-C1'-C2'	5.93	121.71	114.00
1	AA	1109	C	OP2-P-O3'	5.93	118.24	105.20
48	BP	58	THR	N-CA-C	-5.93	95.00	111.00
1	CA	328	C	C2'-C3'-O3'	5.92	123.18	113.70
1	AA	428	G	C2'-C3'-O3'	5.85	123.05	113.70
19	CS	5	LEU	CA-CB-CG	5.84	128.74	115.30
1	AA	1398	A	C5'-C4'-C3'	-5.84	106.66	116.00
35	BA	1819	A	N9-C1'-C2'	5.84	121.59	114.00
35	DA	2732	G	N9-C1'-C2'	5.81	121.56	114.00
35	DA	1493	C	N1-C1'-C2'	5.78	121.51	114.00
35	BA	2172	U	C2'-C3'-O3'	5.75	122.91	113.70
1	CA	1285	A	C2'-C3'-O3'	5.75	122.90	113.70
1	AA	204	U	O4'-C1'-N1	5.72	112.78	108.20
35	BA	1252	G	N9-C1'-C2'	5.71	121.42	114.00
35	DA	2225	A	C2'-C3'-O3'	5.71	122.83	113.70
35	BA	2835	A	N9-C1'-C2'	5.70	121.41	114.00
1	AA	30	U	N1-C1'-C2'	5.70	121.41	114.00
35	BA	1838	C	C2'-C3'-O3'	5.69	122.81	113.70
1	CA	1201	A	C2'-C3'-O3'	5.68	122.79	113.70
35	BA	2345	G	C1'-O4'-C4'	-5.64	105.39	109.90
35	BA	2026	C	C5'-C4'-C3'	-5.62	107.02	116.00
35	BA	479	A	N9-C1'-C2'	5.59	121.27	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	DA	1237	A	N9-C1'-C2'	5.58	121.25	114.00
35	DA	2481	G	N9-C1'-C2'	5.56	121.23	114.00
35	BA	2481	G	N9-C1'-C2'	5.54	121.21	114.00
35	BA	675	A	N9-C1'-C2'	5.54	121.20	114.00
35	BA	1237	A	N9-C1'-C2'	5.54	121.19	114.00
35	DA	2172	U	C2'-C3'-O3'	5.52	122.53	113.70
1	CA	366	C	C2'-C3'-O3'	5.48	122.47	113.70
35	DA	1252	G	N9-C1'-C2'	5.46	121.10	114.00
35	DA	479	A	N9-C1'-C2'	5.44	121.07	114.00
35	DA	906	G	C5'-C4'-C3'	-5.43	107.31	116.00
35	DA	2779	U	O4'-C1'-N1	5.42	112.53	108.20
1	AA	366	C	C2'-C3'-O3'	5.41	122.35	113.70
35	DA	1838	C	C2'-C3'-O3'	5.40	122.34	113.70
35	DA	1904	G	C5'-C4'-C3'	-5.40	107.36	116.00
35	BA	1959	G	C5'-C4'-C3'	-5.37	107.41	116.00
35	BA	1948	G	C5'-C4'-O4'	-5.36	102.66	109.10
35	DA	748	G	N9-C1'-C2'	5.36	120.97	114.00
23	CX	11	U	N1-C1'-C2'	5.32	120.92	114.00
35	DA	2835	A	N9-C1'-C2'	5.31	120.90	114.00
35	BA	1818	U	C5'-C4'-C3'	-5.27	107.56	116.00
1	CA	30	U	N1-C1'-C2'	5.26	120.84	114.00
35	DA	2026	C	C5'-C4'-C3'	-5.25	107.60	116.00
1	AA	481	G	C5'-C4'-C3'	-5.23	107.63	116.00
35	DA	675	A	N9-C1'-C2'	5.22	120.79	114.00
46	BN	3	THR	N-CA-C	-5.22	96.92	111.00
52	BT	29	ARG	N-CA-C	5.22	125.08	111.00
29	D4	53	GLU	N-CA-C	5.21	125.06	111.00
35	DA	2345	G	C1'-O4'-C4'	-5.18	105.75	109.90
35	BA	2126	A	N9-C1'-C2'	5.18	120.73	114.00
24	CY	34	TYR	N-CA-C	-5.18	97.02	111.00
1	AA	812	C	OP2-P-O3'	5.17	116.59	105.20
1	AA	1049	U	N1-C1'-C2'	5.15	120.70	114.00
35	BA	2779	U	O4'-C1'-N1	5.15	112.32	108.20
1	AA	1065	U	N1-C1'-C2'	5.15	120.69	114.00
35	DA	2035	G	N9-C1'-C2'	5.15	120.69	114.00
46	DN	3	THR	N-CA-C	-5.15	97.10	111.00
1	CA	1049	U	N1-C1'-C2'	5.14	120.68	114.00
52	DT	29	ARG	N-CA-C	5.13	124.86	111.00
48	DP	41	ARG	N-CA-C	-5.12	97.17	111.00
35	BA	1459	G	N9-C1'-C2'	5.10	120.63	114.00
41	BG	139	LEU	CA-CB-CG	5.09	127.01	115.30
1	AA	1498	U	OP2-P-O3'	5.09	116.39	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B4	53	GLU	N-CA-C	5.07	124.70	111.00
35	DA	1948	G	C5'-C4'-O4'	-5.06	103.03	109.10
48	BP	41	ARG	N-CA-C	-5.05	97.36	111.00
35	DA	1654	A	N9-C1'-C2'	-5.03	106.47	112.00
1	AA	754	C	N1-C1'-C2'	5.03	120.53	114.00
1	AA	1456	G	N9-C1'-C2'	5.03	120.53	114.00
1	CA	754	C	N1-C1'-C2'	5.02	120.53	114.00
50	DR	4	LEU	CA-CB-CG	5.02	126.85	115.30
35	DA	1351	C	C5'-C4'-C3'	-5.01	107.98	116.00
52	BT	80	SER	N-CA-C	5.01	124.53	111.00
35	BA	848	G	C5'-C4'-C3'	-5.00	107.99	116.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	BA	1799	G	C3'
35	BA	1992	G	C3'
35	DA	1799	G	C3'
35	DA	1992	G	C3'

All (232) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1053	G	Sidechain
1	AA	1055	A	Sidechain
1	AA	1077	G	Sidechain
1	AA	108	G	Sidechain
1	AA	1109	C	Sidechain
1	AA	112	G	Sidechain
1	AA	1184	G	Sidechain
1	AA	1190	G	Sidechain
1	AA	1219	U	Sidechain
1	AA	1226	C	Sidechain
1	AA	1331	G	Sidechain
1	AA	1355	G	Sidechain
1	AA	1370	G	Sidechain
1	AA	1391	U	Sidechain
1	AA	1401	G	Sidechain
1	AA	1402	C	Sidechain
1	AA	1403	C	Sidechain
1	AA	1414	U	Sidechain
1	AA	1485	U	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1498	U	Sidechain
1	AA	1502	A	Sidechain
1	AA	1512	U	Sidechain
1	AA	1519	A	Sidechain
1	AA	30	U	Sidechain
1	AA	309	G	Sidechain
1	AA	361	G	Sidechain
1	AA	387	U	Sidechain
1	AA	39	G	Sidechain
1	AA	436	C	Sidechain
1	AA	5	U	Sidechain
1	AA	573	A	Sidechain
1	AA	582	U	Sidechain
1	AA	598	U	Sidechain
1	AA	672	U	Sidechain
1	AA	691	G	Sidechain
1	AA	724	G	Sidechain
1	AA	741	G	Sidechain
1	AA	748	C	Sidechain
1	AA	760	G	Sidechain
1	AA	781	A	Sidechain
1	AA	835	U	Sidechain
1	AA	887	G	Sidechain
1	AA	898	G	Sidechain
1	AA	963	G	Sidechain
1	AA	969	A	Sidechain
1	AA	971	G	Sidechain
1	AA	981	U	Sidechain
1	AA	991	U	Sidechain
22	AV	29	G	Sidechain
22	AV	4	G	Sidechain
22	AV	8	U	Sidechain
23	AX	12	A	Sidechain
23	AX	17	U	Sidechain
35	BA	1142(A)	A	Sidechain
35	BA	1156	A	Sidechain
35	BA	1215	G	Sidechain
35	BA	1236	G	Sidechain
35	BA	1238	G	Sidechain
35	BA	1253	A	Sidechain
35	BA	1302	A	Sidechain
35	BA	1379	A	Sidechain

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Mol	Chain	Res	Type	Group
35	BA	1496	A	Sidechain
35	BA	1614	A	Sidechain
35	BA	1623	G	Sidechain
35	BA	1633	G	Sidechain
35	BA	1645	G	Sidechain
35	BA	1772	G	Sidechain
35	BA	1776	G	Sidechain
35	BA	1781	C	Sidechain
35	BA	1822	G	Sidechain
35	BA	1827	C	Sidechain
35	BA	1919	A	Sidechain
35	BA	1920	C	Sidechain
35	BA	1926	U	Sidechain
35	BA	1929	G	Sidechain
35	BA	1952	A	Sidechain
35	BA	1992	G	Sidechain
35	BA	200	U	Sidechain
35	BA	2009	G	Sidechain
35	BA	2010	G	Sidechain
35	BA	2031	A	Sidechain
35	BA	2051	A	Sidechain
35	BA	2052	G	Sidechain
35	BA	2053	G	Sidechain
35	BA	2059	A	Sidechain
35	BA	2079	U	Sidechain
35	BA	2126	A	Sidechain
35	BA	2250	G	Sidechain
35	BA	2266	A	Sidechain
35	BA	2296	U	Sidechain
35	BA	2340	G	Sidechain
35	BA	2344	U	Sidechain
35	BA	2401	U	Sidechain
35	BA	2464	C	Sidechain
35	BA	248	G	Sidechain
35	BA	2481	G	Sidechain
35	BA	2494	G	Sidechain
35	BA	2504	U	Sidechain
35	BA	2506	U	Sidechain
35	BA	2508	G	Sidechain
35	BA	2518	A	Sidechain
35	BA	2564	A	Sidechain
35	BA	2569	G	Sidechain

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Mol	Chain	Res	Type	Group
35	BA	2609	U	Sidechain
35	BA	2659	G	Sidechain
35	BA	2685	G	Sidechain
35	BA	2826	A	Sidechain
35	BA	2835	A	Sidechain
35	BA	395	U	Sidechain
35	BA	463	G	Sidechain
35	BA	528	A	Sidechain
35	BA	562	U	Sidechain
35	BA	686	G	Sidechain
35	BA	688	U	Sidechain
35	BA	742	G	Sidechain
35	BA	788	A	Sidechain
35	BA	83	G	Sidechain
35	BA	845	G	Sidechain
35	BA	895	U	Sidechain
35	BA	913	U	Sidechain
35	BA	945	A	Sidechain
35	BA	958	U	Sidechain
36	BB	21	G	Sidechain
37	BC	28	ARG	Sidechain
44	BK	6	ALA	Peptide
1	CA	1053	G	Sidechain
1	CA	1077	G	Sidechain
1	CA	1190	G	Sidechain
1	CA	1226	C	Sidechain
1	CA	1231	G	Sidechain
1	CA	1331	G	Sidechain
1	CA	1355	G	Sidechain
1	CA	1370	G	Sidechain
1	CA	1502	A	Sidechain
1	CA	1505	G	Sidechain
1	CA	1512	U	Sidechain
1	CA	1519	A	Sidechain
1	CA	1525	G	Sidechain
1	CA	1527	C	Sidechain
1	CA	204	U	Sidechain
1	CA	223	U	Sidechain
1	CA	250	A	Sidechain
1	CA	253	U	Sidechain
1	CA	30	U	Sidechain
1	CA	309	G	Sidechain

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Mol	Chain	Res	Type	Group
1	CA	361	G	Sidechain
1	CA	39	G	Sidechain
1	CA	436	C	Sidechain
1	CA	5	U	Sidechain
1	CA	548	G	Sidechain
1	CA	573	A	Sidechain
1	CA	582	U	Sidechain
1	CA	598	U	Sidechain
1	CA	641	U	Sidechain
1	CA	657	G	Sidechain
1	CA	672	U	Sidechain
1	CA	691	G	Sidechain
1	CA	724	G	Sidechain
1	CA	727	G	Sidechain
1	CA	741	G	Sidechain
1	CA	760	G	Sidechain
1	CA	781	A	Sidechain
1	CA	835	U	Sidechain
1	CA	887	G	Sidechain
1	CA	898	G	Sidechain
1	CA	931	C	Sidechain
1	CA	971	G	Sidechain
1	CA	991	U	Sidechain
22	CV	4	G	Sidechain
23	CX	11	U	Sidechain
35	DA	1156	A	Sidechain
35	DA	1236	G	Sidechain
35	DA	1238	G	Sidechain
35	DA	1302	A	Sidechain
35	DA	1379	A	Sidechain
35	DA	1614	A	Sidechain
35	DA	1623	G	Sidechain
35	DA	1645	G	Sidechain
35	DA	1772	G	Sidechain
35	DA	1776	G	Sidechain
35	DA	1781	C	Sidechain
35	DA	1822	G	Sidechain
35	DA	1907	G	Sidechain
35	DA	1919	A	Sidechain
35	DA	1920	C	Sidechain
35	DA	1926	U	Sidechain
35	DA	1952	A	Sidechain

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Mol	Chain	Res	Type	Group
35	DA	1992	G	Sidechain
35	DA	2009	G	Sidechain
35	DA	2010	G	Sidechain
35	DA	2031	A	Sidechain
35	DA	2051	A	Sidechain
35	DA	2052	G	Sidechain
35	DA	2053	G	Sidechain
35	DA	2059	A	Sidechain
35	DA	2061	G	Sidechain
35	DA	2079	U	Sidechain
35	DA	2126	A	Sidechain
35	DA	2250	G	Sidechain
35	DA	2266	A	Sidechain
35	DA	2340	G	Sidechain
35	DA	2344	U	Sidechain
35	DA	2401	U	Sidechain
35	DA	2464	C	Sidechain
35	DA	248	G	Sidechain
35	DA	2481	G	Sidechain
35	DA	2494	G	Sidechain
35	DA	2506	U	Sidechain
35	DA	2508	G	Sidechain
35	DA	2518	A	Sidechain
35	DA	2659	G	Sidechain
35	DA	2685	G	Sidechain
35	DA	2732	G	Sidechain
35	DA	2835	A	Sidechain
35	DA	395	U	Sidechain
35	DA	463	G	Sidechain
35	DA	528	A	Sidechain
35	DA	686	G	Sidechain
35	DA	688	U	Sidechain
35	DA	690	G	Sidechain
35	DA	742	G	Sidechain
35	DA	788	A	Sidechain
35	DA	83	G	Sidechain
35	DA	845	G	Sidechain
35	DA	895	U	Sidechain
35	DA	913	U	Sidechain
35	DA	945	A	Sidechain
35	DA	958	U	Sidechain
36	DB	21	G	Sidechain

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Mol	Chain	Res	Type	Group
37	DC	28	ARG	Sidechain
44	DK	5	VAL	Peptide
46	DN	72	TYR	Sidechain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	233/256 (91%)	139 (60%)	53 (23%)	41 (18%)	0	2
2	CB	233/256 (91%)	140 (60%)	51 (22%)	42 (18%)	0	2
3	AC	205/239 (86%)	133 (65%)	50 (24%)	22 (11%)	0	7
3	CC	205/239 (86%)	132 (64%)	52 (25%)	21 (10%)	0	7
4	AD	206/209 (99%)	134 (65%)	50 (24%)	22 (11%)	0	7
4	CD	206/209 (99%)	134 (65%)	51 (25%)	21 (10%)	0	7
5	AE	149/162 (92%)	119 (80%)	21 (14%)	9 (6%)	1	17
5	CE	149/162 (92%)	117 (78%)	24 (16%)	8 (5%)	2	19
6	AF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1	14
6	CF	99/101 (98%)	74 (75%)	18 (18%)	7 (7%)	1	14
7	AG	153/156 (98%)	109 (71%)	34 (22%)	10 (6%)	1	16
7	CG	153/156 (98%)	110 (72%)	32 (21%)	11 (7%)	1	13
8	AH	136/138 (99%)	103 (76%)	30 (22%)	3 (2%)	6	39
8	CH	136/138 (99%)	105 (77%)	27 (20%)	4 (3%)	4	33
9	AI	121/128 (94%)	81 (67%)	26 (22%)	14 (12%)	0	6
9	CI	121/128 (94%)	82 (68%)	27 (22%)	12 (10%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	97/105 (92%)	60 (62%)	21 (22%)	16 (16%)	0	3
10	CJ	97/105 (92%)	61 (63%)	20 (21%)	16 (16%)	0	3
11	AK	117/129 (91%)	91 (78%)	20 (17%)	6 (5%)	2	20
11	CK	117/129 (91%)	91 (78%)	20 (17%)	6 (5%)	2	20
12	AL	123/132 (93%)	82 (67%)	23 (19%)	18 (15%)	0	3
12	CL	123/132 (93%)	82 (67%)	22 (18%)	19 (15%)	0	3
13	AM	123/126 (98%)	77 (63%)	25 (20%)	21 (17%)	0	2
13	CM	123/126 (98%)	77 (63%)	26 (21%)	20 (16%)	0	3
14	AN	58/61 (95%)	47 (81%)	7 (12%)	4 (7%)	1	14
14	CN	58/61 (95%)	46 (79%)	7 (12%)	5 (9%)	1	10
15	AO	86/89 (97%)	55 (64%)	23 (27%)	8 (9%)	0	9
15	CO	86/89 (97%)	53 (62%)	24 (28%)	9 (10%)	0	7
16	AP	82/88 (93%)	60 (73%)	15 (18%)	7 (8%)	1	10
16	CP	82/88 (93%)	60 (73%)	15 (18%)	7 (8%)	1	10
17	AQ	98/105 (93%)	78 (80%)	15 (15%)	5 (5%)	2	20
17	CQ	98/105 (93%)	78 (80%)	16 (16%)	4 (4%)	3	26
18	AR	68/88 (77%)	52 (76%)	11 (16%)	5 (7%)	1	13
18	CR	68/88 (77%)	51 (75%)	12 (18%)	5 (7%)	1	13
19	AS	77/93 (83%)	43 (56%)	14 (18%)	20 (26%)	0	0
19	CS	77/93 (83%)	43 (56%)	15 (20%)	19 (25%)	0	0
20	AT	97/106 (92%)	52 (54%)	30 (31%)	15 (16%)	0	3
20	CT	97/106 (92%)	53 (55%)	29 (30%)	15 (16%)	0	3
21	AU	23/27 (85%)	14 (61%)	6 (26%)	3 (13%)	0	5
21	CU	23/27 (85%)	14 (61%)	5 (22%)	4 (17%)	0	2
24	AY	663/691 (96%)	435 (66%)	137 (21%)	91 (14%)	0	4
24	CY	663/691 (96%)	449 (68%)	134 (20%)	80 (12%)	0	5
25	B0	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	2	21
25	D0	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	2	21
26	B1	92/98 (94%)	64 (70%)	15 (16%)	13 (14%)	0	4
26	D1	92/98 (94%)	67 (73%)	13 (14%)	12 (13%)	0	5
27	B2	69/72 (96%)	35 (51%)	18 (26%)	16 (23%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	D2	69/72 (96%)	29 (42%)	31 (45%)	9 (13%)	0	5
28	B3	58/60 (97%)	41 (71%)	12 (21%)	5 (9%)	1	10
28	D3	58/60 (97%)	41 (71%)	12 (21%)	5 (9%)	1	10
29	B4	56/71 (79%)	27 (48%)	14 (25%)	15 (27%)	0	0
29	D4	56/71 (79%)	28 (50%)	13 (23%)	15 (27%)	0	0
30	B5	57/60 (95%)	37 (65%)	9 (16%)	11 (19%)	0	2
30	D5	57/60 (95%)	38 (67%)	7 (12%)	12 (21%)	0	1
31	B6	48/54 (89%)	21 (44%)	12 (25%)	15 (31%)	0	0
31	D6	48/54 (89%)	22 (46%)	12 (25%)	14 (29%)	0	0
32	B7	47/49 (96%)	35 (74%)	11 (23%)	1 (2%)	7	40
32	D7	47/49 (96%)	35 (74%)	11 (23%)	1 (2%)	7	40
33	B8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	2
33	D8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	2
34	B9	35/37 (95%)	21 (60%)	9 (26%)	5 (14%)	0	4
34	D9	35/37 (95%)	21 (60%)	8 (23%)	6 (17%)	0	2
37	BC	226/229 (99%)	163 (72%)	51 (23%)	12 (5%)	2	19
37	DC	226/229 (99%)	163 (72%)	50 (22%)	13 (6%)	1	18
38	BD	273/276 (99%)	189 (69%)	50 (18%)	34 (12%)	0	5
38	DD	273/276 (99%)	188 (69%)	50 (18%)	35 (13%)	0	5
39	BE	203/206 (98%)	122 (60%)	45 (22%)	36 (18%)	0	2
39	DE	203/206 (98%)	124 (61%)	44 (22%)	35 (17%)	0	2
40	BF	206/210 (98%)	132 (64%)	44 (21%)	30 (15%)	0	3
40	DF	206/210 (98%)	133 (65%)	42 (20%)	31 (15%)	0	3
41	BG	177/182 (97%)	110 (62%)	43 (24%)	24 (14%)	0	4
41	DG	177/182 (97%)	115 (65%)	36 (20%)	26 (15%)	0	3
42	BH	165/180 (92%)	86 (52%)	40 (24%)	39 (24%)	0	0
42	DH	165/180 (92%)	86 (52%)	40 (24%)	39 (24%)	0	0
44	BK	138/147 (94%)	92 (67%)	35 (25%)	11 (8%)	1	11
44	DK	138/147 (94%)	92 (67%)	35 (25%)	11 (8%)	1	11
46	BN	137/140 (98%)	88 (64%)	28 (20%)	21 (15%)	0	3
46	DN	137/140 (98%)	88 (64%)	28 (20%)	21 (15%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	BO	120/122 (98%)	91 (76%)	19 (16%)	10 (8%)	1	10
47	DO	120/122 (98%)	93 (78%)	17 (14%)	10 (8%)	1	10
48	BP	144/150 (96%)	72 (50%)	45 (31%)	27 (19%)	0	2
48	DP	144/150 (96%)	72 (50%)	44 (31%)	28 (19%)	0	2
49	BQ	139/141 (99%)	106 (76%)	26 (19%)	7 (5%)	2	21
49	DQ	139/141 (99%)	106 (76%)	26 (19%)	7 (5%)	2	21
50	BR	115/118 (98%)	81 (70%)	20 (17%)	14 (12%)	0	5
50	DR	115/118 (98%)	81 (70%)	20 (17%)	14 (12%)	0	5
51	BS	97/112 (87%)	41 (42%)	35 (36%)	21 (22%)	0	1
51	DS	97/112 (87%)	41 (42%)	35 (36%)	21 (22%)	0	1
52	BT	136/146 (93%)	76 (56%)	32 (24%)	28 (21%)	0	1
52	DT	136/146 (93%)	75 (55%)	32 (24%)	29 (21%)	0	1
53	BU	115/118 (98%)	66 (57%)	37 (32%)	12 (10%)	0	7
53	DU	115/118 (98%)	67 (58%)	35 (30%)	13 (11%)	0	6
54	BV	99/101 (98%)	69 (70%)	12 (12%)	18 (18%)	0	2
54	DV	99/101 (98%)	69 (70%)	12 (12%)	18 (18%)	0	2
55	BW	111/113 (98%)	80 (72%)	21 (19%)	10 (9%)	1	9
55	DW	111/113 (98%)	81 (73%)	21 (19%)	9 (8%)	1	11
56	BX	91/96 (95%)	56 (62%)	26 (29%)	9 (10%)	0	8
56	DX	91/96 (95%)	57 (63%)	25 (28%)	9 (10%)	0	8
57	BY	105/110 (96%)	42 (40%)	36 (34%)	27 (26%)	0	0
57	DY	105/110 (96%)	43 (41%)	36 (34%)	26 (25%)	0	0
58	BZ	183/206 (89%)	108 (59%)	42 (23%)	33 (18%)	0	2
58	DZ	183/206 (89%)	114 (62%)	37 (20%)	32 (18%)	0	2
All	All	13200/13966 (94%)	8607 (65%)	2874 (22%)	1719 (13%)	0	5

All (1719) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	12	GLU
2	AB	13	ALA
2	AB	15	VAL
2	AB	20	GLU
2	AB	95	GLN

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Mol	Chain	Res	Type
2	AB	129	GLU
2	AB	190	THR
2	AB	195	ASP
2	AB	233	SER
2	AB	239	VAL
3	AC	12	LEU
3	AC	47	LEU
3	AC	61	ALA
3	AC	95	THR
3	AC	154	SER
3	AC	156	ARG
3	AC	207	VAL
4	AD	3	ARG
4	AD	13	ARG
4	AD	14	ARG
4	AD	18	LYS
4	AD	30	LYS
4	AD	32	ALA
4	AD	44	GLY
4	AD	153	ARG
4	AD	179	GLU
5	AE	11	ILE
6	AF	39	LYS
7	AG	8	GLU
7	AG	52	GLU
7	AG	90	GLU
8	AH	105	ARG
9	AI	41	VAL
9	AI	43	ALA
9	AI	61	ALA
9	AI	89	ASN
10	AJ	33	GLN
10	AJ	36	GLY
10	AJ	55	LYS
10	AJ	56	HIS
10	AJ	57	LYS
10	AJ	59	SER
10	AJ	75	ILE
11	AK	123	LYS
11	AK	127	LYS
12	AL	18	VAL
12	AL	27	LEU

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Mol	Chain	Res	Type
12	AL	28	LYS
12	AL	38	THR
12	AL	45	PRO
12	AL	81	SER
12	AL	91	LYS
13	AM	12	ASN
13	AM	67	GLU
13	AM	70	LEU
13	AM	83	ASP
13	AM	90	LEU
13	AM	91	ARG
13	AM	100	GLY
13	AM	118	ALA
13	AM	124	PRO
14	AN	15	LYS
14	AN	29	ARG
15	AO	24	SER
16	AP	83	GLU
17	AQ	13	ASP
17	AQ	49	GLU
18	AR	37	VAL
18	AR	38	GLU
18	AR	45	SER
19	AS	10	PHE
19	AS	27	GLU
19	AS	28	LYS
19	AS	29	ARG
19	AS	47	HIS
19	AS	61	TYR
20	AT	48	LYS
20	AT	74	LYS
20	AT	99	LEU
21	AU	3	LYS
24	AY	6	GLU
24	AY	19	ALA
24	AY	21	ILE
24	AY	23	ALA
24	AY	66	THR
24	AY	68	ALA
24	AY	84	THR
24	AY	85	PRO
24	AY	88	VAL

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Mol	Chain	Res	Type
24	AY	92	ILE
24	AY	119	GLU
24	AY	121	VAL
24	AY	129	LYS
24	AY	197	ARG
24	AY	203	GLU
24	AY	204	GLU
24	AY	205	TYR
24	AY	206	LEU
24	AY	209	ALA
24	AY	210	ARG
24	AY	251	ILE
24	AY	276	VAL
24	AY	360	ALA
24	AY	385	THR
24	AY	396	ARG
24	AY	402	ILE
24	AY	447	GLY
24	AY	448	GLN
24	AY	456	GLU
24	AY	498	ILE
24	AY	519	ARG
24	AY	530	VAL
24	AY	559	PRO
24	AY	614	GLU
25	B0	74	ARG
26	B1	28	GLY
26	B1	52	ARG
26	B1	53	VAL
26	B1	85	LEU
27	B2	18	PRO
27	B2	19	VAL
27	B2	20	GLU
27	B2	47	ASN
27	B2	48	HIS
28	B3	3	ARG
29	B4	3	GLU
29	B4	26	SER
29	B4	38	LYS
29	B4	43	TYR
29	B4	50	VAL
29	B4	57	GLU

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Mol	Chain	Res	Type
30	B5	49	CYS
30	B5	53	ALA
30	B5	56	LYS
30	B5	57	VAL
31	B6	7	ILE
31	B6	9	LEU
31	B6	18	ARG
31	B6	20	ASN
31	B6	27	LYS
31	B6	31	PRO
31	B6	44	ARG
31	B6	52	VAL
33	B8	31	HIS
33	B8	33	ASN
33	B8	43	GLN
33	B8	49	VAL
34	B9	2	LYS
34	B9	35	ARG
38	BD	19	ALA
38	BD	24	ILE
38	BD	25	THR
38	BD	27	THR
38	BD	30	GLU
38	BD	34	VAL
38	BD	35	LYS
38	BD	127	VAL
38	BD	225	ALA
38	BD	239	ARG
38	BD	246	PRO
39	BE	35	GLN
39	BE	54	GLN
39	BE	77	ILE
39	BE	88	GLY
39	BE	90	THR
39	BE	145	LYS
39	BE	185	LYS
39	BE	189	PRO
40	BF	11	VAL
40	BF	21	ALA
40	BF	64	ILE
40	BF	89	VAL
40	BF	167	ALA

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Mol	Chain	Res	Type
41	BG	4	ASP
41	BG	6	ALA
41	BG	47	LYS
41	BG	87	PRO
41	BG	96	ARG
41	BG	102	PHE
41	BG	109	VAL
41	BG	110	ALA
41	BG	181	ARG
42	BH	13	LYS
42	BH	20	ALA
42	BH	41	MET
42	BH	46	GLU
42	BH	55	PRO
42	BH	83	TYR
42	BH	154	PRO
42	BH	155	SER
42	BH	156	ALA
42	BH	157	TYR
42	BH	160	LYS
42	BH	169	VAL
42	BH	173	PRO
44	BK	51	ALA
44	BK	115	LEU
46	BN	8	GLN
46	BN	36	GLY
46	BN	46	VAL
46	BN	47	ALA
46	BN	57	ALA
46	BN	58	ASP
46	BN	63	THR
46	BN	130	HIS
46	BN	133	GLN
47	BO	35	VAL
47	BO	48	PRO
47	BO	54	GLU
47	BO	68	GLU
48	BP	12	ALA
48	BP	14	LYS
48	BP	17	LYS
48	BP	31	ALA
48	BP	47	ASP

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Mol	Chain	Res	Type
48	BP	48	PRO
48	BP	52	GLU
48	BP	57	THR
48	BP	58	THR
48	BP	111	ARG
48	BP	135	LEU
48	BP	147	LEU
49	BQ	27	VAL
49	BQ	135	ASP
50	BR	8	ARG
50	BR	14	SER
50	BR	58	GLY
50	BR	88	ARG
50	BR	107	ASP
50	BR	117	VAL
51	BS	13	ARG
51	BS	23	ARG
51	BS	97	ARG
51	BS	100	ALA
51	BS	102	ALA
51	BS	103	GLU
52	BT	5	ALA
52	BT	6	LEU
52	BT	24	PRO
52	BT	28	VAL
52	BT	30	VAL
52	BT	55	ASN
52	BT	80	SER
52	BT	91	ARG
52	BT	104	ASN
52	BT	107	ASP
52	BT	130	ALA
52	BT	132	LYS
52	BT	135	ALA
53	BU	91	ASP
53	BU	93	LYS
54	BV	16	PRO
54	BV	18	LEU
54	BV	19	LYS
54	BV	46	VAL
54	BV	67	GLY
55	BW	63	ASP

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Mol	Chain	Res	Type
56	BX	12	VAL
56	BX	42	ALA
57	BY	7	VAL
57	BY	24	VAL
57	BY	48	ALA
57	BY	60	PHE
57	BY	74	PRO
57	BY	77	PRO
57	BY	78	ALA
57	BY	99	CYS
57	BY	100	ALA
57	BY	104	GLY
58	BZ	27	VAL
58	BZ	51	ALA
58	BZ	78	LYS
58	BZ	80	ARG
58	BZ	81	ARG
58	BZ	120	ILE
58	BZ	121	HIS
58	BZ	142	SER
58	BZ	146	ILE
58	BZ	152	ALA
58	BZ	163	LEU
58	BZ	168	GLU
58	BZ	185	GLU
58	BZ	186	GLU
2	CB	12	GLU
2	CB	13	ALA
2	CB	15	VAL
2	CB	20	GLU
2	CB	95	GLN
2	CB	129	GLU
2	CB	195	ASP
2	CB	233	SER
2	CB	239	VAL
3	CC	12	LEU
3	CC	47	LEU
3	CC	61	ALA
3	CC	95	THR
3	CC	154	SER
3	CC	156	ARG
3	CC	207	VAL

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Mol	Chain	Res	Type
4	CD	3	ARG
4	CD	13	ARG
4	CD	14	ARG
4	CD	18	LYS
4	CD	30	LYS
4	CD	32	ALA
4	CD	44	GLY
4	CD	153	ARG
4	CD	171	GLY
5	CE	11	ILE
6	CF	39	LYS
7	CG	8	GLU
7	CG	52	GLU
7	CG	90	GLU
8	CH	105	ARG
9	CI	41	VAL
9	CI	43	ALA
9	CI	61	ALA
9	CI	89	ASN
10	CJ	33	GLN
10	CJ	36	GLY
10	CJ	55	LYS
10	CJ	56	HIS
10	CJ	57	LYS
10	CJ	59	SER
10	CJ	75	ILE
11	CK	123	LYS
11	CK	127	LYS
12	CL	18	VAL
12	CL	27	LEU
12	CL	28	LYS
12	CL	38	THR
12	CL	45	PRO
12	CL	81	SER
12	CL	91	LYS
13	CM	12	ASN
13	CM	67	GLU
13	CM	70	LEU
13	CM	83	ASP
13	CM	90	LEU
13	CM	91	ARG
13	CM	100	GLY

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Mol	Chain	Res	Type
13	CM	118	ALA
13	CM	124	PRO
14	CN	15	LYS
14	CN	29	ARG
15	CO	24	SER
16	CP	83	GLU
17	CQ	13	ASP
17	CQ	49	GLU
18	CR	37	VAL
18	CR	38	GLU
18	CR	45	SER
19	CS	10	PHE
19	CS	27	GLU
19	CS	28	LYS
19	CS	29	ARG
19	CS	47	HIS
19	CS	61	TYR
20	CT	48	LYS
20	CT	74	LYS
20	CT	99	LEU
21	CU	3	LYS
24	CY	21	ILE
24	CY	39	ILE
24	CY	66	THR
24	CY	67	ALA
24	CY	84	THR
24	CY	92	ILE
24	CY	104	ALA
24	CY	138	LYS
24	CY	183	MET
24	CY	209	ALA
24	CY	210	ARG
24	CY	297	GLU
24	CY	299	VAL
24	CY	448	GLN
24	CY	456	GLU
24	CY	498	ILE
24	CY	530	VAL
24	CY	674	ASP
25	D0	74	ARG
26	D1	53	VAL
27	D2	47	ASN

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Mol	Chain	Res	Type
27	D2	48	HIS
28	D3	3	ARG
29	D4	26	SER
29	D4	38	LYS
29	D4	43	TYR
29	D4	50	VAL
29	D4	57	GLU
30	D5	49	CYS
30	D5	53	ALA
30	D5	56	LYS
30	D5	57	VAL
31	D6	7	ILE
31	D6	9	LEU
31	D6	18	ARG
31	D6	20	ASN
31	D6	27	LYS
31	D6	31	PRO
31	D6	44	ARG
31	D6	52	VAL
33	D8	31	HIS
33	D8	33	ASN
33	D8	43	GLN
33	D8	49	VAL
34	D9	2	LYS
34	D9	35	ARG
38	DD	19	ALA
38	DD	24	ILE
38	DD	25	THR
38	DD	27	THR
38	DD	34	VAL
38	DD	35	LYS
38	DD	127	VAL
38	DD	225	ALA
38	DD	239	ARG
38	DD	246	PRO
39	DE	35	GLN
39	DE	54	GLN
39	DE	77	ILE
39	DE	88	GLY
39	DE	90	THR
39	DE	145	LYS
39	DE	185	LYS

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Mol	Chain	Res	Type
39	DE	189	PRO
40	DF	11	VAL
40	DF	21	ALA
40	DF	64	ILE
40	DF	89	VAL
40	DF	167	ALA
41	DG	4	ASP
41	DG	14	GLU
41	DG	47	LYS
41	DG	48	GLU
41	DG	75	LYS
41	DG	81	LYS
41	DG	82	LEU
41	DG	87	PRO
41	DG	96	ARG
41	DG	109	VAL
41	DG	110	ALA
42	DH	13	LYS
42	DH	20	ALA
42	DH	41	MET
42	DH	46	GLU
42	DH	55	PRO
42	DH	83	TYR
42	DH	154	PRO
42	DH	155	SER
42	DH	156	ALA
42	DH	157	TYR
42	DH	160	LYS
42	DH	169	VAL
42	DH	173	PRO
42	DH	176	ALA
44	DK	51	ALA
44	DK	115	LEU
46	DN	8	GLN
46	DN	36	GLY
46	DN	46	VAL
46	DN	47	ALA
46	DN	58	ASP
46	DN	63	THR
46	DN	130	HIS
46	DN	133	GLN
47	DO	35	VAL

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Mol	Chain	Res	Type
47	DO	48	PRO
47	DO	68	GLU
48	DP	12	ALA
48	DP	14	LYS
48	DP	17	LYS
48	DP	31	ALA
48	DP	47	ASP
48	DP	48	PRO
48	DP	52	GLU
48	DP	57	THR
48	DP	58	THR
48	DP	111	ARG
48	DP	135	LEU
48	DP	147	LEU
49	DQ	27	VAL
49	DQ	135	ASP
50	DR	8	ARG
50	DR	14	SER
50	DR	58	GLY
50	DR	88	ARG
50	DR	107	ASP
50	DR	117	VAL
51	DS	13	ARG
51	DS	23	ARG
51	DS	57	LYS
51	DS	97	ARG
51	DS	100	ALA
51	DS	102	ALA
51	DS	103	GLU
52	DT	5	ALA
52	DT	6	LEU
52	DT	24	PRO
52	DT	28	VAL
52	DT	30	VAL
52	DT	55	ASN
52	DT	80	SER
52	DT	91	ARG
52	DT	97	ALA
52	DT	104	ASN
52	DT	107	ASP
52	DT	130	ALA
52	DT	132	LYS

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Mol	Chain	Res	Type
52	DT	135	ALA
53	DU	91	ASP
53	DU	93	LYS
54	DV	16	PRO
54	DV	18	LEU
54	DV	19	LYS
54	DV	46	VAL
54	DV	67	GLY
55	DW	63	ASP
56	DX	12	VAL
56	DX	42	ALA
57	DY	7	VAL
57	DY	24	VAL
57	DY	48	ALA
57	DY	60	PHE
57	DY	74	PRO
57	DY	77	PRO
57	DY	78	ALA
57	DY	99	CYS
57	DY	100	ALA
57	DY	104	GLY
58	DZ	38	TYR
58	DZ	42	VAL
58	DZ	80	ARG
58	DZ	112	ARG
58	DZ	136	PHE
58	DZ	146	ILE
58	DZ	158	PRO
58	DZ	177	PRO
58	DZ	181	GLU
58	DZ	186	GLU
2	AB	18	GLY
2	AB	24	TRP
2	AB	65	GLY
2	AB	83	MET
2	AB	128	GLU
2	AB	151	GLY
2	AB	152	PHE
2	AB	153	ARG
2	AB	165	VAL
2	AB	216	SER
2	AB	221	LEU

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Mol	Chain	Res	Type
2	AB	224	GLN
2	AB	238	LEU
3	AC	26	LYS
3	AC	96	GLY
3	AC	129	ALA
3	AC	131	ARG
3	AC	135	LYS
3	AC	139	GLN
4	AD	5	ILE
4	AD	69	GLY
4	AD	156	GLU
4	AD	171	GLY
5	AE	8	GLU
6	AF	30	LEU
6	AF	34	GLY
6	AF	43	LEU
7	AG	80	VAL
8	AH	2	LEU
9	AI	34	ASN
9	AI	85	LEU
10	AJ	19	SER
10	AJ	61	GLU
10	AJ	83	GLU
10	AJ	84	GLN
10	AJ	85	LEU
11	AK	88	GLY
12	AL	46	LYS
12	AL	71	PRO
12	AL	87	GLY
12	AL	89	ARG
12	AL	121	GLY
13	AM	4	ILE
13	AM	5	ALA
13	AM	7	VAL
13	AM	55	ARG
13	AM	114	ARG
14	AN	14	PRO
16	AP	34	GLU
18	AR	41	LYS
19	AS	14	HIS
19	AS	25	LYS
19	AS	26	GLY

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Mol	Chain	Res	Type
19	AS	62	ILE
19	AS	63	THR
19	AS	73	GLU
20	AT	49	ALA
20	AT	62	LEU
20	AT	69	GLY
24	AY	10	LYS
24	AY	39	ILE
24	AY	112	GLN
24	AY	114	VAL
24	AY	183	MET
24	AY	196	ILE
24	AY	299	VAL
24	AY	347	GLY
24	AY	371	ALA
24	AY	380	LEU
24	AY	386	GLY
24	AY	399	LEU
24	AY	416	LYS
24	AY	418	LYS
24	AY	471	LYS
24	AY	505	GLY
24	AY	657	THR
24	AY	678	GLU
25	B0	20	ARG
26	B1	69	LYS
26	B1	84	GLY
27	B2	21	LEU
27	B2	26	ARG
27	B2	49	LYS
28	B3	29	ARG
29	B4	5	ILE
29	B4	9	LEU
29	B4	20	ASN
29	B4	44	THR
29	B4	48	ARG
29	B4	51	ASP
30	B5	35	GLU
30	B5	36	CYS
30	B5	38	ALA
30	B5	58	LEU
30	B5	59	GLU

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Mol	Chain	Res	Type
31	B6	16	CYS
31	B6	19	ARG
31	B6	23	THR
31	B6	28	ARG
31	B6	43	CYS
32	B7	17	GLY
33	B8	34	TRP
33	B8	37	SER
33	B8	40	GLU
34	B9	11	CYS
34	B9	12	ASP
37	BC	12	LEU
37	BC	30	VAL
37	BC	38	PHE
38	BD	3	VAL
38	BD	12	SER
38	BD	32	SER
38	BD	36	PRO
38	BD	42	GLY
38	BD	125	ILE
38	BD	197	GLY
38	BD	198	ASN
38	BD	234	GLY
38	BD	260	ARG
38	BD	267	SER
38	BD	268	ARG
39	BE	2	LYS
39	BE	46	ALA
39	BE	53	PRO
39	BE	57	LYS
39	BE	66	HIS
39	BE	69	LYS
39	BE	71	GLY
39	BE	72	VAL
39	BE	118	LYS
39	BE	134	ILE
39	BE	144	ARG
39	BE	186	GLY
40	BF	5	ALA
40	BF	10	PRO
40	BF	84	VAL
40	BF	127	GLU

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Mol	Chain	Res	Type
40	BF	169	ASN
40	BF	181	LEU
40	BF	206	ILE
40	BF	207	GLY
41	BG	14	GLU
41	BG	75	LYS
41	BG	81	LYS
41	BG	82	LEU
41	BG	166	ASP
42	BH	21	PRO
42	BH	42	ARG
42	BH	69	ARG
42	BH	138	LYS
42	BH	174	GLY
42	BH	176	ALA
44	BK	10	LEU
44	BK	42	ASN
44	BK	48	MET
44	BK	62	ASP
44	BK	82	ALA
44	BK	87	GLY
46	BN	77	GLY
46	BN	125	GLY
46	BN	129	PRO
47	BO	5	GLN
47	BO	29	ASN
47	BO	89	ASN
47	BO	100	GLY
48	BP	34	GLY
48	BP	98	GLU
49	BQ	52	VAL
49	BQ	62	GLY
49	BQ	71	ASP
50	BR	45	ARG
50	BR	83	ILE
51	BS	37	ALA
51	BS	57	LYS
51	BS	59	LYS
51	BS	85	VAL
51	BS	94	TYR
51	BS	104	GLY
51	BS	107	GLU

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Mol	Chain	Res	Type
52	BT	11	GLU
52	BT	12	SER
52	BT	58	ASN
52	BT	88	ILE
52	BT	97	ALA
52	BT	133	GLU
53	BU	11	ARG
53	BU	27	LEU
53	BU	32	PHE
53	BU	67	ALA
54	BV	2	PHE
54	BV	26	ASP
54	BV	31	ALA
54	BV	47	VAL
54	BV	53	GLU
54	BV	55	ALA
54	BV	78	LYS
55	BW	6	ILE
55	BW	11	ARG
56	BX	87	GLN
57	BY	17	SER
57	BY	38	ILE
57	BY	39	VAL
57	BY	41	GLY
57	BY	59	GLY
57	BY	81	LYS
57	BY	98	VAL
57	BY	107	ASP
58	BZ	5	LEU
58	BZ	42	VAL
58	BZ	85	HIS
58	BZ	112	ARG
58	BZ	148	ASP
58	BZ	158	PRO
58	BZ	180	VAL
2	CB	18	GLY
2	CB	24	TRP
2	CB	65	GLY
2	CB	83	MET
2	CB	128	GLU
2	CB	151	GLY
2	CB	152	PHE

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Mol	Chain	Res	Type
2	CB	153	ARG
2	CB	165	VAL
2	CB	190	THR
2	CB	216	SER
2	CB	221	LEU
2	CB	224	GLN
2	CB	236	TYR
2	CB	238	LEU
3	CC	26	LYS
3	CC	96	GLY
3	CC	129	ALA
3	CC	131	ARG
3	CC	135	LYS
3	CC	139	GLN
4	CD	5	ILE
4	CD	31	CYS
4	CD	69	GLY
4	CD	156	GLU
4	CD	179	GLU
5	CE	8	GLU
6	CF	30	LEU
6	CF	34	GLY
6	CF	43	LEU
7	CG	41	ARG
7	CG	80	VAL
8	CH	2	LEU
9	CI	34	ASN
10	CJ	19	SER
10	CJ	61	GLU
10	CJ	84	GLN
10	CJ	85	LEU
11	CK	88	GLY
12	CL	46	LYS
12	CL	71	PRO
12	CL	72	GLY
12	CL	87	GLY
12	CL	89	ARG
12	CL	121	GLY
13	CM	4	ILE
13	CM	5	ALA
13	CM	7	VAL
13	CM	55	ARG

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Mol	Chain	Res	Type
13	CM	114	ARG
13	CM	121	LYS
16	CP	34	GLU
16	CP	76	GLN
17	CQ	95	TYR
18	CR	41	LYS
19	CS	14	HIS
19	CS	25	LYS
19	CS	26	GLY
19	CS	62	ILE
19	CS	63	THR
19	CS	73	GLU
20	CT	49	ALA
20	CT	62	LEU
20	CT	69	GLY
24	CY	34	TYR
24	CY	86	GLY
24	CY	112	GLN
24	CY	127	LYS
24	CY	129	LYS
24	CY	143	GLY
24	CY	144	ALA
24	CY	172	ASP
24	CY	203	GLU
24	CY	211	GLU
24	CY	300	GLU
24	CY	366	VAL
24	CY	416	LYS
24	CY	505	GLY
24	CY	531	GLY
24	CY	537	GLU
24	CY	547	GLU
24	CY	551	GLN
24	CY	595	GLN
24	CY	664	GLN
24	CY	673	PHE
24	CY	681	LYS
25	D0	20	ARG
26	D1	22	GLY
26	D1	30	VAL
26	D1	83	GLU
26	D1	84	GLY

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Mol	Chain	Res	Type
26	D1	85	LEU
26	D1	94	LEU
26	D1	95	LEU
27	D2	5	GLU
27	D2	49	LYS
28	D3	29	ARG
29	D4	3	GLU
29	D4	5	ILE
29	D4	9	LEU
29	D4	20	ASN
29	D4	44	THR
29	D4	48	ARG
29	D4	51	ASP
30	D5	35	GLU
30	D5	36	CYS
30	D5	38	ALA
30	D5	58	LEU
30	D5	59	GLU
31	D6	16	CYS
31	D6	19	ARG
31	D6	23	THR
31	D6	28	ARG
32	D7	17	GLY
33	D8	34	TRP
33	D8	37	SER
33	D8	40	GLU
34	D9	11	CYS
34	D9	12	ASP
37	DC	12	LEU
37	DC	30	VAL
37	DC	38	PHE
38	DD	3	VAL
38	DD	12	SER
38	DD	30	GLU
38	DD	32	SER
38	DD	36	PRO
38	DD	41	GLY
38	DD	42	GLY
38	DD	125	ILE
38	DD	197	GLY
38	DD	198	ASN
38	DD	236	GLY

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Mol	Chain	Res	Type
38	DD	267	SER
38	DD	268	ARG
39	DE	2	LYS
39	DE	46	ALA
39	DE	53	PRO
39	DE	57	LYS
39	DE	66	HIS
39	DE	69	LYS
39	DE	71	GLY
39	DE	72	VAL
39	DE	118	LYS
39	DE	129	HIS
39	DE	134	ILE
39	DE	144	ARG
39	DE	186	GLY
40	DF	10	PRO
40	DF	82	ILE
40	DF	84	VAL
40	DF	127	GLU
40	DF	169	ASN
40	DF	181	LEU
40	DF	206	ILE
41	DG	3	LEU
41	DG	76	SER
41	DG	104	GLU
41	DG	124	SER
41	DG	181	ARG
42	DH	21	PRO
42	DH	42	ARG
42	DH	69	ARG
42	DH	138	LYS
44	DK	10	LEU
44	DK	42	ASN
44	DK	48	MET
44	DK	62	ASP
44	DK	82	ALA
44	DK	87	GLY
46	DN	57	ALA
46	DN	77	GLY
46	DN	125	GLY
46	DN	129	PRO
47	DO	5	GLN

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Mol	Chain	Res	Type
47	DO	29	ASN
47	DO	54	GLU
47	DO	89	ASN
47	DO	120	GLU
48	DP	34	GLY
48	DP	98	GLU
49	DQ	52	VAL
49	DQ	62	GLY
49	DQ	71	ASP
50	DR	45	ARG
51	DS	37	ALA
51	DS	59	LYS
51	DS	85	VAL
51	DS	94	TYR
51	DS	104	GLY
51	DS	107	GLU
52	DT	12	SER
52	DT	41	ARG
52	DT	88	ILE
52	DT	133	GLU
53	DU	11	ARG
53	DU	27	LEU
53	DU	32	PHE
53	DU	67	ALA
54	DV	2	PHE
54	DV	26	ASP
54	DV	31	ALA
54	DV	47	VAL
54	DV	53	GLU
54	DV	55	ALA
55	DW	6	ILE
55	DW	11	ARG
56	DX	87	GLN
57	DY	17	SER
57	DY	38	ILE
57	DY	39	VAL
57	DY	41	GLY
57	DY	59	GLY
57	DY	81	LYS
57	DY	92	ASN
57	DY	98	VAL
57	DY	107	ASP

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Mol	Chain	Res	Type
58	DZ	17	ALA
58	DZ	18	LEU
58	DZ	37	VAL
58	DZ	40	ASP
58	DZ	142	SER
58	DZ	148	ASP
58	DZ	159	PRO
2	AB	78	GLN
2	AB	79	ASP
2	AB	236	TYR
3	AC	4	LYS
3	AC	168	ALA
4	AD	31	CYS
4	AD	40	PRO
5	AE	140	ARG
5	AE	154	GLY
7	AG	14	PRO
7	AG	41	ARG
7	AG	62	PHE
9	AI	11	LYS
9	AI	44	VAL
9	AI	95	LYS
12	AL	47	LYS
12	AL	51	ALA
12	AL	72	GLY
12	AL	92	ASP
13	AM	11	ARG
13	AM	121	LYS
14	AN	16	PHE
15	AO	14	GLU
15	AO	77	ARG
16	AP	13	HIS
16	AP	76	GLN
17	AQ	95	TYR
20	AT	97	ALA
24	AY	25	LYS
24	AY	34	TYR
24	AY	42	ILE
24	AY	89	ASP
24	AY	120	THR
24	AY	144	ALA
24	AY	148	LEU

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Mol	Chain	Res	Type
24	AY	283	PRO
24	AY	393	ASP
24	AY	458	HIS
24	AY	469	GLU
24	AY	532	GLY
24	AY	535	PRO
24	AY	636	PRO
24	AY	680	PRO
26	B1	95	LEU
27	B2	43	GLN
27	B2	58	ALA
27	B2	68	ARG
28	B3	32	GLN
30	B5	37	LYS
33	B8	35	GLN
33	B8	57	ARG
37	BC	17	PRO
37	BC	127	LYS
38	BD	28	GLU
38	BD	41	GLY
38	BD	74	GLY
38	BD	129	ASN
38	BD	134	ARG
38	BD	236	GLY
38	BD	242	ARG
39	BE	83	ASP
39	BE	86	PRO
39	BE	117	MET
39	BE	129	HIS
40	BF	3	GLU
40	BF	82	ILE
40	BF	108	LYS
40	BF	115	ALA
40	BF	122	LYS
40	BF	168	ARG
40	BF	195	ASP
41	BG	22	ARG
41	BG	43	LEU
41	BG	116	ASP
41	BG	163	ALA
42	BH	18	GLU
42	BH	47	GLU

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Mol	Chain	Res	Type
42	BH	85	LYS
42	BH	98	LEU
42	BH	126	PRO
42	BH	158	HIS
42	BH	165	ALA
42	BH	170	ARG
42	BH	171	LEU
46	BN	40	PRO
46	BN	59	LYS
46	BN	110	GLY
46	BN	136	GLU
47	BO	120	GLU
48	BP	43	GLY
48	BP	49	ARG
48	BP	123	LEU
50	BR	12	ARG
51	BS	71	ARG
51	BS	90	GLY
51	BS	99	LYS
52	BT	3	ARG
52	BT	41	ARG
52	BT	103	ARG
53	BU	83	LEU
53	BU	114	LYS
54	BV	3	ALA
54	BV	50	PRO
55	BW	18	ARG
56	BX	19	ALA
56	BX	22	ALA
56	BX	91	ALA
57	BY	46	LYS
57	BY	92	ASN
58	BZ	30	ASN
58	BZ	83	PRO
58	BZ	122	ARG
58	BZ	128	VAL
58	BZ	166	SER
58	BZ	170	THR
2	CB	78	GLN
2	CB	79	ASP
3	CC	4	LYS
3	CC	15	THR

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Mol	Chain	Res	Type
3	CC	168	ALA
4	CD	40	PRO
5	CE	154	GLY
6	CF	29	ALA
7	CG	14	PRO
7	CG	62	PHE
9	CI	11	LYS
9	CI	44	VAL
9	CI	85	LEU
9	CI	95	LYS
10	CJ	83	GLU
12	CL	47	LYS
12	CL	51	ALA
12	CL	92	ASP
12	CL	116	SER
13	CM	11	ARG
14	CN	14	PRO
14	CN	16	PHE
15	CO	14	GLU
15	CO	77	ARG
16	CP	13	HIS
19	CS	5	LEU
20	CT	97	ALA
24	CY	87	HIS
24	CY	91	THR
24	CY	123	ARG
24	CY	192	LEU
24	CY	239	GLU
24	CY	303	PRO
24	CY	380	LEU
24	CY	400	GLU
24	CY	421	GLN
24	CY	458	HIS
24	CY	502	GLY
24	CY	504	ARG
24	CY	519	ARG
24	CY	620	VAL
24	CY	680	PRO
27	D2	4	SER
27	D2	41	ILE
27	D2	68	ARG
27	D2	71	ASN

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Mol	Chain	Res	Type
28	D3	32	GLN
30	D5	37	LYS
31	D6	43	CYS
33	D8	35	GLN
33	D8	57	ARG
37	DC	17	PRO
37	DC	82	GLU
37	DC	127	LYS
38	DD	28	GLU
38	DD	74	GLY
38	DD	129	ASN
38	DD	134	ARG
38	DD	234	GLY
38	DD	242	ARG
38	DD	260	ARG
39	DE	83	ASP
39	DE	86	PRO
40	DF	3	GLU
40	DF	5	ALA
40	DF	108	LYS
40	DF	115	ALA
40	DF	126	VAL
40	DF	168	ARG
40	DF	195	ASP
40	DF	207	GLY
41	DG	21	ARG
41	DG	115	ARG
41	DG	117	PHE
41	DG	169	ALA
42	DH	18	GLU
42	DH	47	GLU
42	DH	85	LYS
42	DH	98	LEU
42	DH	126	PRO
42	DH	158	HIS
42	DH	165	ALA
42	DH	170	ARG
42	DH	171	LEU
42	DH	174	GLY
46	DN	40	PRO
46	DN	59	LYS
46	DN	110	GLY

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Mol	Chain	Res	Type
46	DN	136	GLU
47	DO	100	GLY
48	DP	43	GLY
48	DP	49	ARG
48	DP	123	LEU
50	DR	12	ARG
50	DR	83	ILE
51	DS	71	ARG
51	DS	90	GLY
51	DS	99	LYS
52	DT	11	GLU
52	DT	58	ASN
53	DU	66	ASN
53	DU	83	LEU
53	DU	110	VAL
53	DU	114	LYS
54	DV	3	ALA
54	DV	50	PRO
54	DV	78	LYS
55	DW	18	ARG
56	DX	6	ASP
56	DX	19	ALA
56	DX	22	ALA
56	DX	91	ALA
57	DY	46	LYS
57	DY	75	ILE
58	DZ	49	ARG
58	DZ	81	ARG
58	DZ	108	PRO
58	DZ	168	GLU
2	AB	29	ALA
2	AB	63	MET
2	AB	64	ARG
2	AB	97	TRP
2	AB	130	ARG
3	AC	15	THR
3	AC	44	GLU
3	AC	63	ASN
3	AC	65	ALA
4	AD	71	SER
5	AE	37	ARG
5	AE	136	MET

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Mol	Chain	Res	Type
5	AE	138	ALA
6	AF	29	ALA
10	AJ	23	ILE
10	AJ	32	ALA
12	AL	19	ARG
12	AL	116	SER
13	AM	36	LYS
13	AM	113	PRO
15	AO	26	GLU
15	AO	80	ALA
15	AO	84	LYS
17	AQ	89	LEU
19	AS	5	LEU
19	AS	42	PRO
19	AS	50	ALA
20	AT	85	MET
20	AT	96	GLY
20	AT	98	PRO
21	AU	25	LYS
24	AY	230	LYS
24	AY	406	GLU
24	AY	444	PRO
24	AY	457	LEU
24	AY	502	GLY
24	AY	506	GLN
24	AY	549	ALA
26	B1	54	ALA
27	B2	51	ARG
27	B2	70	GLN
31	B6	41	PRO
33	B8	3	LYS
34	B9	30	PRO
37	BC	82	GLU
37	BC	168	LYS
37	BC	227	PRO
39	BE	17	ASP
39	BE	64	LYS
39	BE	70	ALA
39	BE	82	ARG
40	BF	62	ARG
40	BF	126	VAL
40	BF	134	GLY

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Mol	Chain	Res	Type
40	BF	180	GLY
41	BG	30	GLU
41	BG	103	LEU
41	BG	126	ASP
44	BK	116	ASN
48	BP	89	ALA
48	BP	106	LEU
48	BP	107	LYS
48	BP	108	LYS
48	BP	119	GLU
49	BQ	139	GLU
50	BR	31	HIS
50	BR	61	HIS
50	BR	86	ARG
51	BS	15	ARG
51	BS	89	ARG
51	BS	105	ALA
52	BT	26	ASP
53	BU	66	ASN
53	BU	110	VAL
55	BW	111	HIS
56	BX	6	ASP
57	BY	67	LEU
57	BY	75	ILE
58	BZ	71	VAL
58	BZ	159	PRO
58	BZ	165	VAL
2	CB	29	ALA
2	CB	63	MET
2	CB	64	ARG
2	CB	97	TRP
2	CB	130	ARG
2	CB	212	GLN
3	CC	65	ALA
4	CD	149	ALA
5	CE	37	ARG
5	CE	136	MET
5	CE	138	ALA
5	CE	140	ARG
7	CG	131	LYS
10	CJ	23	ILE
10	CJ	30	SER

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Mol	Chain	Res	Type
10	CJ	32	ALA
13	CM	36	LYS
13	CM	113	PRO
15	CO	25	THR
15	CO	26	GLU
15	CO	80	ALA
15	CO	84	LYS
16	CP	54	GLU
18	CR	87	ARG
19	CS	30	LEU
19	CS	42	PRO
19	CS	50	ALA
20	CT	34	LYS
20	CT	78	ALA
20	CT	96	GLY
20	CT	98	PRO
21	CU	25	LYS
24	CY	88	VAL
24	CY	137	ASN
24	CY	174	PHE
24	CY	227	ILE
24	CY	371	ALA
24	CY	419	ALA
24	CY	427	ALA
24	CY	470	PHE
24	CY	559	PRO
25	D0	42	GLY
26	D1	24	ALA
27	D2	18	PRO
28	D3	38	GLU
31	D6	41	PRO
33	D8	3	LYS
33	D8	61	LEU
37	DC	168	LYS
37	DC	227	PRO
39	DE	17	ASP
39	DE	45	THR
39	DE	64	LYS
39	DE	70	ALA
39	DE	117	MET
40	DF	90	PHE
40	DF	122	LYS

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Mol	Chain	Res	Type
40	DF	134	GLY
41	DG	97	ASP
41	DG	140	ILE
42	DH	81	GLU
44	DK	116	ASN
48	DP	89	ALA
48	DP	106	LEU
48	DP	107	LYS
49	DQ	139	GLU
50	DR	31	HIS
50	DR	61	HIS
51	DS	15	ARG
51	DS	89	ARG
51	DS	105	ALA
52	DT	3	ARG
52	DT	9	LEU
52	DT	103	ARG
55	DW	99	ARG
57	DY	67	LEU
58	DZ	41	LEU
58	DZ	120	ILE
58	DZ	165	VAL
58	DZ	169	GLU
2	AB	9	GLU
2	AB	84	GLU
2	AB	212	GLN
3	AC	35	GLU
3	AC	179	ARG
4	AD	149	ALA
4	AD	159	ARG
4	AD	186	LEU
6	AF	21	LEU
8	AH	121	ASP
9	AI	94	ALA
9	AI	106	ALA
10	AJ	30	SER
10	AJ	91	PRO
11	AK	34	ASP
13	AM	10	PRO
15	AO	25	THR
16	AP	54	GLU
18	AR	87	ARG

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Mol	Chain	Res	Type
19	AS	30	LEU
19	AS	54	GLY
19	AS	59	PRO
20	AT	34	LYS
20	AT	44	ALA
20	AT	78	ALA
20	AT	104	LEU
21	AU	6	ARG
24	AY	22	ASP
24	AY	65	ILE
24	AY	123	ARG
24	AY	153	MET
24	AY	303	PRO
24	AY	361	ASN
24	AY	415	PRO
24	AY	577	SER
24	AY	598	ASP
24	AY	617	MET
24	AY	652	MET
24	AY	688	ILE
26	B1	30	VAL
26	B1	31	GLY
27	B2	14	ARG
28	B3	38	GLU
29	B4	2	LYS
29	B4	40	HIS
30	B5	4	HIS
33	B8	48	PHE
33	B8	61	LEU
38	BD	10	THR
38	BD	273	ARG
39	BE	45	THR
39	BE	187	ALA
40	BF	90	PHE
41	BG	106	LEU
42	BH	14	GLY
42	BH	81	GLU
42	BH	93	GLY
46	BN	127	ASP
46	BN	134	ARG
48	BP	23	PRO
48	BP	33	ARG

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Mol	Chain	Res	Type
48	BP	83	VAL
50	BR	42	LYS
50	BR	102	GLU
52	BT	9	LEU
52	BT	17	THR
53	BU	46	ALA
54	BV	22	VAL
55	BW	93	ALA
55	BW	99	ARG
56	BX	11	PRO
56	BX	13	LEU
57	BY	37	VAL
58	BZ	46	LYS
2	CB	9	GLU
2	CB	84	GLU
3	CC	35	GLU
3	CC	44	GLU
4	CD	159	ARG
4	CD	186	LEU
5	CE	118	ILE
6	CF	21	LEU
7	CG	42	ILE
8	CH	121	ASP
9	CI	94	ALA
10	CJ	91	PRO
11	CK	34	ASP
11	CK	57	THR
11	CK	95	ILE
12	CL	19	ARG
13	CM	10	PRO
17	CQ	25	ARG
19	CS	54	GLY
19	CS	59	PRO
20	CT	85	MET
20	CT	104	LEU
21	CU	6	ARG
24	CY	36	THR
24	CY	205	TYR
24	CY	206	LEU
24	CY	262	SER
24	CY	283	PRO
24	CY	315	LYS

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Mol	Chain	Res	Type
24	CY	405	PRO
26	D1	63	ALA
29	D4	2	LYS
29	D4	40	HIS
30	D5	4	HIS
33	D8	48	PHE
34	D9	30	PRO
38	DD	10	THR
38	DD	273	ARG
39	DE	187	ALA
40	DF	62	ARG
40	DF	180	GLY
41	DG	12	TYR
41	DG	42	GLY
42	DH	111	HIS
46	DN	127	ASP
46	DN	134	ARG
48	DP	23	PRO
48	DP	33	ARG
48	DP	83	VAL
48	DP	108	LYS
48	DP	119	GLU
50	DR	86	ARG
50	DR	102	GLU
52	DT	17	THR
52	DT	26	ASP
54	DV	22	VAL
55	DW	111	HIS
56	DX	11	PRO
56	DX	13	LEU
57	DY	37	VAL
58	DZ	110	GLY
2	AB	157	ARG
3	AC	165	THR
5	AE	146	ALA
9	AI	127	LYS
11	AK	57	THR
11	AK	95	ILE
13	AM	21	TYR
13	AM	106	ASN
17	AQ	25	ARG
24	AY	24	GLY

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Mol	Chain	Res	Type
24	AY	75	LYS
24	AY	408	VAL
24	AY	591	LYS
25	B0	13	GLY
25	B0	42	GLY
27	B2	44	LEU
28	B3	45	GLY
31	B6	36	LEU
39	BE	52	LEU
39	BE	73	GLU
39	BE	130	GLY
40	BF	14	PRO
40	BF	66	PRO
42	BH	48	GLY
42	BH	92	ILE
42	BH	111	HIS
44	BK	21	PRO
44	BK	73	PRO
46	BN	65	LYS
46	BN	81	GLY
47	BO	18	LYS
48	BP	141	ALA
52	BT	81	PRO
55	BW	14	PRO
55	BW	25	ARG
2	CB	157	ARG
2	CB	204	ASN
3	CC	160	ALA
3	CC	165	THR
4	CD	71	SER
4	CD	88	VAL
8	CH	135	CYS
12	CL	106	ASP
13	CM	116	THR
20	CT	44	ALA
21	CU	9	ARG
24	CY	408	VAL
24	CY	671	MET
25	D0	13	GLY
26	D1	52	ARG
26	D1	73	LEU
39	DE	73	GLU

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Mol	Chain	Res	Type
39	DE	130	GLY
40	DF	2	LYS
40	DF	14	PRO
40	DF	66	PRO
40	DF	85	GLY
41	DG	22	ARG
42	DH	14	GLY
42	DH	45	VAL
42	DH	48	GLY
42	DH	92	ILE
42	DH	93	GLY
44	DK	21	PRO
44	DK	73	PRO
46	DN	65	LYS
46	DN	81	GLY
47	DO	18	LYS
48	DP	67	MET
48	DP	141	ALA
49	DQ	30	GLY
50	DR	42	LYS
52	DT	127	ALA
53	DU	46	ALA
55	DW	14	PRO
55	DW	25	ARG
58	DZ	12	GLY
58	DZ	65	GLN
58	DZ	121	HIS
4	AD	88	VAL
5	AE	118	ILE
7	AG	42	ILE
9	AI	74	ILE
15	AO	75	PRO
26	B1	87	PRO
29	B4	28	LYS
40	BF	177	ALA
42	BH	45	VAL
42	BH	76	VAL
46	BN	5	VAL
49	BQ	30	GLY
52	BT	92	GLY
54	BV	54	GLY
55	BW	59	VAL

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Mol	Chain	Res	Type
57	BY	3	VAL
9	CI	74	ILE
16	CP	2	VAL
19	CS	51	VAL
24	CY	479	PRO
24	CY	670	VAL
28	D3	45	GLY
29	D4	28	LYS
34	D9	21	GLY
39	DE	52	LEU
42	DH	76	VAL
52	DT	81	PRO
55	DW	59	VAL
2	AB	26	PRO
2	AB	131	PRO
2	AB	232	PRO
6	AF	51	PRO
7	AG	9	VAL
9	AI	80	GLY
16	AP	2	VAL
19	AS	51	VAL
26	B1	36	GLY
37	BC	160	GLY
38	BD	228	PRO
40	BF	25	PRO
40	BF	85	GLY
42	BH	39	PRO
48	BP	146	VAL
53	BU	90	VAL
54	BV	36	PRO
57	BY	31	LEU
58	BZ	134	PRO
2	CB	232	PRO
6	CF	51	PRO
7	CG	9	VAL
7	CG	82	GLY
15	CO	75	PRO
24	CY	554	PRO
37	DC	160	GLY
40	DF	25	PRO
40	DF	177	ALA
46	DN	5	VAL

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Mol	Chain	Res	Type
48	DP	146	VAL
53	DU	90	VAL
54	DV	36	PRO
54	DV	54	GLY
57	DY	3	VAL
57	DY	31	LEU
2	AB	230	VAL
7	AG	82	GLY
16	AP	62	VAL
20	AT	100	ILE
27	B2	41	ILE
37	BC	68	GLY
41	BG	129	GLY
51	BS	22	GLY
57	BY	30	VAL
58	BZ	133	ILE
2	CB	131	PRO
2	CB	230	VAL
9	CI	80	GLY
16	CP	62	VAL
20	CT	100	ILE
24	CY	394	ALA
24	CY	600	VAL
38	DD	228	PRO
39	DE	34	VAL
42	DH	39	PRO
51	DS	22	GLY
52	DT	92	GLY
53	DU	9	VAL
2	AB	127	ILE
2	AB	194	PRO
4	AD	92	VAL
4	AD	180	GLY
19	AS	9	VAL
26	B1	86	SER
37	BC	136	GLY
39	BE	14	ILE
39	BE	34	VAL
41	BG	24	GLY
42	BH	107	VAL
52	BT	15	VAL
54	BV	51	VAL

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Mol	Chain	Res	Type
2	CB	127	ILE
2	CB	194	PRO
4	CD	92	VAL
14	CN	55	GLY
15	CO	19	PRO
24	CY	532	GLY
37	DC	68	GLY
37	DC	101	ILE
37	DC	107	GLY
37	DC	136	GLY
39	DE	75	VAL
51	DS	91	PRO
57	DY	30	VAL
58	DZ	166	SER
24	AY	333	GLY
37	BC	107	GLY
39	BE	75	VAL
42	BH	52	VAL
51	BS	91	PRO
57	BY	27	VAL
2	CB	26	PRO
24	CY	293	THR
30	D5	50	GLY
38	DD	11	PRO
39	DE	14	ILE
41	DG	20	ILE
42	DH	52	VAL
42	DH	107	VAL
52	DT	15	VAL
54	DV	51	VAL
58	DZ	14	LYS
58	DZ	134	PRO
38	BD	245	PRO
38	DD	245	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	179 (89%)	23 (11%)	5	29
2	CB	202/220 (92%)	179 (89%)	23 (11%)	5	29
3	AC	160/188 (85%)	142 (89%)	18 (11%)	6	30
3	CC	160/188 (85%)	142 (89%)	18 (11%)	6	30
4	AD	180/181 (99%)	160 (89%)	20 (11%)	6	31
4	CD	180/181 (99%)	160 (89%)	20 (11%)	6	31
5	AE	115/123 (94%)	100 (87%)	15 (13%)	4	24
5	CE	115/123 (94%)	100 (87%)	15 (13%)	4	24
6	AF	90/90 (100%)	83 (92%)	7 (8%)	12	44
6	CF	90/90 (100%)	83 (92%)	7 (8%)	12	44
7	AG	126/127 (99%)	117 (93%)	9 (7%)	14	48
7	CG	126/127 (99%)	117 (93%)	9 (7%)	14	48
8	AH	119/119 (100%)	110 (92%)	9 (8%)	13	45
8	CH	119/119 (100%)	112 (94%)	7 (6%)	19	55
9	AI	98/99 (99%)	90 (92%)	8 (8%)	11	42
9	CI	98/99 (99%)	90 (92%)	8 (8%)	11	42
10	AJ	88/92 (96%)	77 (88%)	11 (12%)	4	25
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	4	25
11	AK	90/99 (91%)	84 (93%)	6 (7%)	16	50
11	CK	90/99 (91%)	84 (93%)	6 (7%)	16	50
12	AL	104/109 (95%)	94 (90%)	10 (10%)	8	37
12	CL	104/109 (95%)	93 (89%)	11 (11%)	6	32
13	AM	99/101 (98%)	91 (92%)	8 (8%)	11	43
13	CM	99/101 (98%)	91 (92%)	8 (8%)	11	43
14	AN	49/50 (98%)	43 (88%)	6 (12%)	5	26
14	CN	49/50 (98%)	43 (88%)	6 (12%)	5	26
15	AO	79/80 (99%)	71 (90%)	8 (10%)	7	34
15	CO	79/80 (99%)	71 (90%)	8 (10%)	7	34
16	AP	72/74 (97%)	67 (93%)	5 (7%)	15	49
16	CP	72/74 (97%)	67 (93%)	5 (7%)	15	49
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	13	46
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	13	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	61/77 (79%)	59 (97%)	2 (3%)	38	69
18	CR	61/77 (79%)	59 (97%)	2 (3%)	38	69
19	AS	69/80 (86%)	59 (86%)	10 (14%)	3	20
19	CS	69/80 (86%)	59 (86%)	10 (14%)	3	20
20	AT	76/82 (93%)	69 (91%)	7 (9%)	9	39
20	CT	76/82 (93%)	69 (91%)	7 (9%)	9	39
21	AU	19/22 (86%)	19 (100%)	0	100	100
21	CU	19/22 (86%)	19 (100%)	0	100	100
24	AY	563/582 (97%)	489 (87%)	74 (13%)	4	23
24	CY	563/582 (97%)	495 (88%)	68 (12%)	5	26
25	B0	66/67 (98%)	57 (86%)	9 (14%)	3	22
25	D0	66/67 (98%)	57 (86%)	9 (14%)	3	22
26	B1	78/83 (94%)	65 (83%)	13 (17%)	2	14
26	D1	78/83 (94%)	70 (90%)	8 (10%)	7	34
27	B2	66/67 (98%)	59 (89%)	7 (11%)	6	32
27	D2	66/67 (98%)	58 (88%)	8 (12%)	5	26
28	B3	51/52 (98%)	47 (92%)	4 (8%)	12	44
28	D3	51/52 (98%)	47 (92%)	4 (8%)	12	44
29	B4	51/63 (81%)	38 (74%)	13 (26%)	0	4
29	D4	51/63 (81%)	37 (72%)	14 (28%)	0	3
30	B5	51/52 (98%)	45 (88%)	6 (12%)	5	28
30	D5	51/52 (98%)	45 (88%)	6 (12%)	5	28
31	B6	49/52 (94%)	39 (80%)	10 (20%)	1	8
31	D6	49/52 (94%)	38 (78%)	11 (22%)	1	6
32	B7	41/42 (98%)	36 (88%)	5 (12%)	5	26
32	D7	41/42 (98%)	36 (88%)	5 (12%)	5	26
33	B8	53/55 (96%)	44 (83%)	9 (17%)	2	14
33	D8	53/55 (96%)	43 (81%)	10 (19%)	1	9
34	B9	34/34 (100%)	30 (88%)	4 (12%)	5	28
34	D9	34/34 (100%)	29 (85%)	5 (15%)	3	20
37	BC	180/181 (99%)	170 (94%)	10 (6%)	21	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DC	180/181 (99%)	169 (94%)	11 (6%)	18	53
38	BD	217/218 (100%)	177 (82%)	40 (18%)	1	10
38	DD	217/218 (100%)	178 (82%)	39 (18%)	1	11
39	BE	165/166 (99%)	139 (84%)	26 (16%)	2	17
39	DE	165/166 (99%)	140 (85%)	25 (15%)	3	19
40	BF	165/166 (99%)	153 (93%)	12 (7%)	14	46
40	DF	165/166 (99%)	153 (93%)	12 (7%)	14	46
41	BG	155/156 (99%)	131 (84%)	24 (16%)	2	18
41	DG	155/156 (99%)	126 (81%)	29 (19%)	1	10
42	BH	136/148 (92%)	126 (93%)	10 (7%)	13	46
42	DH	136/148 (92%)	126 (93%)	10 (7%)	13	46
44	BK	104/111 (94%)	89 (86%)	15 (14%)	3	20
44	DK	104/111 (94%)	90 (86%)	14 (14%)	4	23
46	BN	117/119 (98%)	103 (88%)	14 (12%)	5	27
46	DN	117/119 (98%)	102 (87%)	15 (13%)	4	24
47	BO	100/100 (100%)	92 (92%)	8 (8%)	12	43
47	DO	100/100 (100%)	92 (92%)	8 (8%)	12	43
48	BP	112/116 (97%)	91 (81%)	21 (19%)	1	9
48	DP	112/116 (97%)	91 (81%)	21 (19%)	1	9
49	BQ	111/111 (100%)	95 (86%)	16 (14%)	3	20
49	DQ	111/111 (100%)	97 (87%)	14 (13%)	4	24
50	BR	100/101 (99%)	89 (89%)	11 (11%)	6	31
50	DR	100/101 (99%)	88 (88%)	12 (12%)	5	27
51	BS	77/88 (88%)	68 (88%)	9 (12%)	5	29
51	DS	77/88 (88%)	68 (88%)	9 (12%)	5	29
52	BT	120/127 (94%)	97 (81%)	23 (19%)	1	9
52	DT	120/127 (94%)	97 (81%)	23 (19%)	1	9
53	BU	92/94 (98%)	83 (90%)	9 (10%)	8	36
53	DU	92/94 (98%)	83 (90%)	9 (10%)	8	36
54	BV	82/82 (100%)	71 (87%)	11 (13%)	4	23
54	DV	82/82 (100%)	71 (87%)	11 (13%)	4	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	BW	91/92 (99%)	84 (92%)	7 (8%)	13	45
55	DW	91/92 (99%)	84 (92%)	7 (8%)	13	45
56	BX	74/78 (95%)	64 (86%)	10 (14%)	4	23
56	DX	74/78 (95%)	64 (86%)	10 (14%)	4	23
57	BY	87/91 (96%)	75 (86%)	12 (14%)	3	22
57	DY	87/91 (96%)	75 (86%)	12 (14%)	3	22
58	BZ	162/179 (90%)	134 (83%)	28 (17%)	2	12
58	DZ	162/179 (90%)	144 (89%)	18 (11%)	6	31
All	All	11080/11566 (96%)	9776 (88%)	1304 (12%)	5	28

All (1304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	16	HIS
2	AB	17	PHE
2	AB	24	TRP
2	AB	36	ARG
2	AB	43	ASP
2	AB	44	LEU
2	AB	67	THR
2	AB	79	ASP
2	AB	101	MET
2	AB	111	ARG
2	AB	129	GLU
2	AB	137	ARG
2	AB	157	ARG
2	AB	162	ILE
2	AB	172	ILE
2	AB	178	ARG
2	AB	192	SER
2	AB	200	ILE
2	AB	204	ASN
2	AB	212	GLN
2	AB	220	ASP
2	AB	221	LEU
3	AC	5	ILE
3	AC	16	ARG
3	AC	29	TYR

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Mol	Chain	Res	Type
3	AC	34	LEU
3	AC	56	ASP
3	AC	72	LYS
3	AC	79	ARG
3	AC	85	ARG
3	AC	95	THR
3	AC	98	ASN
3	AC	125	GLU
3	AC	127	ARG
3	AC	152	ILE
3	AC	156	ARG
3	AC	165	THR
3	AC	167	TRP
3	AC	178	LEU
3	AC	179	ARG
4	AD	3	ARG
4	AD	9	CYS
4	AD	12	CYS
4	AD	15	GLU
4	AD	22	LYS
4	AD	36	ARG
4	AD	49	ARG
4	AD	53	ASP
4	AD	57	ARG
4	AD	70	ILE
4	AD	73	ARG
4	AD	78	LEU
4	AD	96	LEU
4	AD	114	ARG
4	AD	127	THR
4	AD	131	ARG
4	AD	132	ARG
4	AD	135	LEU
4	AD	162	LEU
4	AD	168	ARG
5	AE	12	LEU
5	AE	18	ARG
5	AE	20	GLN
5	AE	31	LEU
5	AE	41	VAL
5	AE	47	LYS
5	AE	56	GLN

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Mol	Chain	Res	Type
5	AE	64	ARG
5	AE	72	GLN
5	AE	75	THR
5	AE	76	ILE
5	AE	79	GLU
5	AE	101	ILE
5	AE	117	ASP
5	AE	144	THR
6	AF	15	ASP
6	AF	32	ASN
6	AF	43	LEU
6	AF	47	ARG
6	AF	69	GLU
6	AF	86	ARG
6	AF	98	LEU
7	AG	27	ILE
7	AG	57	GLU
7	AG	66	VAL
7	AG	79	ARG
7	AG	104	LEU
7	AG	113	GLU
7	AG	124	LEU
7	AG	137	LYS
7	AG	151	TYR
8	AH	1	MET
8	AH	25	ASP
8	AH	54	ASP
8	AH	83	ILE
8	AH	91	ARG
8	AH	92	ARG
8	AH	98	LYS
8	AH	102	ARG
8	AH	118	VAL
9	AI	4	TYR
9	AI	10	ARG
9	AI	29	ASN
9	AI	59	PHE
9	AI	95	LYS
9	AI	114	TYR
9	AI	121	ARG
9	AI	128	ARG
10	AJ	22	LYS

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Mol	Chain	Res	Type
10	AJ	40	LEU
10	AJ	43	ARG
10	AJ	50	ILE
10	AJ	55	LYS
10	AJ	59	SER
10	AJ	62	HIS
10	AJ	63	PHE
10	AJ	74	ILE
10	AJ	76	ASN
10	AJ	96	ILE
11	AK	29	ILE
11	AK	87	THR
11	AK	91	ARG
11	AK	92	GLU
11	AK	117	ASN
11	AK	124	LYS
12	AL	7	ILE
12	AL	20	LYS
12	AL	38	THR
12	AL	41	ARG
12	AL	47	LYS
12	AL	53	ARG
12	AL	70	ILE
12	AL	81	SER
12	AL	85	ILE
12	AL	113	ARG
13	AM	64	TRP
13	AM	66	LEU
13	AM	108	ARG
13	AM	113	PRO
13	AM	115	LYS
13	AM	120	LYS
13	AM	121	LYS
13	AM	124	PRO
14	AN	14	PRO
14	AN	16	PHE
14	AN	29	ARG
14	AN	41	ARG
14	AN	42	ILE
14	AN	44	LEU
15	AO	10	LYS
15	AO	39	LEU

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Mol	Chain	Res	Type
15	AO	41	GLU
15	AO	57	LEU
15	AO	65	ARG
15	AO	82	ILE
15	AO	85	LEU
15	AO	88	ARG
16	AP	1	MET
16	AP	2	VAL
16	AP	6	LEU
16	AP	11	SER
16	AP	32	TYR
17	AQ	7	THR
17	AQ	9	VAL
17	AQ	23	VAL
17	AQ	35	VAL
17	AQ	48	GLU
17	AQ	52	LYS
17	AQ	78	GLU
18	AR	29	PHE
18	AR	31	LEU
19	AS	5	LEU
19	AS	6	LYS
19	AS	7	LYS
19	AS	15	LEU
19	AS	19	VAL
19	AS	29	ARG
19	AS	37	ARG
19	AS	44	MET
19	AS	66	MET
19	AS	77	THR
20	AT	13	LEU
20	AT	24	LEU
20	AT	26	ASN
20	AT	36	LEU
20	AT	74	LYS
20	AT	84	LEU
20	AT	93	GLU
24	AY	20	HIS
24	AY	21	ILE
24	AY	40	HIS
24	AY	65	ILE
24	AY	83	ASP

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Mol	Chain	Res	Type
24	AY	85	PRO
24	AY	88	VAL
24	AY	89	ASP
24	AY	92	ILE
24	AY	96	ARG
24	AY	100	VAL
24	AY	101	LEU
24	AY	102	ASP
24	AY	111	SER
24	AY	117	GLN
24	AY	122	TRP
24	AY	124	GLN
24	AY	130	VAL
24	AY	132	ARG
24	AY	137	ASN
24	AY	152	THR
24	AY	157	LEU
24	AY	170	ARG
24	AY	191	ASP
24	AY	192	LEU
24	AY	240	GLU
24	AY	242	LEU
24	AY	252	ASP
24	AY	255	ILE
24	AY	260	LEU
24	AY	270	GLN
24	AY	289	ILE
24	AY	298	VAL
24	AY	312	LEU
24	AY	319	ASP
24	AY	326	THR
24	AY	337	SER
24	AY	343	ASN
24	AY	357	ARG
24	AY	378	VAL
24	AY	381	LYS
24	AY	388	THR
24	AY	399	LEU
24	AY	409	ILE
24	AY	410	ASP
24	AY	420	ASP
24	AY	421	GLN

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Mol	Chain	Res	Type
24	AY	426	GLN
24	AY	428	LEU
24	AY	438	PHE
24	AY	440	VAL
24	AY	468	ARG
24	AY	476	VAL
24	AY	481	VAL
24	AY	487	ILE
24	AY	501	THR
24	AY	504	ARG
24	AY	509	HIS
24	AY	512	ILE
24	AY	515	GLU
24	AY	525	PHE
24	AY	527	ASN
24	AY	567	LEU
24	AY	572	TYR
24	AY	574	GLU
24	AY	595	GLN
24	AY	598	ASP
24	AY	614	GLU
24	AY	630	GLN
24	AY	631	ILE
24	AY	634	MET
24	AY	644	ARG
24	AY	657	THR
24	AY	685	GLU
25	B0	5	LYS
25	B0	11	ARG
25	B0	20	ARG
25	B0	27	GLU
25	B0	41	ARG
25	B0	60	PHE
25	B0	75	LEU
25	B0	78	TYR
25	B0	84	LEU
26	B1	18	ILE
26	B1	35	THR
26	B1	45	ASN
26	B1	46	LEU
26	B1	56	GLN
26	B1	65	SER

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Mol	Chain	Res	Type
26	B1	72	GLU
26	B1	73	LEU
26	B1	75	GLU
26	B1	80	LEU
26	B1	83	GLU
26	B1	94	LEU
26	B1	95	LEU
27	B2	3	LEU
27	B2	30	ARG
27	B2	32	LEU
27	B2	44	LEU
27	B2	52	ASP
27	B2	59	ARG
27	B2	64	LEU
28	B3	8	LEU
28	B3	28	LEU
28	B3	38	GLU
28	B3	48	GLU
29	B4	1	MET
29	B4	5	ILE
29	B4	8	LYS
29	B4	9	LEU
29	B4	13	ARG
29	B4	20	ASN
29	B4	32	TYR
29	B4	40	HIS
29	B4	42	PHE
29	B4	43	TYR
29	B4	49	PHE
29	B4	51	ASP
29	B4	55	ARG
30	B5	3	LYS
30	B5	4	HIS
30	B5	23	HIS
30	B5	36	CYS
30	B5	55	ARG
30	B5	58	LEU
31	B6	6	ARG
31	B6	9	LEU
31	B6	10	LEU
31	B6	11	LEU
31	B6	15	GLU

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Mol	Chain	Res	Type
31	B6	23	THR
31	B6	30	THR
31	B6	31	PRO
31	B6	39	TYR
31	B6	42	TRP
32	B7	1	MET
32	B7	4	THR
32	B7	8	ASN
32	B7	41	ARG
32	B7	48	LYS
33	B8	6	THR
33	B8	30	ARG
33	B8	32	LEU
33	B8	33	ASN
33	B8	34	TRP
33	B8	44	LYS
33	B8	48	PHE
33	B8	49	VAL
33	B8	61	LEU
34	B9	1	MET
34	B9	10	ILE
34	B9	11	CYS
34	B9	29	ASN
37	BC	18	ASN
37	BC	53	ARG
37	BC	54	ARG
37	BC	74	ARG
37	BC	149	ASN
37	BC	184	GLU
37	BC	185	LYS
37	BC	189	ASN
37	BC	191	ARG
37	BC	212	SER
38	BD	10	THR
38	BD	23	GLU
38	BD	24	ILE
38	BD	26	LYS
38	BD	35	LYS
38	BD	37	LEU
38	BD	43	ARG
38	BD	61	LEU
38	BD	63	ARG

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Mol	Chain	Res	Type
38	BD	65	ILE
38	BD	87	ASN
38	BD	89	SER
38	BD	92	ILE
38	BD	94	LEU
38	BD	95	LEU
38	BD	96	HIS
38	BD	104	TYR
38	BD	106	ILE
38	BD	111	LEU
38	BD	117	VAL
38	BD	131	LEU
38	BD	157	ARG
38	BD	166	GLN
38	BD	183	ARG
38	BD	190	TYR
38	BD	192	THR
38	BD	202	LYS
38	BD	211	ARG
38	BD	212	SER
38	BD	221	VAL
38	BD	227	ASN
38	BD	228	PRO
38	BD	244	ARG
38	BD	246	PRO
38	BD	257	LEU
38	BD	260	ARG
38	BD	263	ARG
38	BD	270	ILE
38	BD	273	ARG
38	BD	275	LYS
39	BE	4	ILE
39	BE	9	VAL
39	BE	18	ASP
39	BE	24	THR
39	BE	36	ARG
39	BE	49	LEU
39	BE	54	GLN
39	BE	55	ASN
39	BE	61	ARG
39	BE	67	PHE
39	BE	69	LYS

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Mol	Chain	Res	Type
39	BE	78	LEU
39	BE	79	ARG
39	BE	94	GLU
39	BE	95	ILE
39	BE	118	LYS
39	BE	119	ARG
39	BE	121	ASN
39	BE	134	ILE
39	BE	144	ARG
39	BE	178	GLU
39	BE	184	VAL
39	BE	192	ASN
39	BE	197	ILE
39	BE	202	LYS
39	BE	203	LYS
40	BF	19	GLU
40	BF	28	ILE
40	BF	41	LEU
40	BF	64	ILE
40	BF	66	PRO
40	BF	83	PHE
40	BF	125	LEU
40	BF	149	ASP
40	BF	160	ASN
40	BF	165	ARG
40	BF	175	THR
40	BF	179	GLU
41	BG	4	ASP
41	BG	5	VAL
41	BG	16	ARG
41	BG	22	ARG
41	BG	33	ARG
41	BG	34	LEU
41	BG	36	LYS
41	BG	60	LEU
41	BG	71	THR
41	BG	80	PHE
41	BG	83	ARG
41	BG	91	ARG
41	BG	98	ARG
41	BG	118	ARG
41	BG	128	ARG

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Mol	Chain	Res	Type
41	BG	133	LEU
41	BG	135	LEU
41	BG	145	THR
41	BG	147	ASP
41	BG	148	MET
41	BG	152	LEU
41	BG	159	VAL
41	BG	164	GLU
41	BG	166	ASP
42	BH	46	GLU
42	BH	49	VAL
42	BH	53	GLU
42	BH	54	ARG
42	BH	83	TYR
42	BH	89	ILE
42	BH	104	GLU
42	BH	105	LEU
42	BH	143	GLN
42	BH	158	HIS
44	BK	2	LYS
44	BK	3	LYS
44	BK	5	VAL
44	BK	29	GLN
44	BK	30	HIS
44	BK	34	ILE
44	BK	38	VAL
44	BK	47	ASN
44	BK	65	PHE
44	BK	70	LYS
44	BK	77	LEU
44	BK	86	LYS
44	BK	95	LYS
44	BK	105	LEU
44	BK	117	THR
46	BN	1	MET
46	BN	4	TYR
46	BN	23	LEU
46	BN	26	LEU
46	BN	39	ARG
46	BN	41	ASP
46	BN	45	ASN
46	BN	48	MET

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Mol	Chain	Res	Type
46	BN	56	ASN
46	BN	63	THR
46	BN	65	LYS
46	BN	96	GLU
46	BN	109	LYS
46	BN	123	TYR
47	BO	23	ARG
47	BO	38	VAL
47	BO	40	VAL
47	BO	48	PRO
47	BO	49	ARG
47	BO	80	ASP
47	BO	87	ILE
47	BO	117	LEU
48	BP	7	ARG
48	BP	13	ASN
48	BP	16	ARG
48	BP	18	ARG
48	BP	39	LYS
48	BP	41	ARG
48	BP	42	SER
48	BP	51	PHE
48	BP	57	THR
48	BP	60	MET
48	BP	61	ARG
48	BP	62	LEU
48	BP	64	LYS
48	BP	70	GLN
48	BP	81	GLN
48	BP	85	LEU
48	BP	91	PHE
48	BP	108	LYS
48	BP	114	ILE
48	BP	123	LEU
48	BP	149	GLU
49	BQ	14	ARG
49	BQ	17	LEU
49	BQ	45	GLN
49	BQ	46	GLN
49	BQ	55	VAL
49	BQ	56	ARG
49	BQ	58	PHE

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Mol	Chain	Res	Type
49	BQ	65	PHE
49	BQ	67	ARG
49	BQ	76	LYS
49	BQ	79	LEU
49	BQ	81	VAL
49	BQ	106	VAL
49	BQ	134	ARG
49	BQ	135	ASP
49	BQ	139	GLU
50	BR	8	ARG
50	BR	27	SER
50	BR	30	THR
50	BR	33	ARG
50	BR	54	LEU
50	BR	71	GLN
50	BR	75	LEU
50	BR	94	TYR
50	BR	97	VAL
50	BR	99	LYS
50	BR	100	LEU
51	BS	11	LYS
51	BS	12	PHE
51	BS	36	TYR
51	BS	63	THR
51	BS	67	ARG
51	BS	92	TYR
51	BS	97	ARG
51	BS	101	LEU
51	BS	106	ARG
52	BT	6	LEU
52	BT	13	ARG
52	BT	16	ARG
52	BT	24	PRO
52	BT	32	TYR
52	BT	38	ASN
52	BT	49	VAL
52	BT	53	ARG
52	BT	58	ASN
52	BT	62	THR
52	BT	65	LYS
52	BT	78	LEU
52	BT	82	LEU

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Mol	Chain	Res	Type
52	BT	90	GLN
52	BT	93	ARG
52	BT	96	ARG
52	BT	108	ARG
52	BT	115	ARG
52	BT	124	ASP
52	BT	125	ARG
52	BT	128	GLU
52	BT	129	ARG
52	BT	132	LYS
53	BU	20	LEU
53	BU	49	HIS
53	BU	74	LEU
53	BU	76	TYR
53	BU	79	PHE
53	BU	92	ARG
53	BU	101	ARG
53	BU	108	GLU
53	BU	112	ARG
54	BV	1	MET
54	BV	18	LEU
54	BV	19	LYS
54	BV	21	ARG
54	BV	39	LEU
54	BV	40	LEU
54	BV	82	ARG
54	BV	89	GLN
54	BV	95	LEU
54	BV	98	GLU
54	BV	99	ILE
55	BW	11	ARG
55	BW	40	ASN
55	BW	52	GLU
55	BW	75	TYR
55	BW	88	ARG
55	BW	98	LYS
55	BW	107	LEU
56	BX	3	THR
56	BX	11	PRO
56	BX	27	THR
56	BX	28	PHE
56	BX	51	VAL

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Mol	Chain	Res	Type
56	BX	56	THR
56	BX	57	LEU
56	BX	68	ARG
56	BX	75	ASP
56	BX	76	ARG
57	BY	2	ARG
57	BY	7	VAL
57	BY	9	LYS
57	BY	29	GLU
57	BY	32	PRO
57	BY	51	VAL
57	BY	53	PRO
57	BY	55	TYR
57	BY	77	PRO
57	BY	79	CYS
57	BY	90	LEU
57	BY	102	CYS
58	BZ	5	LEU
58	BZ	6	LYS
58	BZ	8	TYR
58	BZ	28	MET
58	BZ	30	ASN
58	BZ	31	ARG
58	BZ	34	ASN
58	BZ	55	HIS
58	BZ	63	ASP
58	BZ	68	PRO
58	BZ	72	ARG
58	BZ	78	LYS
58	BZ	83	PRO
58	BZ	87	ASP
58	BZ	92	SER
58	BZ	107	THR
58	BZ	112	ARG
58	BZ	123	ASP
58	BZ	127	LYS
58	BZ	140	ASP
58	BZ	146	ILE
58	BZ	150	LEU
58	BZ	154	ASP
58	BZ	158	PRO
58	BZ	163	LEU

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Mol	Chain	Res	Type
58	BZ	166	SER
58	BZ	171	ILE
58	BZ	186	GLU
2	CB	15	VAL
2	CB	16	HIS
2	CB	17	PHE
2	CB	24	TRP
2	CB	36	ARG
2	CB	43	ASP
2	CB	44	LEU
2	CB	67	THR
2	CB	79	ASP
2	CB	101	MET
2	CB	111	ARG
2	CB	129	GLU
2	CB	137	ARG
2	CB	157	ARG
2	CB	162	ILE
2	CB	172	ILE
2	CB	178	ARG
2	CB	192	SER
2	CB	200	ILE
2	CB	204	ASN
2	CB	212	GLN
2	CB	220	ASP
2	CB	221	LEU
3	CC	5	ILE
3	CC	16	ARG
3	CC	29	TYR
3	CC	34	LEU
3	CC	56	ASP
3	CC	72	LYS
3	CC	79	ARG
3	CC	85	ARG
3	CC	95	THR
3	CC	98	ASN
3	CC	125	GLU
3	CC	127	ARG
3	CC	152	ILE
3	CC	156	ARG
3	CC	165	THR
3	CC	167	TRP

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Mol	Chain	Res	Type
3	CC	178	LEU
3	CC	179	ARG
4	CD	3	ARG
4	CD	9	CYS
4	CD	12	CYS
4	CD	15	GLU
4	CD	22	LYS
4	CD	36	ARG
4	CD	49	ARG
4	CD	53	ASP
4	CD	57	ARG
4	CD	70	ILE
4	CD	73	ARG
4	CD	78	LEU
4	CD	96	LEU
4	CD	114	ARG
4	CD	127	THR
4	CD	131	ARG
4	CD	132	ARG
4	CD	135	LEU
4	CD	162	LEU
4	CD	168	ARG
5	CE	12	LEU
5	CE	18	ARG
5	CE	20	GLN
5	CE	31	LEU
5	CE	41	VAL
5	CE	47	LYS
5	CE	56	GLN
5	CE	64	ARG
5	CE	72	GLN
5	CE	75	THR
5	CE	76	ILE
5	CE	79	GLU
5	CE	101	ILE
5	CE	117	ASP
5	CE	144	THR
6	CF	15	ASP
6	CF	32	ASN
6	CF	43	LEU
6	CF	47	ARG
6	CF	69	GLU

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Mol	Chain	Res	Type
6	CF	86	ARG
6	CF	98	LEU
7	CG	27	ILE
7	CG	57	GLU
7	CG	66	VAL
7	CG	79	ARG
7	CG	104	LEU
7	CG	113	GLU
7	CG	124	LEU
7	CG	137	LYS
7	CG	151	TYR
8	CH	1	MET
8	CH	25	ASP
8	CH	54	ASP
8	CH	91	ARG
8	CH	98	LYS
8	CH	102	ARG
8	CH	118	VAL
9	CI	4	TYR
9	CI	10	ARG
9	CI	29	ASN
9	CI	59	PHE
9	CI	95	LYS
9	CI	114	TYR
9	CI	121	ARG
9	CI	128	ARG
10	CJ	22	LYS
10	CJ	40	LEU
10	CJ	43	ARG
10	CJ	50	ILE
10	CJ	55	LYS
10	CJ	59	SER
10	CJ	62	HIS
10	CJ	63	PHE
10	CJ	74	ILE
10	CJ	76	ASN
10	CJ	96	ILE
11	CK	29	ILE
11	CK	87	THR
11	CK	91	ARG
11	CK	92	GLU
11	CK	117	ASN

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Mol	Chain	Res	Type
11	CK	124	LYS
12	CL	7	ILE
12	CL	20	LYS
12	CL	38	THR
12	CL	41	ARG
12	CL	47	LYS
12	CL	53	ARG
12	CL	70	ILE
12	CL	81	SER
12	CL	85	ILE
12	CL	98	TYR
12	CL	113	ARG
13	CM	64	TRP
13	CM	66	LEU
13	CM	108	ARG
13	CM	113	PRO
13	CM	115	LYS
13	CM	120	LYS
13	CM	121	LYS
13	CM	124	PRO
14	CN	14	PRO
14	CN	16	PHE
14	CN	29	ARG
14	CN	41	ARG
14	CN	42	ILE
14	CN	44	LEU
15	CO	10	LYS
15	CO	39	LEU
15	CO	41	GLU
15	CO	57	LEU
15	CO	65	ARG
15	CO	82	ILE
15	CO	85	LEU
15	CO	88	ARG
16	CP	1	MET
16	CP	2	VAL
16	CP	6	LEU
16	CP	11	SER
16	CP	32	TYR
17	CQ	7	THR
17	CQ	9	VAL
17	CQ	23	VAL

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Mol	Chain	Res	Type
17	CQ	35	VAL
17	CQ	48	GLU
17	CQ	52	LYS
17	CQ	78	GLU
18	CR	29	PHE
18	CR	31	LEU
19	CS	5	LEU
19	CS	6	LYS
19	CS	7	LYS
19	CS	15	LEU
19	CS	19	VAL
19	CS	29	ARG
19	CS	37	ARG
19	CS	44	MET
19	CS	66	MET
19	CS	77	THR
20	CT	13	LEU
20	CT	24	LEU
20	CT	26	ASN
20	CT	36	LEU
20	CT	74	LYS
20	CT	84	LEU
20	CT	93	GLU
24	CY	6	GLU
24	CY	13	ARG
24	CY	14	ASN
24	CY	21	ILE
24	CY	34	TYR
24	CY	65	ILE
24	CY	66	THR
24	CY	79	ILE
24	CY	81	ILE
24	CY	88	VAL
24	CY	90	PHE
24	CY	92	ILE
24	CY	95	GLU
24	CY	100	VAL
24	CY	101	LEU
24	CY	102	ASP
24	CY	117	GLN
24	CY	128	TYR
24	CY	130	VAL

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Mol	Chain	Res	Type
24	CY	132	ARG
24	CY	137	ASN
24	CY	157	LEU
24	CY	175	SER
24	CY	191	ASP
24	CY	192	LEU
24	CY	216	LEU
24	CY	225	GLU
24	CY	232	LEU
24	CY	255	ILE
24	CY	260	LEU
24	CY	278	ASP
24	CY	312	LEU
24	CY	326	THR
24	CY	343	ASN
24	CY	357	ARG
24	CY	381	LYS
24	CY	388	THR
24	CY	396	ARG
24	CY	397	VAL
24	CY	399	LEU
24	CY	415	PRO
24	CY	420	ASP
24	CY	421	GLN
24	CY	422	GLU
24	CY	428	LEU
24	CY	438	PHE
24	CY	459	LEU
24	CY	476	VAL
24	CY	487	ILE
24	CY	492	ASP
24	CY	499	ARG
24	CY	504	ARG
24	CY	507	TYR
24	CY	512	ILE
24	CY	527	ASN
24	CY	548	GLU
24	CY	572	TYR
24	CY	575	VAL
24	CY	580	MET
24	CY	598	ASP
24	CY	614	GLU

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Mol	Chain	Res	Type
24	CY	634	MET
24	CY	641	GLN
24	CY	644	ARG
24	CY	647	VAL
24	CY	661	SER
24	CY	674	ASP
24	CY	683	VAL
25	D0	5	LYS
25	D0	11	ARG
25	D0	20	ARG
25	D0	27	GLU
25	D0	41	ARG
25	D0	60	PHE
25	D0	75	LEU
25	D0	78	TYR
25	D0	84	LEU
26	D1	20	ARG
26	D1	39	LYS
26	D1	45	ASN
26	D1	46	LEU
26	D1	50	ARG
26	D1	61	ARG
26	D1	80	LEU
26	D1	83	GLU
27	D2	20	GLU
27	D2	37	PHE
27	D2	53	LEU
27	D2	56	GLN
27	D2	57	ILE
27	D2	59	ARG
27	D2	60	LEU
27	D2	63	VAL
28	D3	8	LEU
28	D3	28	LEU
28	D3	38	GLU
28	D3	48	GLU
29	D4	1	MET
29	D4	5	ILE
29	D4	8	LYS
29	D4	9	LEU
29	D4	13	ARG
29	D4	20	ASN

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Mol	Chain	Res	Type
29	D4	32	TYR
29	D4	39	CYS
29	D4	40	HIS
29	D4	42	PHE
29	D4	43	TYR
29	D4	49	PHE
29	D4	51	ASP
29	D4	55	ARG
30	D5	3	LYS
30	D5	4	HIS
30	D5	23	HIS
30	D5	36	CYS
30	D5	55	ARG
30	D5	58	LEU
31	D6	6	ARG
31	D6	9	LEU
31	D6	10	LEU
31	D6	11	LEU
31	D6	15	GLU
31	D6	23	THR
31	D6	28	ARG
31	D6	30	THR
31	D6	31	PRO
31	D6	39	TYR
31	D6	42	TRP
32	D7	1	MET
32	D7	4	THR
32	D7	8	ASN
32	D7	41	ARG
32	D7	48	LYS
33	D8	6	THR
33	D8	30	ARG
33	D8	32	LEU
33	D8	33	ASN
33	D8	34	TRP
33	D8	44	LYS
33	D8	48	PHE
33	D8	49	VAL
33	D8	61	LEU
33	D8	64	TYR
34	D9	1	MET
34	D9	2	LYS

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Mol	Chain	Res	Type
34	D9	10	ILE
34	D9	11	CYS
34	D9	29	ASN
37	DC	18	ASN
37	DC	53	ARG
37	DC	54	ARG
37	DC	74	ARG
37	DC	121	MET
37	DC	149	ASN
37	DC	184	GLU
37	DC	185	LYS
37	DC	189	ASN
37	DC	191	ARG
37	DC	212	SER
38	DD	10	THR
38	DD	23	GLU
38	DD	24	ILE
38	DD	26	LYS
38	DD	35	LYS
38	DD	37	LEU
38	DD	43	ARG
38	DD	61	LEU
38	DD	63	ARG
38	DD	65	ILE
38	DD	87	ASN
38	DD	89	SER
38	DD	92	ILE
38	DD	94	LEU
38	DD	95	LEU
38	DD	96	HIS
38	DD	104	TYR
38	DD	106	ILE
38	DD	111	LEU
38	DD	117	VAL
38	DD	131	LEU
38	DD	157	ARG
38	DD	166	GLN
38	DD	183	ARG
38	DD	190	TYR
38	DD	192	THR
38	DD	202	LYS
38	DD	212	SER

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Mol	Chain	Res	Type
38	DD	221	VAL
38	DD	227	ASN
38	DD	228	PRO
38	DD	244	ARG
38	DD	246	PRO
38	DD	257	LEU
38	DD	260	ARG
38	DD	270	ILE
38	DD	271	ILE
38	DD	273	ARG
38	DD	275	LYS
39	DE	4	ILE
39	DE	9	VAL
39	DE	18	ASP
39	DE	36	ARG
39	DE	49	LEU
39	DE	55	ASN
39	DE	61	ARG
39	DE	67	PHE
39	DE	69	LYS
39	DE	78	LEU
39	DE	79	ARG
39	DE	94	GLU
39	DE	95	ILE
39	DE	113	PHE
39	DE	118	LYS
39	DE	119	ARG
39	DE	121	ASN
39	DE	134	ILE
39	DE	144	ARG
39	DE	178	GLU
39	DE	184	VAL
39	DE	192	ASN
39	DE	197	ILE
39	DE	202	LYS
39	DE	203	LYS
40	DF	19	GLU
40	DF	28	ILE
40	DF	41	LEU
40	DF	64	ILE
40	DF	66	PRO
40	DF	83	PHE

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Mol	Chain	Res	Type
40	DF	125	LEU
40	DF	149	ASP
40	DF	160	ASN
40	DF	165	ARG
40	DF	175	THR
40	DF	179	GLU
41	DG	4	ASP
41	DG	22	ARG
41	DG	26	GLN
41	DG	33	ARG
41	DG	34	LEU
41	DG	37	VAL
41	DG	38	VAL
41	DG	40	ASN
41	DG	43	LEU
41	DG	45	GLU
41	DG	47	LYS
41	DG	49	ASP
41	DG	51	ARG
41	DG	62	LEU
41	DG	67	LYS
41	DG	80	PHE
41	DG	82	LEU
41	DG	83	ARG
41	DG	98	ARG
41	DG	118	ARG
41	DG	120	LEU
41	DG	123	ASN
41	DG	135	LEU
41	DG	143	GLU
41	DG	145	THR
41	DG	148	MET
41	DG	159	VAL
41	DG	166	ASP
41	DG	167	GLU
42	DH	46	GLU
42	DH	49	VAL
42	DH	53	GLU
42	DH	54	ARG
42	DH	83	TYR
42	DH	89	ILE
42	DH	104	GLU

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Mol	Chain	Res	Type
42	DH	105	LEU
42	DH	143	GLN
42	DH	158	HIS
44	DK	2	LYS
44	DK	3	LYS
44	DK	29	GLN
44	DK	30	HIS
44	DK	34	ILE
44	DK	38	VAL
44	DK	47	ASN
44	DK	65	PHE
44	DK	70	LYS
44	DK	77	LEU
44	DK	86	LYS
44	DK	95	LYS
44	DK	105	LEU
44	DK	117	THR
46	DN	1	MET
46	DN	4	TYR
46	DN	23	LEU
46	DN	26	LEU
46	DN	39	ARG
46	DN	41	ASP
46	DN	45	ASN
46	DN	48	MET
46	DN	56	ASN
46	DN	63	THR
46	DN	65	LYS
46	DN	78	TYR
46	DN	96	GLU
46	DN	109	LYS
46	DN	123	TYR
47	DO	23	ARG
47	DO	38	VAL
47	DO	40	VAL
47	DO	48	PRO
47	DO	49	ARG
47	DO	80	ASP
47	DO	87	ILE
47	DO	117	LEU
48	DP	7	ARG
48	DP	13	ASN

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Mol	Chain	Res	Type
48	DP	16	ARG
48	DP	18	ARG
48	DP	39	LYS
48	DP	41	ARG
48	DP	42	SER
48	DP	51	PHE
48	DP	57	THR
48	DP	60	MET
48	DP	61	ARG
48	DP	62	LEU
48	DP	64	LYS
48	DP	70	GLN
48	DP	81	GLN
48	DP	85	LEU
48	DP	91	PHE
48	DP	108	LYS
48	DP	114	ILE
48	DP	123	LEU
48	DP	149	GLU
49	DQ	14	ARG
49	DQ	45	GLN
49	DQ	46	GLN
49	DQ	55	VAL
49	DQ	56	ARG
49	DQ	58	PHE
49	DQ	65	PHE
49	DQ	67	ARG
49	DQ	76	LYS
49	DQ	79	LEU
49	DQ	81	VAL
49	DQ	134	ARG
49	DQ	135	ASP
49	DQ	139	GLU
50	DR	8	ARG
50	DR	27	SER
50	DR	30	THR
50	DR	33	ARG
50	DR	54	LEU
50	DR	65	LEU
50	DR	71	GLN
50	DR	75	LEU
50	DR	94	TYR

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Mol	Chain	Res	Type
50	DR	97	VAL
50	DR	99	LYS
50	DR	100	LEU
51	DS	11	LYS
51	DS	12	PHE
51	DS	36	TYR
51	DS	63	THR
51	DS	67	ARG
51	DS	92	TYR
51	DS	97	ARG
51	DS	101	LEU
51	DS	106	ARG
52	DT	6	LEU
52	DT	13	ARG
52	DT	16	ARG
52	DT	24	PRO
52	DT	32	TYR
52	DT	38	ASN
52	DT	49	VAL
52	DT	53	ARG
52	DT	58	ASN
52	DT	62	THR
52	DT	65	LYS
52	DT	78	LEU
52	DT	82	LEU
52	DT	90	GLN
52	DT	93	ARG
52	DT	96	ARG
52	DT	108	ARG
52	DT	115	ARG
52	DT	124	ASP
52	DT	125	ARG
52	DT	128	GLU
52	DT	129	ARG
52	DT	132	LYS
53	DU	20	LEU
53	DU	49	HIS
53	DU	74	LEU
53	DU	76	TYR
53	DU	79	PHE
53	DU	92	ARG
53	DU	101	ARG

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Mol	Chain	Res	Type
53	DU	108	GLU
53	DU	112	ARG
54	DV	1	MET
54	DV	18	LEU
54	DV	19	LYS
54	DV	21	ARG
54	DV	39	LEU
54	DV	40	LEU
54	DV	82	ARG
54	DV	89	GLN
54	DV	95	LEU
54	DV	98	GLU
54	DV	99	ILE
55	DW	11	ARG
55	DW	40	ASN
55	DW	52	GLU
55	DW	75	TYR
55	DW	88	ARG
55	DW	98	LYS
55	DW	107	LEU
56	DX	3	THR
56	DX	11	PRO
56	DX	27	THR
56	DX	28	PHE
56	DX	51	VAL
56	DX	56	THR
56	DX	57	LEU
56	DX	68	ARG
56	DX	75	ASP
56	DX	76	ARG
57	DY	2	ARG
57	DY	7	VAL
57	DY	9	LYS
57	DY	29	GLU
57	DY	32	PRO
57	DY	51	VAL
57	DY	53	PRO
57	DY	55	TYR
57	DY	77	PRO
57	DY	79	CYS
57	DY	90	LEU
57	DY	102	CYS

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Mol	Chain	Res	Type
58	DZ	5	LEU
58	DZ	6	LYS
58	DZ	8	TYR
58	DZ	20	ARG
58	DZ	24	LEU
58	DZ	31	ARG
58	DZ	72	ARG
58	DZ	81	ARG
58	DZ	87	ASP
58	DZ	92	SER
58	DZ	112	ARG
58	DZ	123	ASP
58	DZ	140	ASP
58	DZ	150	LEU
58	DZ	154	ASP
58	DZ	168	GLU
58	DZ	171	ILE
58	DZ	179	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (348) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	37	ASN
2	AB	40	HIS
2	AB	78	GLN
2	AB	94	ASN
2	AB	110	GLN
2	AB	113	HIS
2	AB	146	GLN
2	AB	204	ASN
3	AC	28	GLN
3	AC	31	HIS
3	AC	37	GLN
3	AC	108	ASN
3	AC	118	GLN
3	AC	170	GLN
3	AC	176	HIS
3	AC	181	ASN
4	AD	62	GLN
4	AD	74	GLN
4	AD	77	ASN
4	AD	129	ASN

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Mol	Chain	Res	Type
5	AE	20	GLN
5	AE	72	GLN
5	AE	73	ASN
6	AF	16	GLN
6	AF	18	GLN
6	AF	27	GLN
6	AF	32	ASN
6	AF	73	ASN
6	AF	100	ASN
7	AG	13	GLN
7	AG	68	ASN
7	AG	84	ASN
7	AG	96	GLN
7	AG	97	GLN
7	AG	106	GLN
8	AH	82	HIS
9	AI	3	GLN
9	AI	58	HIS
9	AI	124	GLN
10	AJ	56	HIS
10	AJ	68	HIS
10	AJ	76	ASN
10	AJ	84	GLN
11	AK	22	HIS
11	AK	117	ASN
12	AL	9	GLN
12	AL	49	ASN
12	AL	75	HIS
12	AL	99	HIS
13	AM	40	ASN
13	AM	77	ASN
14	AN	49	HIS
15	AO	9	GLN
15	AO	13	GLN
15	AO	37	ASN
15	AO	62	GLN
17	AQ	16	GLN
19	AS	14	HIS
19	AS	47	HIS
20	AT	26	ASN
20	AT	42	GLN
20	AT	45	GLN

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Mol	Chain	Res	Type
20	AT	75	ASN
24	AY	14	ASN
24	AY	124	GLN
24	AY	137	ASN
24	AY	165	GLN
24	AY	208	GLN
24	AY	343	ASN
24	AY	421	GLN
24	AY	458	HIS
24	AY	475	ASN
24	AY	500	GLN
24	AY	527	ASN
24	AY	573	HIS
24	AY	630	GLN
24	AY	641	GLN
25	B0	70	GLN
26	B1	45	ASN
26	B1	56	GLN
27	B2	38	GLN
27	B2	47	ASN
27	B2	56	GLN
28	B3	19	GLN
28	B3	46	ASN
30	B5	22	HIS
30	B5	23	HIS
30	B5	43	HIS
31	B6	20	ASN
31	B6	26	ASN
31	B6	32	ASN
31	B6	49	HIS
32	B7	8	ASN
33	B8	31	HIS
33	B8	33	ASN
33	B8	43	GLN
34	B9	29	ASN
37	BC	58	ASN
37	BC	149	ASN
37	BC	166	ASN
38	BD	58	HIS
38	BD	115	GLN
38	BD	116	GLN
38	BD	126	GLN

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Mol	Chain	Res	Type
38	BD	166	GLN
38	BD	186	HIS
38	BD	198	ASN
38	BD	227	ASN
39	BE	48	GLN
39	BE	54	GLN
39	BE	55	ASN
39	BE	129	HIS
39	BE	143	ASN
39	BE	169	ASN
39	BE	192	ASN
40	BF	8	GLN
40	BF	69	HIS
40	BF	75	HIS
40	BF	133	ASN
40	BF	160	ASN
40	BF	169	ASN
40	BF	204	ASN
41	BG	27	ASN
42	BH	65	HIS
42	BH	147	ASN
42	BH	158	HIS
44	BK	29	GLN
44	BK	47	ASN
44	BK	89	HIS
46	BN	45	ASN
46	BN	56	ASN
46	BN	101	HIS
46	BN	131	GLN
47	BO	5	GLN
47	BO	82	ASN
48	BP	9	ASN
48	BP	13	ASN
48	BP	27	HIS
48	BP	84	ASN
48	BP	128	HIS
49	BQ	12	GLN
49	BQ	13	GLN
49	BQ	45	GLN
50	BR	3	HIS
50	BR	16	HIS
50	BR	23	ASN

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Mol	Chain	Res	Type
50	BR	61	HIS
52	BT	38	ASN
52	BT	43	GLN
52	BT	58	ASN
52	BT	84	GLN
52	BT	90	GLN
53	BU	14	HIS
53	BU	44	ASN
53	BU	49	HIS
53	BU	66	ASN
53	BU	81	HIS
53	BU	94	ASN
53	BU	117	GLN
54	BV	11	GLN
55	BW	61	ASN
55	BW	102	HIS
56	BX	41	ASN
56	BX	55	ASN
56	BX	82	GLN
58	BZ	54	HIS
58	BZ	65	GLN
58	BZ	118	GLN
58	BZ	121	HIS
2	CB	37	ASN
2	CB	40	HIS
2	CB	78	GLN
2	CB	94	ASN
2	CB	110	GLN
2	CB	113	HIS
2	CB	146	GLN
2	CB	204	ASN
3	CC	28	GLN
3	CC	31	HIS
3	CC	37	GLN
3	CC	108	ASN
3	CC	118	GLN
3	CC	170	GLN
3	CC	176	HIS
3	CC	181	ASN
4	CD	62	GLN
4	CD	74	GLN
4	CD	77	ASN

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Mol	Chain	Res	Type
4	CD	129	ASN
5	CE	20	GLN
5	CE	72	GLN
5	CE	73	ASN
6	CF	16	GLN
6	CF	18	GLN
6	CF	27	GLN
6	CF	32	ASN
6	CF	73	ASN
6	CF	100	ASN
7	CG	13	GLN
7	CG	68	ASN
7	CG	84	ASN
7	CG	96	GLN
7	CG	97	GLN
7	CG	106	GLN
8	CH	82	HIS
9	CI	3	GLN
9	CI	58	HIS
9	CI	124	GLN
10	CJ	56	HIS
10	CJ	68	HIS
10	CJ	76	ASN
10	CJ	84	GLN
11	CK	22	HIS
11	CK	117	ASN
12	CL	9	GLN
12	CL	49	ASN
12	CL	75	HIS
13	CM	40	ASN
13	CM	77	ASN
13	CM	101	GLN
14	CN	49	HIS
15	CO	9	GLN
15	CO	13	GLN
15	CO	37	ASN
15	CO	62	GLN
17	CQ	16	GLN
19	CS	14	HIS
19	CS	47	HIS
20	CT	16	HIS
20	CT	26	ASN

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Mol	Chain	Res	Type
20	CT	42	GLN
20	CT	45	GLN
20	CT	75	ASN
24	CY	40	HIS
24	CY	117	GLN
24	CY	137	ASN
24	CY	165	GLN
24	CY	270	GLN
24	CY	343	ASN
24	CY	421	GLN
24	CY	448	GLN
24	CY	458	HIS
24	CY	480	GLN
24	CY	500	GLN
24	CY	527	ASN
24	CY	543	GLN
24	CY	573	HIS
24	CY	625	ASN
24	CY	630	GLN
24	CY	664	GLN
25	D0	12	ASN
25	D0	70	GLN
26	D1	45	ASN
26	D1	56	GLN
27	D2	38	GLN
27	D2	47	ASN
27	D2	65	ASN
28	D3	19	GLN
28	D3	46	ASN
30	D5	43	HIS
31	D6	20	ASN
31	D6	26	ASN
31	D6	32	ASN
31	D6	49	HIS
32	D7	8	ASN
33	D8	31	HIS
33	D8	33	ASN
33	D8	43	GLN
34	D9	29	ASN
37	DC	58	ASN
37	DC	149	ASN
37	DC	166	ASN

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Mol	Chain	Res	Type
38	DD	58	HIS
38	DD	96	HIS
38	DD	115	GLN
38	DD	116	GLN
38	DD	126	GLN
38	DD	166	GLN
38	DD	186	HIS
38	DD	198	ASN
38	DD	227	ASN
38	DD	253	GLN
39	DE	48	GLN
39	DE	54	GLN
39	DE	55	ASN
39	DE	129	HIS
39	DE	143	ASN
39	DE	169	ASN
39	DE	192	ASN
40	DF	8	GLN
40	DF	69	HIS
40	DF	75	HIS
40	DF	133	ASN
40	DF	160	ASN
40	DF	169	ASN
40	DF	204	ASN
41	DG	27	ASN
41	DG	41	GLN
41	DG	58	GLN
42	DH	65	HIS
42	DH	147	ASN
42	DH	158	HIS
44	DK	29	GLN
44	DK	47	ASN
44	DK	89	HIS
46	DN	45	ASN
46	DN	56	ASN
46	DN	101	HIS
46	DN	131	GLN
47	DO	5	GLN
47	DO	82	ASN
48	DP	9	ASN
48	DP	13	ASN
48	DP	27	HIS

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Mol	Chain	Res	Type
48	DP	84	ASN
48	DP	128	HIS
49	DQ	12	GLN
49	DQ	13	GLN
49	DQ	45	GLN
50	DR	3	HIS
50	DR	16	HIS
50	DR	23	ASN
50	DR	61	HIS
50	DR	71	GLN
51	DS	16	ASN
52	DT	38	ASN
52	DT	43	GLN
52	DT	58	ASN
52	DT	84	GLN
52	DT	90	GLN
53	DU	44	ASN
53	DU	49	HIS
53	DU	66	ASN
53	DU	81	HIS
53	DU	94	ASN
53	DU	117	GLN
54	DV	11	GLN
55	DW	61	ASN
55	DW	102	HIS
56	DX	41	ASN
56	DX	55	ASN
56	DX	82	GLN
57	DY	6	HIS
58	DZ	54	HIS
58	DZ	55	HIS
58	DZ	65	GLN
58	DZ	73	GLN
58	DZ	118	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	270 (17%)	43 (2%)
1	CA	1503/1522 (98%)	266 (17%)	43 (2%)
22	AV	76/77 (98%)	15 (19%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	AW	76/77 (98%)	25 (32%)	1 (1%)
22	CV	76/77 (98%)	14 (18%)	0
22	CW	76/77 (98%)	19 (25%)	1 (1%)
23	AX	11/25 (44%)	4 (36%)	1 (9%)
23	CX	11/25 (44%)	4 (36%)	1 (9%)
35	BA	2900/2915 (99%)	597 (20%)	71 (2%)
35	DA	2900/2915 (99%)	594 (20%)	71 (2%)
36	BB	118/122 (96%)	25 (21%)	0
36	DB	118/122 (96%)	25 (21%)	0
All	All	9368/9476 (98%)	1858 (19%)	232 (2%)

All (1858) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	33	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	51	A
1	AA	60	A
1	AA	61	G
1	AA	62	U
1	AA	81	U
1	AA	88	A
1	AA	89	C
1	AA	90	U
1	AA	91	C
1	AA	97	G
1	AA	98	G
1	AA	101	A
1	AA	104	G
1	AA	116	A
1	AA	120	A
1	AA	121	C
1	AA	129	U
1	AA	129(A)	G
1	AA	131	C
1	AA	144	G
1	AA	146	G

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Mol	Chain	Res	Type
1	AA	147	G
1	AA	149	A
1	AA	160	A
1	AA	163	C
1	AA	181	G
1	AA	182	U
1	AA	189(G)	G
1	AA	189(H)	G
1	AA	195	A
1	AA	197	A
1	AA	198	G
1	AA	202	U
1	AA	203	U
1	AA	204	U
1	AA	216	G
1	AA	243	A
1	AA	244	U
1	AA	247	G
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	268	C
1	AA	281	G
1	AA	289	G
1	AA	316	G
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	332	G
1	AA	344	A
1	AA	345	C
1	AA	346	G
1	AA	350	G
1	AA	352	C
1	AA	353	A
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	397	A
1	AA	398	C
1	AA	412	A
1	AA	413	G

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Mol	Chain	Res	Type
1	AA	414	A
1	AA	422	C
1	AA	428	G
1	AA	429	U
1	AA	430	A
1	AA	435	C
1	AA	437	U
1	AA	439	A
1	AA	444	C
1	AA	452	A
1	AA	460	G
1	AA	461	A
1	AA	471	G
1	AA	481	G
1	AA	484	G
1	AA	485	G
1	AA	496	A
1	AA	498	U
1	AA	509	A
1	AA	510	A
1	AA	511	C
1	AA	527	G
1	AA	531	U
1	AA	532	A
1	AA	533	A
1	AA	534	U
1	AA	536	C
1	AA	547	A
1	AA	553	A
1	AA	559	A
1	AA	560	U
1	AA	561	U
1	AA	562	C
1	AA	572	A
1	AA	573	A
1	AA	575	G
1	AA	576	G
1	AA	577	G
1	AA	588	G
1	AA	596	C
1	AA	631	G
1	AA	632	A

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Mol	Chain	Res	Type
1	AA	650	G
1	AA	653	A
1	AA	665	A
1	AA	682	G
1	AA	683	G
1	AA	686	U
1	AA	687	A
1	AA	688	G
1	AA	704	A
1	AA	721	G
1	AA	722	A
1	AA	723	U
1	AA	724	G
1	AA	728	A
1	AA	731	G
1	AA	744	C
1	AA	748	C
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	813	U
1	AA	816	A
1	AA	817	C
1	AA	828	A
1	AA	839	U
1	AA	840	C
1	AA	841	U
1	AA	848	C
1	AA	858	G
1	AA	859	A
1	AA	867	G
1	AA	874	G
1	AA	895	G
1	AA	907	A
1	AA	914	A
1	AA	921	U
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	951	G
1	AA	960	U

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Mol	Chain	Res	Type
1	AA	961	U
1	AA	968	A
1	AA	969	A
1	AA	974	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	978	A
1	AA	980	C
1	AA	981	U
1	AA	991	U
1	AA	992	U
1	AA	993	G
1	AA	997	U
1	AA	1003	G
1	AA	1004	A
1	AA	1005	A
1	AA	1010	G
1	AA	1027	C
1	AA	1030	C
1	AA	1030(B)	C
1	AA	1050	G
1	AA	1054	C
1	AA	1064	G
1	AA	1065	U
1	AA	1066	C
1	AA	1068	G
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1102	A
1	AA	1117	G
1	AA	1124	G
1	AA	1125	U
1	AA	1129	C
1	AA	1130	A
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1146	A
1	AA	1152	A
1	AA	1154	G

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Mol	Chain	Res	Type
1	AA	1159	U
1	AA	1184	G
1	AA	1187	G
1	AA	1196	U
1	AA	1197	G
1	AA	1199	U
1	AA	1202	G
1	AA	1212	U
1	AA	1214	C
1	AA	1217	C
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1238	A
1	AA	1240	U
1	AA	1241	G
1	AA	1249	C
1	AA	1256	A
1	AA	1257	U
1	AA	1273	G
1	AA	1280	A
1	AA	1281	U
1	AA	1285	A
1	AA	1286	A
1	AA	1287	A
1	AA	1298	C
1	AA	1299	A
1	AA	1300	G
1	AA	1301	U
1	AA	1302	U
1	AA	1317	C
1	AA	1320	C
1	AA	1322	C
1	AA	1323	G
1	AA	1331	G
1	AA	1335	C
1	AA	1336	C
1	AA	1337	G
1	AA	1338	G
1	AA	1346	A
1	AA	1348	U
1	AA	1354	C

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Mol	Chain	Res	Type
1	AA	1363	C
1	AA	1364	U
1	AA	1365	G
1	AA	1370	G
1	AA	1379	G
1	AA	1394	A
1	AA	1397	C
1	AA	1398	A
1	AA	1404	C
1	AA	1419	G
1	AA	1434	A
1	AA	1442	G
1	AA	1442(A)	G
1	AA	1443	G
1	AA	1447	A
1	AA	1452	C
1	AA	1456	G
1	AA	1490	C
1	AA	1492	A
1	AA	1493	A
1	AA	1494	G
1	AA	1499	A
1	AA	1503	A
1	AA	1504	G
1	AA	1505	G
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1519	A
1	AA	1520	G
1	AA	1529	G
1	AA	1530	G
22	AV	4	G
22	AV	5	G
22	AV	8	U
22	AV	17	C
22	AV	17(A)	U
22	AV	18	G
22	AV	19	G
22	AV	20	U
22	AV	21	A
22	AV	47	U

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Mol	Chain	Res	Type
22	AV	48	C
22	AV	63	G
22	AV	71	C
22	AV	75	C
22	AV	76	A
22	AW	5	G
22	AW	7	G
22	AW	8	U
22	AW	9	G
22	AW	10	G
22	AW	15	G
22	AW	18	U
22	AW	19	G
22	AW	20	G
22	AW	21	U
22	AW	22	A
22	AW	28	U
22	AW	48	U
22	AW	49	C
22	AW	50	G
22	AW	53	G
22	AW	62	C
22	AW	64	G
22	AW	66	C
22	AW	68	C
22	AW	69	C
22	AW	72	C
22	AW	73	A
22	AW	74	A
22	AW	75	C
23	AX	12	A
23	AX	13	A
23	AX	14	A
23	AX	19	U
35	BA	9	U
35	BA	18	C
35	BA	28	A
35	BA	35	G
35	BA	42	G
35	BA	43	A
35	BA	45	C
35	BA	49	A

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Mol	Chain	Res	Type
35	BA	50	U
35	BA	61	G
35	BA	63	U
35	BA	72	U
35	BA	75	G
35	BA	83	G
35	BA	84	A
35	BA	85	G
35	BA	88	G
35	BA	90	U
35	BA	92	A
35	BA	94	C
35	BA	95	G
35	BA	100	G
35	BA	102	G
35	BA	106	C
35	BA	116	C
35	BA	118	A
35	BA	119	A
35	BA	121	G
35	BA	125	G
35	BA	129	C
35	BA	139(A)	G
35	BA	141	A
35	BA	142(A)	C
35	BA	155	U
35	BA	156	U
35	BA	157	U
35	BA	171	G
35	BA	174	C
35	BA	190	A
35	BA	196	A
35	BA	199	A
35	BA	204	A
35	BA	205	G
35	BA	212	G
35	BA	215	G
35	BA	216	A
35	BA	221	A
35	BA	222	A
35	BA	227	A
35	BA	241	A

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Mol	Chain	Res	Type
35	BA	248	G
35	BA	252	G
35	BA	261	G
35	BA	271(J)	C
35	BA	271(K)	U
35	BA	271(L)	U
35	BA	271(O)	C
35	BA	271(Y)	U
35	BA	272	G
35	BA	272(A)	U
35	BA	272(B)	G
35	BA	272(H)	C
35	BA	272(I)	U
35	BA	276	A
35	BA	280	C
35	BA	283	A
35	BA	286	C
35	BA	299	A
35	BA	310	A
35	BA	311	A
35	BA	329	G
35	BA	330	A
35	BA	332	A
35	BA	333	G
35	BA	336	C
35	BA	345	A
35	BA	346	A
35	BA	352	G
35	BA	353	G
35	BA	362	U
35	BA	363	G
35	BA	363(F)	A
35	BA	364	C
35	BA	365	C
35	BA	371	A
35	BA	372	G
35	BA	386	G
35	BA	396	G
35	BA	405	U
35	BA	406	G
35	BA	407	G
35	BA	411	G

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Mol	Chain	Res	Type
35	BA	412	A
35	BA	428	A
35	BA	444	C
35	BA	448	U
35	BA	449	A
35	BA	455	C
35	BA	458	G
35	BA	475	U
35	BA	480	A
35	BA	481	G
35	BA	504	U
35	BA	505	A
35	BA	508	G
35	BA	509	C
35	BA	526	A
35	BA	527	C
35	BA	528	A
35	BA	529	A
35	BA	530	G
35	BA	531	C
35	BA	532	A
35	BA	544	G
35	BA	548	A
35	BA	552	G
35	BA	555	U
35	BA	556	G
35	BA	562	U
35	BA	563	G
35	BA	573	G
35	BA	575	A
35	BA	587	C
35	BA	591	C
35	BA	592	G
35	BA	604	G
35	BA	607	U
35	BA	613	G
35	BA	614(B)	G
35	BA	615	G
35	BA	620	G
35	BA	622	G
35	BA	627	A
35	BA	637	A

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Mol	Chain	Res	Type
35	BA	645	C
35	BA	646	A
35	BA	651	G
35	BA	653	A
35	BA	654	A
35	BA	654(I)	C
35	BA	654(J)	A
35	BA	654(K)	C
35	BA	654(M)	C
35	BA	654(T)	C
35	BA	655	A
35	BA	675	A
35	BA	682	G
35	BA	686	G
35	BA	695	G
35	BA	699	A
35	BA	722	A
35	BA	727	A
35	BA	729	G
35	BA	730	C
35	BA	740	U
35	BA	745	G
35	BA	753	C
35	BA	764	A
35	BA	765	G
35	BA	775	G
35	BA	776	G
35	BA	782	A
35	BA	784	A
35	BA	785	G
35	BA	788	A
35	BA	789	A
35	BA	790	C
35	BA	791	C
35	BA	792	G
35	BA	793	A
35	BA	794	G
35	BA	800	A
35	BA	805	G
35	BA	811	U
35	BA	812	C
35	BA	827	U

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Mol	Chain	Res	Type
35	BA	828	U
35	BA	830	G
35	BA	840	C
35	BA	841	A
35	BA	859	G
35	BA	878	A
35	BA	889	C
35	BA	896	A
35	BA	897	C
35	BA	900	A
35	BA	904	C
35	BA	910	A
35	BA	926	A
35	BA	932	G
35	BA	940	G
35	BA	941	A
35	BA	945	A
35	BA	946	G
35	BA	959	A
35	BA	961	C
35	BA	962	G
35	BA	969	U
35	BA	974	G
35	BA	975	C
35	BA	980	A
35	BA	983	A
35	BA	985	C
35	BA	990	A
35	BA	991	C
35	BA	996	A
35	BA	1005	C
35	BA	1011	G
35	BA	1012	U
35	BA	1013	C
35	BA	1021	A
35	BA	1022	G
35	BA	1023	U
35	BA	1026	U
35	BA	1033	U
35	BA	1034	G
35	BA	1039	G
35	BA	1044	G

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Mol	Chain	Res	Type
35	BA	1045	A
35	BA	1047	G
35	BA	1048	A
35	BA	1049	C
35	BA	1052	C
35	BA	1053	C
35	BA	1054	A
35	BA	1058	G
35	BA	1062	G
35	BA	1067	A
35	BA	1070	A
35	BA	1073	A
35	BA	1076	C
35	BA	1088	A
35	BA	1090	U
35	BA	1109	C
35	BA	1111	A
35	BA	1112	G
35	BA	1114	G
35	BA	1115	G
35	BA	1122	G
35	BA	1126	A
35	BA	1135	C
35	BA	1136	G
35	BA	1141	U
35	BA	1142	U
35	BA	1142(A)	A
35	BA	1143	A
35	BA	1146	C
35	BA	1155	A
35	BA	1157	G
35	BA	1158	C
35	BA	1159	U
35	BA	1170	G
35	BA	1173	G
35	BA	1174	A
35	BA	1175	U
35	BA	1176	G
35	BA	1177	A
35	BA	1204	A
35	BA	1210	A
35	BA	1211	U

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Mol	Chain	Res	Type
35	BA	1212	G
35	BA	1213	A
35	BA	1220	A
35	BA	1221	C
35	BA	1224	C
35	BA	1238	G
35	BA	1247	A
35	BA	1248	G
35	BA	1250	G
35	BA	1251	C
35	BA	1252	G
35	BA	1255	U
35	BA	1256	G
35	BA	1266	G
35	BA	1271	G
35	BA	1272	A
35	BA	1273	U
35	BA	1287	A
35	BA	1300	U
35	BA	1302	A
35	BA	1314	C
35	BA	1326	U
35	BA	1329	U
35	BA	1330	C
35	BA	1332	G
35	BA	1342	A
35	BA	1345	C
35	BA	1349	A
35	BA	1359	A
35	BA	1365	A
35	BA	1379	A
35	BA	1380	G
35	BA	1384	A
35	BA	1385	G
35	BA	1386	C
35	BA	1396	U
35	BA	1403	C
35	BA	1406	U
35	BA	1411	C
35	BA	1416	G
35	BA	1420	U
35	BA	1421	G

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Mol	Chain	Res	Type
35	BA	1427	A
35	BA	1428	C
35	BA	1434	A
35	BA	1435	G
35	BA	1445	A
35	BA	1445(A)	C
35	BA	1453	U
35	BA	1455	G
35	BA	1459	G
35	BA	1460	A
35	BA	1461	G
35	BA	1467	C
35	BA	1476	C
35	BA	1477	A
35	BA	1478	G
35	BA	1482	G
35	BA	1484	G
35	BA	1485	G
35	BA	1488	G
35	BA	1490	A
35	BA	1491	G
35	BA	1493	C
35	BA	1494	A
35	BA	1495	A
35	BA	1496	A
35	BA	1497	U
35	BA	1505	C
35	BA	1509	C
35	BA	1509(A)	A
35	BA	1517	G
35	BA	1528(A)	A
35	BA	1541	G
35	BA	1542	A
35	BA	1544	A
35	BA	1553	A
35	BA	1554	A
35	BA	1559	G
35	BA	1569	A
35	BA	1578	U
35	BA	1579	A
35	BA	1584	C
35	BA	1586	A

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Mol	Chain	Res	Type
35	BA	1588	C
35	BA	1603	A
35	BA	1608	A
35	BA	1609	A
35	BA	1610	A
35	BA	1615	C
35	BA	1616	A
35	BA	1618	A
35	BA	1634	A
35	BA	1640	C
35	BA	1644	C
35	BA	1648	C
35	BA	1668	A
35	BA	1674	G
35	BA	1678	G
35	BA	1698	A
35	BA	1699	G
35	BA	1718	G
35	BA	1722	A
35	BA	1739	U
35	BA	1740	G
35	BA	1744	C
35	BA	1748	G
35	BA	1763	G
35	BA	1764	G
35	BA	1773	A
35	BA	1780	A
35	BA	1781	C
35	BA	1784	A
35	BA	1787	A
35	BA	1791	A
35	BA	1799	G
35	BA	1800	C
35	BA	1801	G
35	BA	1815	A
35	BA	1816	G
35	BA	1820	U
35	BA	1821	A
35	BA	1829	A
35	BA	1839	G
35	BA	1846	G
35	BA	1847	A

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Mol	Chain	Res	Type
35	BA	1850	G
35	BA	1858	G
35	BA	1862	G
35	BA	1866	C
35	BA	1878	G
35	BA	1885	A
35	BA	1888	G
35	BA	1889	A
35	BA	1900	A
35	BA	1906	G
35	BA	1912	A
35	BA	1929	G
35	BA	1930	G
35	BA	1931	U
35	BA	1937	A
35	BA	1938	A
35	BA	1943	U
35	BA	1944	U
35	BA	1945	G
35	BA	1948	G
35	BA	1955	U
35	BA	1960	A
35	BA	1963	U
35	BA	1964	G
35	BA	1967	C
35	BA	1969	A
35	BA	1970	A
35	BA	1971	A
35	BA	1972	A
35	BA	1987	G
35	BA	1993	U
35	BA	1997	G
35	BA	2004	G
35	BA	2021	C
35	BA	2022	U
35	BA	2023	G
35	BA	2031	A
35	BA	2033	A
35	BA	2034	U
35	BA	2043	C
35	BA	2055	C
35	BA	2056	G

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Mol	Chain	Res	Type
35	BA	2060	A
35	BA	2061	G
35	BA	2062	A
35	BA	2065	C
35	BA	2069	G
35	BA	2076	U
35	BA	2100	G
35	BA	2103	C
35	BA	2104	G
35	BA	2112	G
35	BA	2116	G
35	BA	2118	U
35	BA	2127	G
35	BA	2131	G
35	BA	2132	U
35	BA	2133	G
35	BA	2134	A
35	BA	2157	G
35	BA	2158	A
35	BA	2159	G
35	BA	2163	C
35	BA	2172	U
35	BA	2173	A
35	BA	2185	C
35	BA	2187	G
35	BA	2189	U
35	BA	2190	G
35	BA	2192	G
35	BA	2193	G
35	BA	2198	A
35	BA	2199	A
35	BA	2200	C
35	BA	2202	C
35	BA	2203	U
35	BA	2205	C
35	BA	2206	G
35	BA	2207	G
35	BA	2208	A
35	BA	2219	G
35	BA	2225	A
35	BA	2226	C
35	BA	2238	G

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Mol	Chain	Res	Type
35	BA	2239	G
35	BA	2263	C
35	BA	2273	A
35	BA	2283	C
35	BA	2286	A
35	BA	2288	A
35	BA	2297	C
35	BA	2302	G
35	BA	2305	A
35	BA	2306	C
35	BA	2307	G
35	BA	2308	G
35	BA	2309	A
35	BA	2313	C
35	BA	2319	G
35	BA	2320	A
35	BA	2325	G
35	BA	2334	G
35	BA	2336	A
35	BA	2345	G
35	BA	2346	A
35	BA	2347	C
35	BA	2348	U
35	BA	2349	G
35	BA	2350	C
35	BA	2383	G
35	BA	2385	C
35	BA	2402	C
35	BA	2406	U
35	BA	2423	U
35	BA	2424	C
35	BA	2425	A
35	BA	2427	C
35	BA	2428	G
35	BA	2429	G
35	BA	2430	A
35	BA	2431	U
35	BA	2434	A
35	BA	2435	A
35	BA	2439	A
35	BA	2441	C
35	BA	2448	A

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Mol	Chain	Res	Type
35	BA	2461	C
35	BA	2465	C
35	BA	2469	A
35	BA	2470	G
35	BA	2473	U
35	BA	2474	C
35	BA	2475	C
35	BA	2476	A
35	BA	2477	C
35	BA	2478	A
35	BA	2482	G
35	BA	2484	G
35	BA	2502	G
35	BA	2503	A
35	BA	2505	G
35	BA	2519	U
35	BA	2520	C
35	BA	2524	G
35	BA	2529	G
35	BA	2543	G
35	BA	2554	U
35	BA	2566	A
35	BA	2567	G
35	BA	2572	A
35	BA	2577	A
35	BA	2585	U
35	BA	2586	C
35	BA	2602	A
35	BA	2609	U
35	BA	2610	C
35	BA	2611	U
35	BA	2612	C
35	BA	2615	U
35	BA	2630	G
35	BA	2646	C
35	BA	2655	G
35	BA	2657	A
35	BA	2658	C
35	BA	2670	A
35	BA	2673	G
35	BA	2682	U
35	BA	2690	C

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Mol	Chain	Res	Type
35	BA	2691	C
35	BA	2702	U
35	BA	2703	C
35	BA	2706	G
35	BA	2712	U
35	BA	2712(A)	A
35	BA	2713	A
35	BA	2726	U
35	BA	2733	A
35	BA	2750	A
35	BA	2751	G
35	BA	2755	C
35	BA	2756	U
35	BA	2757	A
35	BA	2758	A
35	BA	2762	G
35	BA	2764	A
35	BA	2765	A
35	BA	2766	G
35	BA	2778	A
35	BA	2779	U
35	BA	2780	G
35	BA	2790	A
35	BA	2791	C
35	BA	2796	U
35	BA	2799	C
35	BA	2801	A
35	BA	2802	G
35	BA	2803	C
35	BA	2808	U
35	BA	2820	A
35	BA	2821	A
35	BA	2824	C
35	BA	2833	G
35	BA	2834	G
35	BA	2836	U
35	BA	2849	U
35	BA	2872	G
35	BA	2879	C
35	BA	2880	C
35	BA	2892	A
35	BA	2894	G

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Mol	Chain	Res	Type
35	BA	2895	U
36	BB	8	U
36	BB	13	A
36	BB	15	A
36	BB	16	G
36	BB	22	U
36	BB	25	A
36	BB	33	G
36	BB	35	U
36	BB	41	U
36	BB	42	C
36	BB	45	A
36	BB	52	A
36	BB	53	A
36	BB	56	G
36	BB	67	G
36	BB	73	A
36	BB	81	G
36	BB	82	G
36	BB	88	C
36	BB	89	G
36	BB	90	A
36	BB	103	G
36	BB	104	U
36	BB	110	G
36	BB	113	G
1	CA	9	G
1	CA	31	G
1	CA	32	A
1	CA	33	A
1	CA	39	G
1	CA	47	C
1	CA	48	C
1	CA	51	A
1	CA	60	A
1	CA	61	G
1	CA	62	U
1	CA	81	U
1	CA	88	A
1	CA	89	C
1	CA	90	U
1	CA	91	C

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Mol	Chain	Res	Type
1	CA	97	G
1	CA	98	G
1	CA	101	A
1	CA	104	G
1	CA	116	A
1	CA	120	A
1	CA	121	C
1	CA	129	U
1	CA	129(A)	G
1	CA	131	C
1	CA	144	G
1	CA	146	G
1	CA	147	G
1	CA	149	A
1	CA	160	A
1	CA	163	C
1	CA	181	G
1	CA	182	U
1	CA	189(G)	G
1	CA	189(H)	G
1	CA	195	A
1	CA	197	A
1	CA	198	G
1	CA	202	U
1	CA	203	U
1	CA	204	U
1	CA	216	G
1	CA	243	A
1	CA	244	U
1	CA	247	G
1	CA	251	G
1	CA	266	G
1	CA	267	C
1	CA	268	C
1	CA	281	G
1	CA	289	G
1	CA	316	G
1	CA	321	A
1	CA	328	C
1	CA	329	A
1	CA	332	G
1	CA	344	A

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Mol	Chain	Res	Type
1	CA	345	C
1	CA	346	G
1	CA	350	G
1	CA	352	C
1	CA	353	A
1	CA	354	G
1	CA	367	U
1	CA	372	C
1	CA	397	A
1	CA	398	C
1	CA	412	A
1	CA	413	G
1	CA	414	A
1	CA	422	C
1	CA	428	G
1	CA	429	U
1	CA	430	A
1	CA	435	C
1	CA	437	U
1	CA	439	A
1	CA	444	C
1	CA	452	A
1	CA	460	G
1	CA	461	A
1	CA	471	G
1	CA	481	G
1	CA	484	G
1	CA	485	G
1	CA	496	A
1	CA	498	U
1	CA	509	A
1	CA	510	A
1	CA	511	C
1	CA	527	G
1	CA	531	U
1	CA	532	A
1	CA	533	A
1	CA	534	U
1	CA	536	C
1	CA	547	A
1	CA	559	A
1	CA	560	U

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Mol	Chain	Res	Type
1	CA	561	U
1	CA	562	C
1	CA	572	A
1	CA	573	A
1	CA	575	G
1	CA	576	G
1	CA	577	G
1	CA	588	G
1	CA	596	C
1	CA	631	G
1	CA	632	A
1	CA	650	G
1	CA	653	A
1	CA	665	A
1	CA	682	G
1	CA	683	G
1	CA	686	U
1	CA	687	A
1	CA	688	G
1	CA	704	A
1	CA	721	G
1	CA	722	A
1	CA	723	U
1	CA	724	G
1	CA	728	A
1	CA	731	G
1	CA	744	C
1	CA	748	C
1	CA	755	G
1	CA	777	A
1	CA	793	U
1	CA	794	A
1	CA	813	U
1	CA	816	A
1	CA	817	C
1	CA	828	A
1	CA	839	U
1	CA	840	C
1	CA	841	U
1	CA	848	C
1	CA	858	G
1	CA	859	A

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Mol	Chain	Res	Type
1	CA	867	G
1	CA	874	G
1	CA	895	G
1	CA	907	A
1	CA	914	A
1	CA	921	U
1	CA	927	G
1	CA	934	C
1	CA	935	A
1	CA	951	G
1	CA	960	U
1	CA	961	U
1	CA	968	A
1	CA	969	A
1	CA	974	A
1	CA	975	A
1	CA	976	G
1	CA	977	A
1	CA	978	A
1	CA	980	C
1	CA	981	U
1	CA	991	U
1	CA	992	U
1	CA	993	G
1	CA	997	U
1	CA	1003	G
1	CA	1004	A
1	CA	1005	A
1	CA	1010	G
1	CA	1027	C
1	CA	1030	C
1	CA	1030(B)	C
1	CA	1050	G
1	CA	1054	C
1	CA	1064	G
1	CA	1065	U
1	CA	1066	C
1	CA	1068	G
1	CA	1094	G
1	CA	1095	U
1	CA	1101	A
1	CA	1102	A

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Mol	Chain	Res	Type
1	CA	1117	G
1	CA	1124	G
1	CA	1125	U
1	CA	1129	C
1	CA	1130	A
1	CA	1137	C
1	CA	1138	G
1	CA	1139	G
1	CA	1146	A
1	CA	1152	A
1	CA	1154	G
1	CA	1159	U
1	CA	1184	G
1	CA	1187	G
1	CA	1196	U
1	CA	1197	G
1	CA	1199	U
1	CA	1202	G
1	CA	1212	U
1	CA	1214	C
1	CA	1217	C
1	CA	1225	A
1	CA	1226	C
1	CA	1227	A
1	CA	1238	A
1	CA	1240	U
1	CA	1241	G
1	CA	1249	C
1	CA	1256	A
1	CA	1257	U
1	CA	1273	G
1	CA	1280	A
1	CA	1281	U
1	CA	1285	A
1	CA	1286	A
1	CA	1287	A
1	CA	1298	C
1	CA	1299	A
1	CA	1300	G
1	CA	1301	U
1	CA	1302	U
1	CA	1317	C

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Mol	Chain	Res	Type
1	CA	1322	C
1	CA	1323	G
1	CA	1331	G
1	CA	1335	C
1	CA	1336	C
1	CA	1337	G
1	CA	1338	G
1	CA	1346	A
1	CA	1348	U
1	CA	1354	C
1	CA	1363	C
1	CA	1364	U
1	CA	1365	G
1	CA	1370	G
1	CA	1379	G
1	CA	1394	A
1	CA	1397	C
1	CA	1398	A
1	CA	1404	C
1	CA	1419	G
1	CA	1442	G
1	CA	1442(A)	G
1	CA	1447	A
1	CA	1452	C
1	CA	1456	G
1	CA	1490	C
1	CA	1492	A
1	CA	1493	A
1	CA	1494	G
1	CA	1498	U
1	CA	1499	A
1	CA	1503	A
1	CA	1504	G
1	CA	1505	G
1	CA	1506	U
1	CA	1517	G
1	CA	1519	A
1	CA	1520	G
1	CA	1529	G
1	CA	1530	G
22	CV	3	C
22	CV	4	G

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Mol	Chain	Res	Type
22	CV	5	G
22	CV	17	C
22	CV	17(A)	U
22	CV	18	G
22	CV	19	G
22	CV	20	U
22	CV	21	A
22	CV	47	U
22	CV	48	C
22	CV	63	G
22	CV	75	C
22	CV	76	A
22	CW	4	G
22	CW	5	G
22	CW	7	G
22	CW	9	G
22	CW	10	G
22	CW	15	G
22	CW	18	U
22	CW	19	G
22	CW	20	G
22	CW	21	U
22	CW	22	A
22	CW	48	U
22	CW	49	C
22	CW	53	G
22	CW	66	C
22	CW	72	C
22	CW	73	A
22	CW	74	A
22	CW	75	C
23	CX	12	A
23	CX	13	A
23	CX	14	A
23	CX	19	U
35	DA	9	U
35	DA	18	C
35	DA	28	A
35	DA	35	G
35	DA	42	G
35	DA	43	A
35	DA	45	C

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Mol	Chain	Res	Type
35	DA	49	A
35	DA	50	U
35	DA	61	G
35	DA	63	U
35	DA	72	U
35	DA	75	G
35	DA	83	G
35	DA	84	A
35	DA	85	G
35	DA	88	G
35	DA	90	U
35	DA	92	A
35	DA	94	C
35	DA	95	G
35	DA	100	G
35	DA	102	G
35	DA	106	C
35	DA	116	C
35	DA	118	A
35	DA	119	A
35	DA	121	G
35	DA	125	G
35	DA	129	C
35	DA	139(A)	G
35	DA	141	A
35	DA	142(A)	C
35	DA	155	U
35	DA	156	U
35	DA	157	U
35	DA	171	G
35	DA	174	C
35	DA	190	A
35	DA	196	A
35	DA	199	A
35	DA	204	A
35	DA	205	G
35	DA	212	G
35	DA	215	G
35	DA	216	A
35	DA	221	A
35	DA	222	A
35	DA	227	A

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Mol	Chain	Res	Type
35	DA	241	A
35	DA	248	G
35	DA	252	G
35	DA	261	G
35	DA	271(J)	C
35	DA	271(K)	U
35	DA	271(L)	U
35	DA	271(O)	C
35	DA	271(Y)	U
35	DA	272	G
35	DA	272(A)	U
35	DA	272(B)	G
35	DA	272(H)	C
35	DA	272(I)	U
35	DA	276	A
35	DA	280	C
35	DA	283	A
35	DA	286	C
35	DA	299	A
35	DA	310	A
35	DA	311	A
35	DA	329	G
35	DA	330	A
35	DA	332	A
35	DA	333	G
35	DA	336	C
35	DA	345	A
35	DA	346	A
35	DA	352	G
35	DA	353	G
35	DA	362	U
35	DA	363	G
35	DA	363(F)	A
35	DA	364	C
35	DA	365	C
35	DA	371	A
35	DA	372	G
35	DA	386	G
35	DA	396	G
35	DA	405	U
35	DA	406	G
35	DA	407	G

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Mol	Chain	Res	Type
35	DA	411	G
35	DA	412	A
35	DA	428	A
35	DA	444	C
35	DA	448	U
35	DA	449	A
35	DA	455	C
35	DA	458	G
35	DA	475	U
35	DA	480	A
35	DA	481	G
35	DA	504	U
35	DA	505	A
35	DA	508	G
35	DA	509	C
35	DA	526	A
35	DA	527	C
35	DA	528	A
35	DA	529	A
35	DA	530	G
35	DA	531	C
35	DA	532	A
35	DA	544	G
35	DA	548	A
35	DA	552	G
35	DA	555	U
35	DA	556	G
35	DA	562	U
35	DA	563	G
35	DA	573	G
35	DA	575	A
35	DA	587	C
35	DA	591	C
35	DA	592	G
35	DA	604	G
35	DA	607	U
35	DA	613	G
35	DA	614(B)	G
35	DA	615	G
35	DA	620	G
35	DA	622	G
35	DA	627	A

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Mol	Chain	Res	Type
35	DA	637	A
35	DA	645	C
35	DA	646	A
35	DA	651	G
35	DA	653	A
35	DA	654	A
35	DA	654(I)	C
35	DA	654(J)	A
35	DA	654(K)	C
35	DA	654(M)	C
35	DA	654(T)	C
35	DA	655	A
35	DA	675	A
35	DA	682	G
35	DA	686	G
35	DA	695	G
35	DA	699	A
35	DA	722	A
35	DA	727	A
35	DA	729	G
35	DA	730	C
35	DA	740	U
35	DA	745	G
35	DA	753	C
35	DA	764	A
35	DA	765	G
35	DA	775	G
35	DA	776	G
35	DA	782	A
35	DA	784	A
35	DA	785	G
35	DA	788	A
35	DA	789	A
35	DA	790	C
35	DA	791	C
35	DA	792	G
35	DA	793	A
35	DA	794	G
35	DA	800	A
35	DA	805	G
35	DA	811	U
35	DA	812	C

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Mol	Chain	Res	Type
35	DA	827	U
35	DA	828	U
35	DA	830	G
35	DA	840	C
35	DA	841	A
35	DA	859	G
35	DA	878	A
35	DA	889	C
35	DA	896	A
35	DA	897	C
35	DA	900	A
35	DA	904	C
35	DA	910	A
35	DA	926	A
35	DA	932	G
35	DA	940	G
35	DA	941	A
35	DA	945	A
35	DA	946	G
35	DA	959	A
35	DA	961	C
35	DA	962	G
35	DA	969	U
35	DA	974	G
35	DA	975	C
35	DA	980	A
35	DA	983	A
35	DA	985	C
35	DA	990	A
35	DA	991	C
35	DA	996	A
35	DA	1005	C
35	DA	1011	G
35	DA	1012	U
35	DA	1013	C
35	DA	1021	A
35	DA	1022	G
35	DA	1023	U
35	DA	1026	U
35	DA	1033	U
35	DA	1034	G
35	DA	1039	G

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Mol	Chain	Res	Type
35	DA	1044	G
35	DA	1045	A
35	DA	1047	G
35	DA	1048	A
35	DA	1049	C
35	DA	1052	C
35	DA	1053	C
35	DA	1054	A
35	DA	1058	G
35	DA	1062	G
35	DA	1067	A
35	DA	1070	A
35	DA	1073	A
35	DA	1076	C
35	DA	1088	A
35	DA	1090	U
35	DA	1109	C
35	DA	1111	A
35	DA	1112	G
35	DA	1114	G
35	DA	1115	G
35	DA	1122	G
35	DA	1126	A
35	DA	1135	C
35	DA	1136	G
35	DA	1141	U
35	DA	1142	U
35	DA	1142(A)	A
35	DA	1143	A
35	DA	1146	C
35	DA	1155	A
35	DA	1157	G
35	DA	1158	C
35	DA	1159	U
35	DA	1170	G
35	DA	1173	G
35	DA	1174	A
35	DA	1175	U
35	DA	1176	G
35	DA	1177	A
35	DA	1204	A
35	DA	1210	A

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Mol	Chain	Res	Type
35	DA	1211	U
35	DA	1212	G
35	DA	1213	A
35	DA	1220	A
35	DA	1221	C
35	DA	1224	C
35	DA	1238	G
35	DA	1247	A
35	DA	1248	G
35	DA	1250	G
35	DA	1251	C
35	DA	1252	G
35	DA	1255	U
35	DA	1256	G
35	DA	1266	G
35	DA	1271	G
35	DA	1272	A
35	DA	1273	U
35	DA	1287	A
35	DA	1300	U
35	DA	1302	A
35	DA	1314	C
35	DA	1326	U
35	DA	1329	U
35	DA	1330	C
35	DA	1332	G
35	DA	1342	A
35	DA	1345	C
35	DA	1349	A
35	DA	1359	A
35	DA	1365	A
35	DA	1379	A
35	DA	1380	G
35	DA	1384	A
35	DA	1385	G
35	DA	1386	C
35	DA	1396	U
35	DA	1403	C
35	DA	1406	U
35	DA	1411	C
35	DA	1416	G
35	DA	1420	U

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Mol	Chain	Res	Type
35	DA	1421	G
35	DA	1427	A
35	DA	1428	C
35	DA	1434	A
35	DA	1435	G
35	DA	1445	A
35	DA	1445(A)	C
35	DA	1453	U
35	DA	1455	G
35	DA	1459	G
35	DA	1460	A
35	DA	1461	G
35	DA	1467	C
35	DA	1476	C
35	DA	1477	A
35	DA	1478	G
35	DA	1482	G
35	DA	1484	G
35	DA	1485	G
35	DA	1488	G
35	DA	1490	A
35	DA	1491	G
35	DA	1493	C
35	DA	1494	A
35	DA	1495	A
35	DA	1496	A
35	DA	1497	U
35	DA	1505	C
35	DA	1509	C
35	DA	1509(A)	A
35	DA	1517	G
35	DA	1528(A)	A
35	DA	1541	G
35	DA	1542	A
35	DA	1544	A
35	DA	1553	A
35	DA	1554	A
35	DA	1559	G
35	DA	1569	A
35	DA	1578	U
35	DA	1579	A
35	DA	1584	C

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Mol	Chain	Res	Type
35	DA	1586	A
35	DA	1588	C
35	DA	1603	A
35	DA	1608	A
35	DA	1609	A
35	DA	1610	A
35	DA	1615	C
35	DA	1616	A
35	DA	1618	A
35	DA	1634	A
35	DA	1640	C
35	DA	1644	C
35	DA	1648	C
35	DA	1668	A
35	DA	1674	G
35	DA	1678	G
35	DA	1698	A
35	DA	1699	G
35	DA	1718	G
35	DA	1722	A
35	DA	1739	U
35	DA	1740	G
35	DA	1744	C
35	DA	1748	G
35	DA	1763	G
35	DA	1764	G
35	DA	1773	A
35	DA	1780	A
35	DA	1781	C
35	DA	1784	A
35	DA	1787	A
35	DA	1791	A
35	DA	1799	G
35	DA	1800	C
35	DA	1801	G
35	DA	1815	A
35	DA	1816	G
35	DA	1820	U
35	DA	1821	A
35	DA	1829	A
35	DA	1839	G
35	DA	1846	G

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Mol	Chain	Res	Type
35	DA	1847	A
35	DA	1850	G
35	DA	1858	G
35	DA	1862	G
35	DA	1866	C
35	DA	1878	G
35	DA	1885	A
35	DA	1888	G
35	DA	1889	A
35	DA	1900	A
35	DA	1906	G
35	DA	1912	A
35	DA	1929	G
35	DA	1930	G
35	DA	1931	U
35	DA	1937	A
35	DA	1938	A
35	DA	1943	U
35	DA	1944	U
35	DA	1945	G
35	DA	1948	G
35	DA	1955	U
35	DA	1960	A
35	DA	1963	U
35	DA	1964	G
35	DA	1967	C
35	DA	1969	A
35	DA	1970	A
35	DA	1971	A
35	DA	1972	A
35	DA	1993	U
35	DA	1997	G
35	DA	2004	G
35	DA	2021	C
35	DA	2022	U
35	DA	2023	G
35	DA	2031	A
35	DA	2033	A
35	DA	2034	U
35	DA	2043	C
35	DA	2055	C
35	DA	2056	G

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Mol	Chain	Res	Type
35	DA	2060	A
35	DA	2061	G
35	DA	2062	A
35	DA	2065	C
35	DA	2069	G
35	DA	2076	U
35	DA	2100	G
35	DA	2103	C
35	DA	2104	G
35	DA	2112	G
35	DA	2116	G
35	DA	2118	U
35	DA	2127	G
35	DA	2132	U
35	DA	2133	G
35	DA	2134	A
35	DA	2157	G
35	DA	2158	A
35	DA	2159	G
35	DA	2163	C
35	DA	2172	U
35	DA	2173	A
35	DA	2185	C
35	DA	2187	G
35	DA	2189	U
35	DA	2190	G
35	DA	2192	G
35	DA	2193	G
35	DA	2198	A
35	DA	2199	A
35	DA	2200	C
35	DA	2202	C
35	DA	2203	U
35	DA	2205	C
35	DA	2206	G
35	DA	2207	G
35	DA	2208	A
35	DA	2219	G
35	DA	2225	A
35	DA	2226	C
35	DA	2238	G
35	DA	2239	G

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Mol	Chain	Res	Type
35	DA	2263	C
35	DA	2273	A
35	DA	2283	C
35	DA	2286	A
35	DA	2288	A
35	DA	2297	C
35	DA	2302	G
35	DA	2305	A
35	DA	2306	C
35	DA	2307	G
35	DA	2308	G
35	DA	2309	A
35	DA	2313	C
35	DA	2319	G
35	DA	2320	A
35	DA	2325	G
35	DA	2334	G
35	DA	2336	A
35	DA	2345	G
35	DA	2346	A
35	DA	2347	C
35	DA	2348	U
35	DA	2349	G
35	DA	2350	C
35	DA	2383	G
35	DA	2385	C
35	DA	2402	C
35	DA	2423	U
35	DA	2424	C
35	DA	2425	A
35	DA	2427	C
35	DA	2428	G
35	DA	2429	G
35	DA	2430	A
35	DA	2431	U
35	DA	2434	A
35	DA	2435	A
35	DA	2439	A
35	DA	2441	C
35	DA	2448	A
35	DA	2461	C
35	DA	2465	C

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Mol	Chain	Res	Type
35	DA	2469	A
35	DA	2470	G
35	DA	2473	U
35	DA	2474	C
35	DA	2475	C
35	DA	2476	A
35	DA	2477	C
35	DA	2478	A
35	DA	2482	G
35	DA	2484	G
35	DA	2502	G
35	DA	2503	A
35	DA	2505	G
35	DA	2519	U
35	DA	2520	C
35	DA	2524	G
35	DA	2529	G
35	DA	2543	G
35	DA	2554	U
35	DA	2566	A
35	DA	2567	G
35	DA	2572	A
35	DA	2573	C
35	DA	2577	A
35	DA	2585	U
35	DA	2586	C
35	DA	2602	A
35	DA	2609	U
35	DA	2610	C
35	DA	2611	U
35	DA	2612	C
35	DA	2615	U
35	DA	2630	G
35	DA	2646	C
35	DA	2655	G
35	DA	2657	A
35	DA	2658	C
35	DA	2670	A
35	DA	2673	G
35	DA	2682	U
35	DA	2690	C
35	DA	2691	C

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Mol	Chain	Res	Type
35	DA	2702	U
35	DA	2703	C
35	DA	2712	U
35	DA	2712(A)	A
35	DA	2713	A
35	DA	2726	U
35	DA	2733	A
35	DA	2750	A
35	DA	2751	G
35	DA	2755	C
35	DA	2756	U
35	DA	2757	A
35	DA	2758	A
35	DA	2762	G
35	DA	2764	A
35	DA	2765	A
35	DA	2766	G
35	DA	2778	A
35	DA	2779	U
35	DA	2780	G
35	DA	2790	A
35	DA	2791	C
35	DA	2796	U
35	DA	2799	C
35	DA	2801	A
35	DA	2802	G
35	DA	2803	C
35	DA	2808	U
35	DA	2820	A
35	DA	2821	A
35	DA	2824	C
35	DA	2833	G
35	DA	2834	G
35	DA	2836	U
35	DA	2849	U
35	DA	2872	G
35	DA	2879	C
35	DA	2880	C
35	DA	2892	A
35	DA	2894	G
35	DA	2895	U
36	DB	8	U

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Mol	Chain	Res	Type
36	DB	13	A
36	DB	15	A
36	DB	16	G
36	DB	22	U
36	DB	25	A
36	DB	33	G
36	DB	35	U
36	DB	41	U
36	DB	42	C
36	DB	45	A
36	DB	52	A
36	DB	53	A
36	DB	56	G
36	DB	67	G
36	DB	73	A
36	DB	81	G
36	DB	82	G
36	DB	88	C
36	DB	89	G
36	DB	90	A
36	DB	103	G
36	DB	104	U
36	DB	110	G
36	DB	113	G

All (232) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	30	U
1	AA	60	A
1	AA	115	G
1	AA	119	A
1	AA	203	U
1	AA	243	A
1	AA	250	A
1	AA	266	G
1	AA	315	A
1	AA	328	C
1	AA	344	A
1	AA	353	A
1	AA	366	C
1	AA	428	G

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Mol	Chain	Res	Type
1	AA	429	U
1	AA	438	G
1	AA	532	A
1	AA	533	A
1	AA	535	A
1	AA	560	U
1	AA	575	G
1	AA	576	G
1	AA	631	G
1	AA	703	G
1	AA	812	C
1	AA	913	A
1	AA	992	U
1	AA	1049	U
1	AA	1065	U
1	AA	1101	A
1	AA	1129	C
1	AA	1201	A
1	AA	1225	A
1	AA	1226	C
1	AA	1285	A
1	AA	1299	A
1	AA	1300	G
1	AA	1337	G
1	AA	1347	G
1	AA	1364	U
1	AA	1493	A
1	AA	1498	U
1	AA	1505	G
22	AW	73	A
23	AX	11	U
35	BA	27	G
35	BA	49	A
35	BA	74	A
35	BA	120	U
35	BA	128	C
35	BA	221	A
35	BA	226	G
35	BA	329	G
35	BA	331	A
35	BA	332	A
35	BA	363(F)	A

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Mol	Chain	Res	Type
35	BA	474	G
35	BA	503	A
35	BA	603	A
35	BA	614(A)	U
35	BA	614(C)	A
35	BA	728	G
35	BA	739	G
35	BA	752	A
35	BA	764	A
35	BA	961	C
35	BA	1020	A
35	BA	1022	G
35	BA	1052	C
35	BA	1057	A
35	BA	1156	A
35	BA	1173	G
35	BA	1210	A
35	BA	1212	G
35	BA	1237	A
35	BA	1301	A
35	BA	1378	A
35	BA	1427	A
35	BA	1453	U
35	BA	1494	A
35	BA	1541	G
35	BA	1558	A
35	BA	1799	G
35	BA	1819	A
35	BA	1838	C
35	BA	1846	G
35	BA	1930	G
35	BA	1943	U
35	BA	1948	G
35	BA	1992	G
35	BA	2033	A
35	BA	2111	C
35	BA	2126	A
35	BA	2172	U
35	BA	2198	A
35	BA	2225	A
35	BA	2282	G
35	BA	2296	U

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Mol	Chain	Res	Type
35	BA	2344	U
35	BA	2345	G
35	BA	2422	A
35	BA	2425	A
35	BA	2428	G
35	BA	2481	G
35	BA	2611	U
35	BA	2689	U
35	BA	2690	C
35	BA	2756	U
35	BA	2762	G
35	BA	2778	A
35	BA	2779	U
35	BA	2799	C
35	BA	2801(A)	A
35	BA	2835	A
35	BA	2849	U
35	BA	2891	G
1	CA	30	U
1	CA	60	A
1	CA	115	G
1	CA	119	A
1	CA	203	U
1	CA	243	A
1	CA	250	A
1	CA	266	G
1	CA	315	A
1	CA	328	C
1	CA	344	A
1	CA	353	A
1	CA	366	C
1	CA	428	G
1	CA	429	U
1	CA	438	G
1	CA	532	A
1	CA	533	A
1	CA	534	U
1	CA	535	A
1	CA	560	U
1	CA	575	G
1	CA	576	G
1	CA	631	G

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Mol	Chain	Res	Type
1	CA	703	G
1	CA	812	C
1	CA	913	A
1	CA	992	U
1	CA	1049	U
1	CA	1065	U
1	CA	1101	A
1	CA	1129	C
1	CA	1201	A
1	CA	1225	A
1	CA	1226	C
1	CA	1285	A
1	CA	1299	A
1	CA	1300	G
1	CA	1337	G
1	CA	1347	G
1	CA	1364	U
1	CA	1493	A
1	CA	1498	U
22	CW	73	A
23	CX	11	U
35	DA	27	G
35	DA	49	A
35	DA	74	A
35	DA	120	U
35	DA	128	C
35	DA	221	A
35	DA	226	G
35	DA	329	G
35	DA	331	A
35	DA	332	A
35	DA	363(F)	A
35	DA	474	G
35	DA	503	A
35	DA	603	A
35	DA	614(A)	U
35	DA	614(C)	A
35	DA	728	G
35	DA	739	G
35	DA	752	A
35	DA	764	A
35	DA	961	C

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Mol	Chain	Res	Type
35	DA	1020	A
35	DA	1022	G
35	DA	1052	C
35	DA	1057	A
35	DA	1156	A
35	DA	1173	G
35	DA	1210	A
35	DA	1212	G
35	DA	1237	A
35	DA	1301	A
35	DA	1378	A
35	DA	1427	A
35	DA	1453	U
35	DA	1494	A
35	DA	1541	G
35	DA	1558	A
35	DA	1799	G
35	DA	1819	A
35	DA	1838	C
35	DA	1846	G
35	DA	1930	G
35	DA	1943	U
35	DA	1948	G
35	DA	1992	G
35	DA	2033	A
35	DA	2111	C
35	DA	2126	A
35	DA	2172	U
35	DA	2198	A
35	DA	2225	A
35	DA	2282	G
35	DA	2296	U
35	DA	2344	U
35	DA	2345	G
35	DA	2422	A
35	DA	2425	A
35	DA	2428	G
35	DA	2481	G
35	DA	2611	U
35	DA	2689	U
35	DA	2690	C
35	DA	2756	U

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Mol	Chain	Res	Type
35	DA	2762	G
35	DA	2778	A
35	DA	2779	U
35	DA	2799	C
35	DA	2801(A)	A
35	DA	2835	A
35	DA	2849	U
35	DA	2891	G

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

4 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	$\#\|Z\| > 2$
22	5MU	AV	54	22	18,21,23	0.40	0	26,30,35	0.49	0
22	5MU	AW	55	22	18,21,23	0.28	0	26,30,35	0.49	0
22	5MU	CW	55	22	18,21,23	0.30	0	26,30,35	0.50	0
22	5MU	CV	54	22	18,21,23	0.29	0	26,30,35	0.47	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
22	5MU	AV	54	22	-	0/7/25/26	0/2/2/2
22	5MU	AW	55	22	-	0/7/25/26	0/2/2/2
22	5MU	CW	55	22	-	0/7/25/26	0/2/2/2
22	5MU	CV	54	22	-	0/7/25/26	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
62	GDP	AY	703	60	24,30,30	1.29	2 (8%)	30,47,47	1.57	6 (20%)
61	FUA	CY	702	-	39,40,40	1.67	7 (17%)	49,64,64	1.44	9 (18%)
62	GDP	CY	703	60	24,30,30	1.30	2 (8%)	30,47,47	1.69	6 (20%)
61	FUA	AY	702	-	39,40,40	1.68	7 (17%)	49,64,64	1.51	5 (10%)

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
62	GDP	AY	703	60	-	3/12/32/32	0/3/3/3
61	FUA	CY	702	-	-	9/15/92/92	0/4/4/4
62	GDP	CY	703	60	-	3/12/32/32	0/3/3/3
61	FUA	AY	702	-	-	6/15/92/92	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CY	702	FUA	C23-C22	-4.50	1.39	1.51
61	AY	702	FUA	C23-C22	-4.38	1.39	1.51
61	AY	702	FUA	C23-C24	-4.27	1.39	1.53
61	CY	702	FUA	C23-C24	-4.26	1.39	1.53
61	AY	702	FUA	C29-C22	4.19	1.53	1.47
62	AY	703	GDP	C5-C6	-3.95	1.39	1.47
61	CY	702	FUA	C29-C22	3.91	1.53	1.47
62	CY	703	GDP	C5-C6	-3.90	1.39	1.47
61	CY	702	FUA	C24-C25	-3.40	1.39	1.50
61	AY	702	FUA	C24-C25	-3.28	1.39	1.50
61	AY	702	FUA	C14-C8	-3.11	1.53	1.59
61	CY	702	FUA	C14-C8	-3.08	1.53	1.59
61	CY	702	FUA	C25-C26	2.55	1.39	1.32
62	CY	703	GDP	O4'-C1'	2.52	1.44	1.41
61	AY	702	FUA	C25-C26	2.38	1.39	1.32
61	CY	702	FUA	C10-C9	-2.22	1.53	1.57
62	AY	703	GDP	O4'-C1'	2.21	1.44	1.41
61	AY	702	FUA	C10-C9	-2.18	1.53	1.57

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AY	702	FUA	C13-C12-C11	-4.33	105.84	111.90
62	CY	703	GDP	PA-O3A-PB	-4.29	118.11	132.83
61	CY	702	FUA	C16-O2-C31	-4.20	110.67	117.06
62	AY	703	GDP	PA-O3A-PB	-3.92	119.36	132.83
61	AY	702	FUA	C16-O2-C31	-3.91	111.12	117.06
62	CY	703	GDP	C2'-C3'-C4'	-3.62	95.61	102.64
61	AY	702	FUA	C8-C9-C10	-3.43	112.82	116.34
62	CY	703	GDP	C2-N1-C6	-3.18	119.25	125.10
62	AY	703	GDP	C2-N1-C6	-3.17	119.27	125.10
61	CY	702	FUA	C13-C12-C11	-3.16	107.47	111.90
62	CY	703	GDP	C8-N7-C5	3.10	108.89	102.99
61	AY	702	FUA	O2-C31-C32	2.95	116.52	111.09
62	AY	703	GDP	C8-N7-C5	2.88	108.47	102.99
61	CY	702	FUA	C8-C9-C10	-2.87	113.40	116.34
62	CY	703	GDP	C5-C6-N1	2.74	118.78	113.95
62	AY	703	GDP	C5-C6-N1	2.65	118.63	113.95
62	AY	703	GDP	O4'-C1'-C2'	-2.64	103.07	106.93
61	CY	702	FUA	C28-C26-C27	2.41	119.93	114.60
61	AY	702	FUA	C28-C26-C27	2.33	119.75	114.60
61	CY	702	FUA	C23-C24-C25	2.29	119.39	111.88
61	CY	702	FUA	O2-C31-C32	2.29	115.29	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	CY	702	FUA	C24-C25-C26	-2.15	120.39	127.75
62	AY	703	GDP	O6-C6-C5	-2.11	120.25	124.37
61	CY	702	FUA	C19-C10-C9	-2.10	108.03	113.09
61	CY	702	FUA	C21-C14-C8	-2.02	110.41	112.27
62	CY	703	GDP	O6-C6-C5	-2.00	120.46	124.37

There are no chirality outliers.

All (21) torsion outliers are listed below:

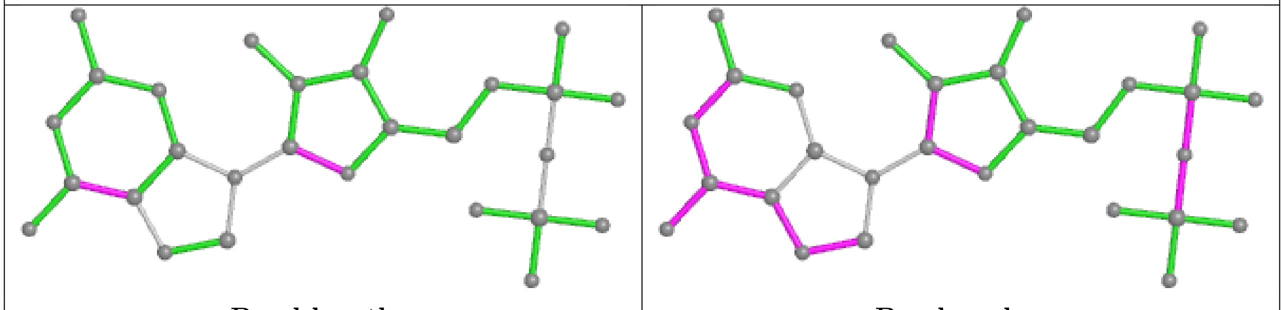
Mol	Chain	Res	Type	Atoms
61	AY	702	FUA	C13-C17-C22-C29
61	AY	702	FUA	C17-C22-C23-C24
61	AY	702	FUA	C29-C22-C23-C24
61	CY	702	FUA	C13-C17-C22-C29
61	CY	702	FUA	C17-C22-C23-C24
61	CY	702	FUA	C29-C22-C23-C24
62	AY	703	GDP	C5'-O5'-PA-O3A
62	AY	703	GDP	C5'-O5'-PA-O1A
62	CY	703	GDP	C5'-O5'-PA-O1A
61	AY	702	FUA	C32-C31-O2-C16
61	AY	702	FUA	O3-C31-O2-C16
61	CY	702	FUA	C23-C22-C29-O4
61	CY	702	FUA	C23-C22-C29-O5
61	CY	702	FUA	C15-C16-O2-C31
62	CY	703	GDP	C5'-O5'-PA-O3A
62	CY	703	GDP	C5'-O5'-PA-O2A
61	AY	702	FUA	C23-C24-C25-C26
61	CY	702	FUA	C23-C24-C25-C26
62	AY	703	GDP	C5'-O5'-PA-O2A
61	CY	702	FUA	C17-C22-C29-O4
61	CY	702	FUA	C17-C16-O2-C31

There are no ring outliers.

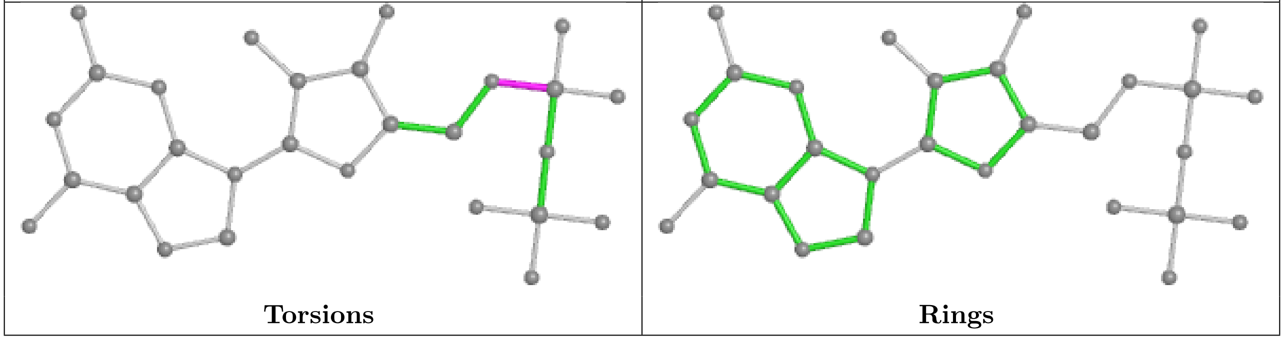
No monomer is involved in short contacts.

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

Ligand GDP AY 703

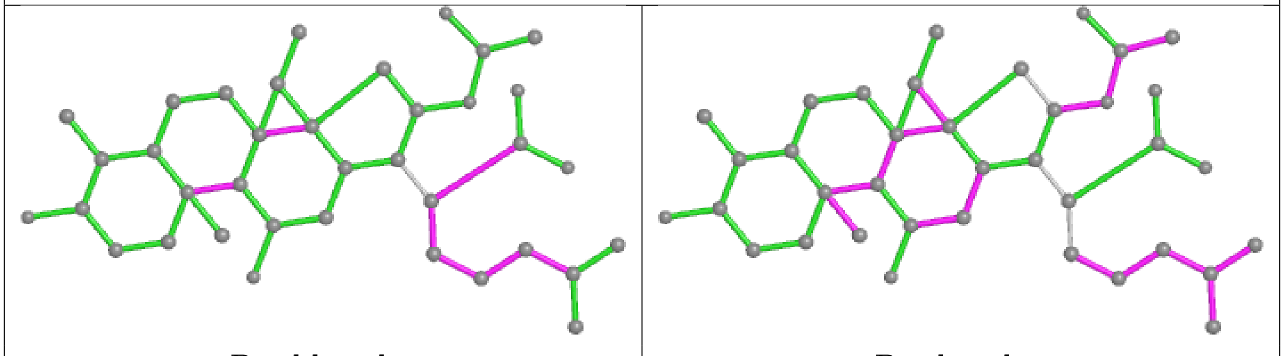


Bond lengths **Bond angles**

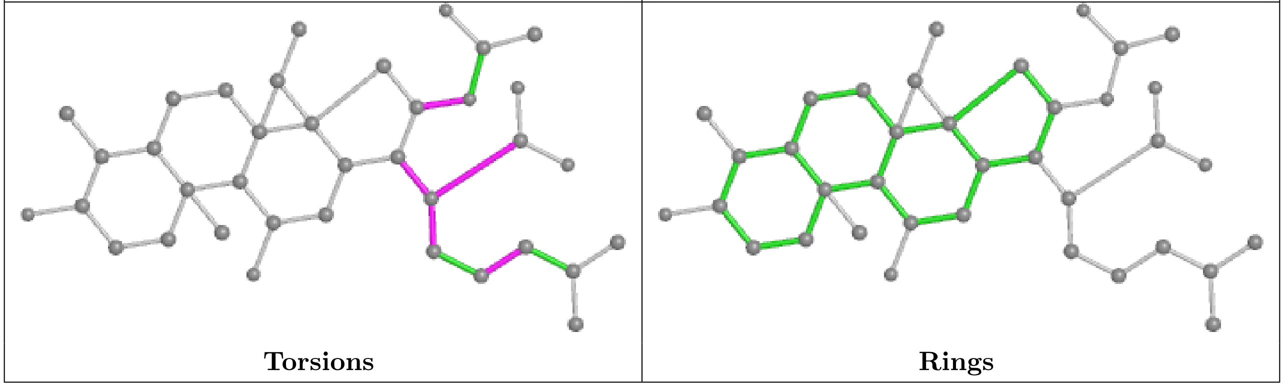


Torsions **Rings**

Ligand FUA CY 702

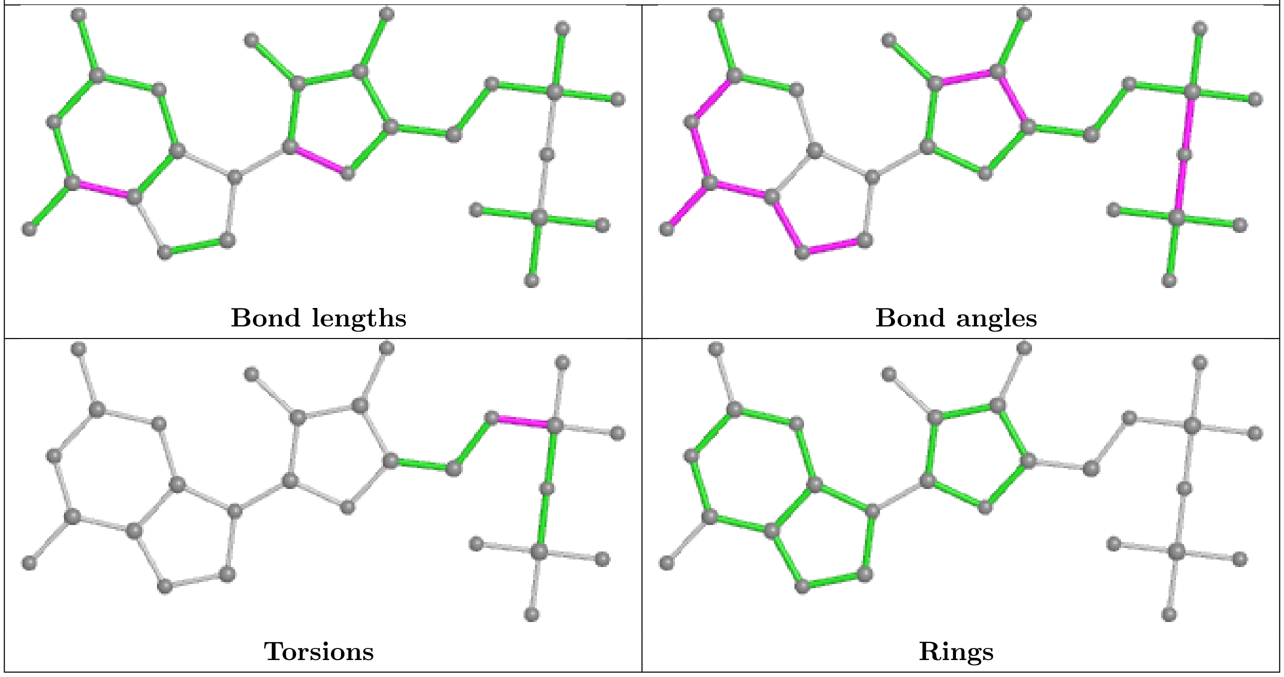


Bond lengths **Bond angles**



Torsions **Rings**

Ligand GDP CY 703



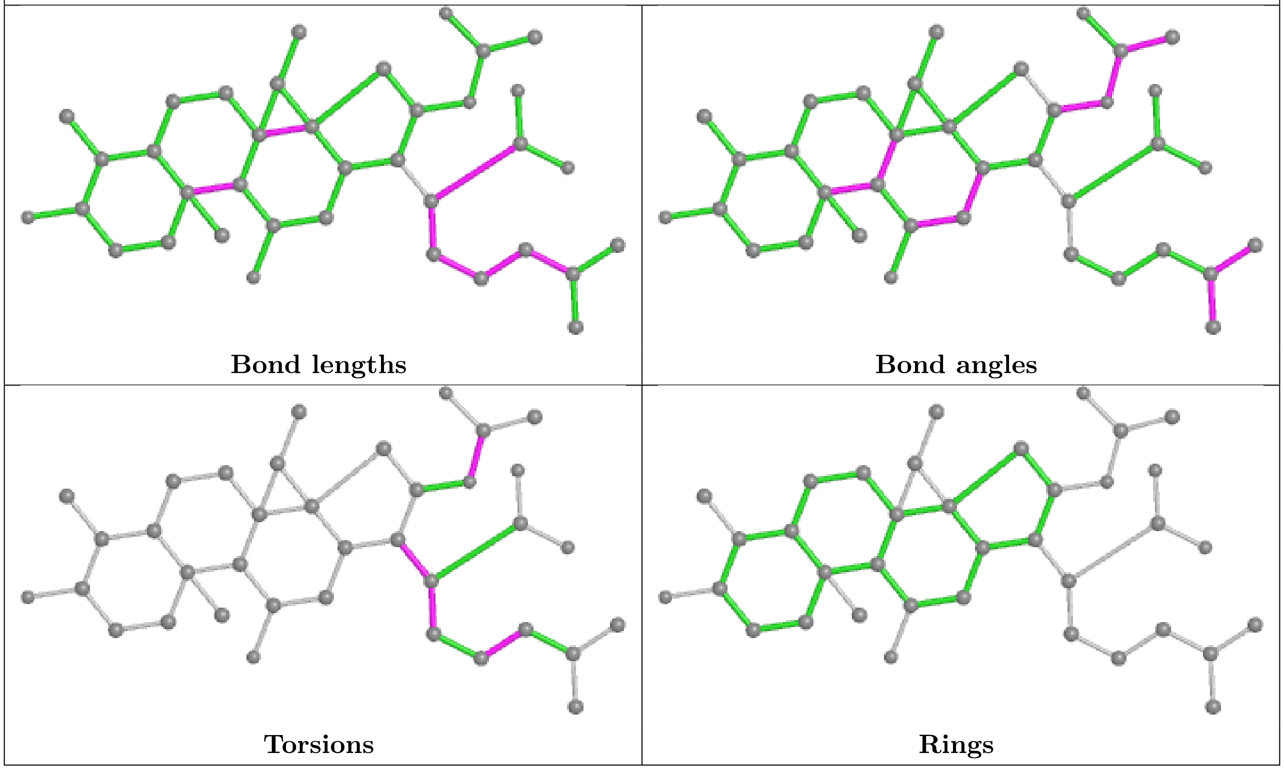
Bond lengths

Bond angles

Torsions

Rings

Ligand FUA AY 702



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	CI	2
9	AI	2
45	DL	1
45	BL	1
41	BG	1
41	DG	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DL	30:UNK	C	52:UNK	N	38.40
1	BL	30:UNK	C	52:UNK	N	36.36
1	BG	112:PRO	C	113:ARG	N	3.27
1	DG	112:PRO	C	113:ARG	N	3.05
1	CI	53:VAL	C	54:ASP	N	2.98
1	AI	53:VAL	C	54:ASP	N	2.92
1	AI	104:ARG	C	105:ASP	N	2.54
1	CI	104:ARG	C	105:ASP	N	2.54

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	1504/1522 (98%)	-0.27	22 (1%)	73	60	23, 62, 148, 220	0
1	CA	1504/1522 (98%)	-0.51	15 (0%)	82	70	26, 65, 148, 220	0
2	AB	235/256 (91%)	-0.30	3 (1%)	77	63	40, 81, 147, 159	0
2	CB	235/256 (91%)	-0.32	1 (0%)	92	86	43, 82, 147, 158	0
3	AC	207/239 (86%)	-0.41	0	100	100	31, 72, 113, 118	0
3	CC	207/239 (86%)	-0.38	0	100	100	33, 75, 115, 121	0
4	AD	208/209 (99%)	-0.39	0	100	100	46, 79, 115, 124	0
4	CD	208/209 (99%)	-0.43	0	100	100	48, 80, 116, 125	0
5	AE	151/162 (93%)	-0.49	1 (0%)	87	78	25, 50, 90, 112	0
5	CE	151/162 (93%)	-0.46	1 (0%)	87	78	27, 52, 91, 112	0
6	AF	101/101 (100%)	-0.44	0	100	100	55, 85, 110, 118	0
6	CF	101/101 (100%)	-0.29	0	100	100	60, 87, 111, 118	0
7	AG	155/156 (99%)	-0.38	1 (0%)	89	81	51, 79, 109, 136	0
7	CG	155/156 (99%)	-0.39	2 (1%)	77	63	55, 81, 111, 136	0
8	AH	138/138 (100%)	-0.41	0	100	100	32, 54, 75, 82	0
8	CH	138/138 (100%)	-0.49	0	100	100	35, 56, 76, 83	0
9	AI	127/128 (99%)	-0.23	1 (0%)	86	75	50, 83, 114, 120	0
9	CI	127/128 (99%)	-0.36	1 (0%)	86	75	53, 86, 114, 120	0
10	AJ	99/105 (94%)	0.08	6 (6%)	21	12	47, 100, 155, 159	0
10	CJ	99/105 (94%)	0.18	3 (3%)	50	34	50, 102, 156, 159	0
11	AK	119/129 (92%)	-0.34	2 (1%)	70	55	42, 59, 100, 123	0
11	CK	119/129 (92%)	-0.28	1 (0%)	86	75	44, 60, 102, 124	0
12	AL	125/132 (94%)	-0.49	0	100	100	38, 57, 87, 127	0
12	CL	125/132 (94%)	-0.43	2 (1%)	72	57	39, 58, 88, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	AM	125/126 (99%)	-0.15	6 (4%)	30	19	68, 111, 139, 171	0
13	CM	125/126 (99%)	-0.16	8 (6%)	19	11	70, 112, 139, 172	0
14	AN	60/61 (98%)	-0.41	1 (1%)	70	55	39, 59, 92, 97	0
14	CN	60/61 (98%)	-0.42	0	100	100	44, 61, 93, 98	0
15	AO	88/89 (98%)	-0.57	0	100	100	35, 61, 91, 100	0
15	CO	88/89 (98%)	-0.54	0	100	100	38, 61, 94, 100	0
16	AP	84/88 (95%)	-0.45	0	100	100	54, 73, 96, 131	0
16	CP	84/88 (95%)	-0.43	1 (1%)	79	66	57, 74, 98, 132	0
17	AQ	100/105 (95%)	-0.56	0	100	100	43, 64, 89, 98	0
17	CQ	100/105 (95%)	-0.50	0	100	100	46, 66, 90, 97	0
18	AR	70/88 (79%)	-0.42	1 (1%)	75	61	42, 69, 94, 108	0
18	CR	70/88 (79%)	-0.51	1 (1%)	75	61	45, 70, 95, 109	0
19	AS	79/93 (84%)	-0.02	2 (2%)	57	41	77, 106, 144, 149	0
19	CS	79/93 (84%)	0.15	4 (5%)	28	17	78, 107, 144, 150	0
20	AT	99/106 (93%)	-0.37	0	100	100	63, 84, 126, 129	0
20	CT	99/106 (93%)	-0.37	0	100	100	64, 85, 127, 129	0
21	AU	25/27 (92%)	-0.24	0	100	100	63, 82, 118, 122	0
21	CU	25/27 (92%)	0.12	0	100	100	66, 86, 120, 123	0
22	AV	76/77 (98%)	-0.48	0	100	100	32, 67, 110, 127	0
22	AW	76/77 (98%)	-0.43	1 (1%)	77	63	71, 168, 192, 201	0
22	CV	76/77 (98%)	-0.61	0	100	100	47, 84, 121, 151	0
22	CW	76/77 (98%)	-0.37	1 (1%)	77	63	78, 176, 200, 210	0
23	AX	11/25 (44%)	0.09	0	100	100	28, 94, 149, 166	0
23	CX	11/25 (44%)	0.01	0	100	100	45, 106, 156, 168	0
24	AY	667/691 (96%)	-0.17	9 (1%)	77	63	61, 99, 140, 150	0
24	CY	667/691 (96%)	0.08	23 (3%)	45	30	73, 108, 148, 161	0
25	B0	84/85 (98%)	0.05	6 (7%)	16	9	67, 82, 140, 163	0
25	D0	84/85 (98%)	0.37	9 (10%)	6	3	69, 84, 141, 163	0
26	B1	94/98 (95%)	-0.46	1 (1%)	80	68	41, 70, 118, 128	0
26	D1	94/98 (95%)	-0.34	0	100	100	53, 80, 123, 131	0
27	B2	71/72 (98%)	-0.30	2 (2%)	53	37	77, 116, 150, 161	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
27	D2	71/72 (98%)	-0.15	2 (2%) 53 37	95, 119, 146, 163	0
28	B3	60/60 (100%)	-0.08	1 (1%) 70 55	63, 88, 114, 135	0
28	D3	60/60 (100%)	-0.02	2 (3%) 46 31	64, 89, 114, 134	0
29	B4	58/71 (81%)	0.07	3 (5%) 27 17	76, 135, 220, 222	0
29	D4	58/71 (81%)	0.27	7 (12%) 4 3	77, 137, 220, 222	0
30	B5	59/60 (98%)	-0.08	3 (5%) 28 17	52, 80, 153, 172	0
30	D5	59/60 (98%)	-0.03	4 (6%) 17 10	52, 80, 153, 172	0
31	B6	50/54 (92%)	0.00	2 (4%) 38 25	56, 89, 107, 117	0
31	D6	50/54 (92%)	-0.26	1 (2%) 65 49	56, 90, 108, 117	0
32	B7	49/49 (100%)	-0.34	2 (4%) 37 24	47, 64, 119, 132	0
32	D7	49/49 (100%)	-0.39	0 100 100	47, 64, 120, 132	0
33	B8	64/65 (98%)	-0.37	1 (1%) 72 57	63, 75, 105, 125	0
33	D8	64/65 (98%)	-0.26	1 (1%) 72 57	65, 76, 105, 126	0
34	B9	37/37 (100%)	-0.43	0 100 100	60, 71, 85, 89	0
34	D9	37/37 (100%)	-0.30	1 (2%) 54 38	60, 73, 87, 91	0
35	BA	2901/2915 (99%)	-0.39	27 (0%) 84 73	30, 76, 162, 221	0
35	DA	2901/2915 (99%)	-0.52	32 (1%) 80 68	29, 77, 162, 221	0
36	BB	119/122 (97%)	-0.54	0 100 100	65, 106, 138, 183	0
36	DB	119/122 (97%)	-0.72	0 100 100	66, 108, 138, 183	0
37	BC	228/229 (99%)	-0.13	4 (1%) 68 53	42, 97, 147, 160	0
37	DC	228/229 (99%)	0.09	12 (5%) 26 16	43, 98, 148, 162	0
38	BD	275/276 (99%)	-0.52	0 100 100	31, 52, 82, 101	0
38	DD	275/276 (99%)	-0.51	1 (0%) 92 86	32, 52, 82, 101	0
39	BE	205/206 (99%)	-0.33	4 (1%) 65 49	44, 77, 128, 135	0
39	DE	205/206 (99%)	-0.29	3 (1%) 73 60	44, 77, 128, 134	0
40	BF	208/210 (99%)	0.01	10 (4%) 30 19	53, 110, 166, 177	0
40	DF	208/210 (99%)	-0.01	11 (5%) 26 16	53, 111, 166, 176	0
41	BG	181/182 (99%)	-0.27	4 (2%) 62 45	63, 95, 131, 143	0
41	DG	181/182 (99%)	-0.03	6 (3%) 46 31	86, 110, 137, 151	0
42	BH	167/180 (92%)	0.06	6 (3%) 42 28	81, 117, 143, 159	0
42	DH	167/180 (92%)	0.04	4 (2%) 59 42	81, 118, 143, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
43	BJ	0/173	-	-			-	-
43	DJ	0/173	-	-			-	-
44	BK	140/147 (95%)	1.96	61 (43%)	0	0	162, 180, 186, 188	0
44	DK	140/147 (95%)	1.68	49 (35%)	0	0	162, 180, 186, 187	0
45	BL	0/125	-	-			-	-
45	BM	0/125	-	-			-	-
45	Bl	0/125	-	-			-	-
45	Bm	0/125	-	-			-	-
45	DL	0/125	-	-			-	-
45	DM	0/125	-	-			-	-
45	Dl	0/125	-	-			-	-
45	Dm	0/125	-	-			-	-
46	BN	139/140 (99%)	-0.30	2 (1%)	75	61	60, 91, 132, 137	0
46	DN	139/140 (99%)	-0.25	1 (0%)	87	78	61, 91, 132, 137	0
47	BO	122/122 (100%)	-0.45	0	100	100	35, 60, 73, 86	0
47	DO	122/122 (100%)	-0.43	0	100	100	36, 61, 73, 88	0
48	BP	146/150 (97%)	0.02	4 (2%)	54	38	46, 111, 137, 157	0
48	DP	146/150 (97%)	0.10	4 (2%)	54	38	50, 113, 137, 157	0
49	BQ	141/141 (100%)	-0.38	0	100	100	45, 65, 88, 119	0
49	DQ	141/141 (100%)	-0.41	0	100	100	45, 66, 89, 120	0
50	BR	117/118 (99%)	-0.37	1 (0%)	84	73	49, 81, 101, 128	0
50	DR	117/118 (99%)	-0.28	1 (0%)	84	73	53, 82, 101, 128	0
51	BS	99/112 (88%)	-0.19	2 (2%)	65	49	82, 116, 140, 144	0
51	DS	99/112 (88%)	0.28	5 (5%)	28	17	83, 117, 141, 145	0
52	BT	138/146 (94%)	-0.13	4 (2%)	51	35	55, 83, 149, 176	0
52	DT	138/146 (94%)	-0.18	5 (3%)	42	28	57, 84, 149, 177	0
53	BU	117/118 (99%)	-0.36	0	100	100	62, 80, 114, 135	0
53	DU	117/118 (99%)	-0.36	0	100	100	62, 81, 115, 134	0
54	BV	101/101 (100%)	-0.02	1 (0%)	82	70	59, 116, 133, 141	0
54	DV	101/101 (100%)	0.18	6 (5%)	22	13	61, 116, 134, 140	0
55	BW	113/113 (100%)	-0.28	0	100	100	61, 79, 119, 158	0
55	DW	113/113 (100%)	-0.16	0	100	100	63, 80, 120, 159	0
56	BX	93/96 (96%)	-0.18	0	100	100	76, 91, 110, 114	0
56	DX	93/96 (96%)	-0.22	0	100	100	76, 92, 111, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
57	BY	107/110 (97%)	0.08	2 (1%)	66	51	78, 127, 149, 155	0
57	DY	107/110 (97%)	0.41	4 (3%)	41	27	78, 127, 149, 155	0
58	BZ	185/206 (89%)	-0.23	1 (0%)	91	83	47, 90, 135, 143	0
58	DZ	185/206 (89%)	-0.09	1 (0%)	91	83	68, 99, 138, 146	0
All	All	22794/24788 (91%)	-0.29	446 (1%)	65	49	23, 82, 154, 222	0

All (446) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BA	654(K)	C	14.8
1	CA	1036	G	13.4
52	BT	138	ALA	13.1
35	DA	654(D)	G	13.0
35	BA	654(F)	C	11.4
35	BA	654(I)	C	11.3
1	AA	1026	G	11.3
44	BK	16	LYS	10.9
1	AA	1030(B)	C	10.0
1	CA	89	C	9.9
1	AA	1036	G	9.7
1	AA	89	C	9.6
41	DG	49	ASP	9.4
35	DA	654(J)	A	9.3
52	DT	134	GLU	9.3
35	DA	654(E)	G	9.2
44	BK	50	ASP	9.1
35	BA	654(D)	G	9.0
35	DA	654(K)	C	8.8
35	DA	654(G)	C	8.4
35	DA	654(F)	C	8.3
30	B5	60	VAL	8.2
35	BA	654(E)	G	8.2
35	BA	2802	G	8.2
11	CK	129	SER	8.0
44	BK	11	GLN	7.9
30	B5	59	GLU	7.9
44	DK	51	ALA	7.8
1	CA	1030(B)	C	7.8
33	D8	65	GLU	7.8
22	AW	1	C	7.4
44	DK	11	GLN	7.3

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Mol	Chain	Res	Type	RSRZ
35	BA	654(J)	A	7.3
35	BA	2897	U	7.2
1	CA	1030(A)	G	7.1
35	BA	654(L)	G	7.1
35	DA	2897	U	6.9
30	D5	60	VAL	6.9
35	BA	654(H)	G	6.9
1	AA	1029	C	6.9
41	BG	49	ASP	6.8
44	BK	51	ALA	6.7
1	AA	1028	C	6.6
35	BA	2795	G	6.6
44	BK	61	ALA	6.5
24	CY	42	ILE	6.5
1	AA	1030(A)	G	6.4
24	AY	41	LYS	6.4
25	D0	6	GLY	6.3
44	DK	52	ILE	6.3
44	DK	9	LYS	6.2
52	BT	137	LYS	6.2
44	DK	16	LYS	6.2
30	D5	59	GLU	6.1
35	DA	2802	G	6.0
1	CA	88	A	6.0
40	BF	12	LEU	6.0
35	DA	654(H)	G	5.9
35	DA	654(I)	C	5.9
57	DY	107	ASP	5.9
35	DA	2796	U	5.9
24	CY	116	PRO	5.8
35	DA	654(S)	G	5.8
41	BG	48	GLU	5.7
35	BA	654(C)	G	5.7
57	DY	28	LYS	5.7
13	CM	126	LYS	5.7
40	DF	1	MET	5.6
37	DC	147	GLY	5.6
35	BA	654(G)	C	5.6
41	DG	48	GLU	5.6
44	DK	26	ALA	5.5
32	B7	49	ARG	5.5
25	D0	5	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
24	AY	116	PRO	5.5
44	DK	50	ASP	5.4
1	CA	1035	A	5.4
24	AY	43	GLY	5.4
13	CM	122	LYS	5.4
1	CA	82	U	5.2
44	DK	2	LYS	5.2
25	B0	4	LYS	5.2
1	AA	1030(C)	G	5.2
44	DK	18	THR	5.1
40	BF	8	GLN	5.1
1	CA	1026	G	5.1
44	BK	15	GLY	5.1
22	CW	1	C	5.0
44	DK	27	LEU	5.0
44	DK	3	LYS	4.9
44	BK	7	VAL	4.8
1	CA	81	U	4.8
25	D0	3	HIS	4.8
44	BK	17	ALA	4.8
1	AA	81	U	4.8
44	BK	63	ARG	4.8
44	DK	10	LEU	4.7
35	DA	654(L)	G	4.7
44	DK	65	PHE	4.7
30	B5	58	LEU	4.6
44	BK	60	TYR	4.6
1	AA	1031	G	4.6
57	DY	106	LEU	4.6
13	CM	125	ARG	4.5
44	BK	97	GLY	4.5
29	D4	57	GLU	4.5
24	CY	64	THR	4.5
25	D0	7	LEU	4.5
25	D0	8	GLY	4.5
37	DC	116	ALA	4.4
24	CY	690	GLY	4.4
35	DA	1174	A	4.4
24	AY	113	GLY	4.4
44	DK	55	VAL	4.4
24	AY	114	VAL	4.4
35	BA	275	G	4.4

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Mol	Chain	Res	Type	RSRZ
44	DK	20	ALA	4.3
44	DK	54	PRO	4.3
40	DF	133	ASN	4.3
37	DC	79	ALA	4.3
44	DK	22	PRO	4.3
44	BK	31	GLY	4.3
44	BK	83	GLY	4.3
40	BF	25	PRO	4.3
52	BT	136	GLN	4.2
35	DA	2793	G	4.2
40	DF	208	GLY	4.2
37	DC	78	ILE	4.2
44	BK	32	ALA	4.1
44	DK	21	PRO	4.1
12	CL	128	ALA	4.1
41	BG	50	ALA	4.0
35	BA	2896	C	4.0
27	B2	72	ALA	4.0
35	DA	2896	C	4.0
39	DE	205	ALA	4.0
2	CB	7	VAL	4.0
24	CY	4	LYS	4.0
25	D0	4	LYS	4.0
52	DT	135	ALA	4.0
51	DS	109	GLY	4.0
28	D3	1	MET	3.9
37	BC	2	PRO	3.9
44	BK	35	MET	3.9
1	CA	80	G	3.9
44	BK	64	SER	3.9
13	CM	123	ALA	3.9
48	DP	149	GLU	3.9
5	CE	154	GLY	3.9
1	AA	88	A	3.9
44	BK	62	ASP	3.8
31	B6	42	TRP	3.8
44	BK	49	GLY	3.8
5	AE	155	GLU	3.8
44	BK	18	THR	3.8
44	BK	12	LEU	3.8
44	BK	47	ASN	3.8
13	CM	124	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
44	DK	74	ALA	3.7
44	BK	2	LYS	3.7
37	DC	97	GLY	3.7
35	DA	157	U	3.7
24	CY	41	LYS	3.7
44	BK	14	ALA	3.7
40	DF	17	ARG	3.6
35	BA	2794	C	3.6
25	B0	8	GLY	3.6
44	BK	82	ALA	3.6
35	DA	654(C)	G	3.6
13	AM	7	VAL	3.6
44	BK	66	THR	3.6
50	DR	2	ARG	3.6
48	BP	87	ASP	3.6
44	BK	52	ILE	3.6
7	AG	84	ASN	3.6
11	AK	129	SER	3.6
52	DT	137	LYS	3.6
40	BF	1	MET	3.5
44	DK	36	GLU	3.5
44	BK	8	VAL	3.5
44	DK	37	PHE	3.5
44	BK	22	PRO	3.5
25	B0	6	GLY	3.5
54	DV	48	GLY	3.5
35	DA	275	G	3.5
44	DK	141	ALA	3.5
13	AM	122	LYS	3.5
51	DS	61	ASN	3.4
29	D4	32	TYR	3.4
13	AM	125	ARG	3.4
44	BK	27	LEU	3.4
44	DK	13	PRO	3.4
13	CM	120	LYS	3.4
44	BK	37	PHE	3.4
18	CR	88	LYS	3.4
1	AA	1035	A	3.4
44	DK	17	ALA	3.4
37	DC	124	VAL	3.4
40	BF	24	LEU	3.4
44	BK	65	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	AA	82	U	3.4
1	CA	1001(A)	G	3.3
24	CY	84	THR	3.3
44	BK	13	PRO	3.3
54	DV	36	PRO	3.3
39	BE	76	ARG	3.3
25	B0	3	HIS	3.3
13	CM	7	VAL	3.3
44	BK	36	GLU	3.2
44	DK	61	ALA	3.2
37	DC	96	GLY	3.2
51	BS	60	GLY	3.2
44	BK	30	HIS	3.2
35	DA	2799	C	3.2
35	DA	2804	C	3.2
44	DK	118	THR	3.2
52	DT	39	ARG	3.2
35	DA	2795	G	3.2
37	DC	98	GLU	3.1
24	CY	40	HIS	3.1
29	B4	47	GLN	3.1
48	DP	150	ALA	3.1
44	BK	21	PRO	3.1
35	BA	2894	G	3.1
40	BF	133	ASN	3.1
44	BK	84	LEU	3.1
1	AA	1030(D)	A	3.1
7	CG	82	GLY	3.1
44	DK	30	HIS	3.1
41	DG	113	ARG	3.1
58	DZ	159	PRO	3.1
39	DE	204	ALA	3.1
1	AA	1027	C	3.1
44	DK	4	VAL	3.1
35	DA	156	U	3.1
51	DS	57	LYS	3.1
9	CI	95	LYS	3.0
31	B6	26	ASN	3.0
44	BK	33	ASN	3.0
44	DK	137	GLU	3.0
44	DK	82	ALA	3.0
40	BF	11	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
44	BK	69	THR	3.0
25	D0	2	ALA	3.0
35	BA	2796	U	3.0
24	CY	203	GLU	3.0
44	BK	48	MET	3.0
24	CY	202	PRO	3.0
35	DA	654(R)	C	3.0
27	D2	71	ASN	3.0
1	CA	1028	C	2.9
19	AS	82	GLY	2.9
35	BA	2799	C	2.9
44	BK	28	GLY	2.9
19	CS	82	GLY	2.9
51	DS	59	LYS	2.9
35	BA	888	C	2.9
44	BK	41	PHE	2.9
40	DF	23	ASP	2.9
35	DA	1534	U	2.9
13	AM	124	PRO	2.8
44	DK	19	PRO	2.8
37	DC	80	LYS	2.8
44	BK	45	THR	2.8
40	BF	10	PRO	2.8
44	BK	10	LEU	2.8
46	BN	68	GLU	2.8
19	CS	81	ARG	2.8
41	BG	115	ARG	2.8
10	CJ	88	LEU	2.8
44	BK	67	PHE	2.8
24	AY	40	HIS	2.8
24	CY	114	VAL	2.8
30	D5	2	ALA	2.8
24	AY	115	GLU	2.8
24	CY	17	ILE	2.8
42	BH	42	ARG	2.8
40	BF	9	ILE	2.8
1	CA	1257	U	2.8
12	CL	129	ALA	2.8
29	D4	56	VAL	2.7
1	AA	1030	C	2.7
30	D5	54	GLY	2.7
54	DV	20	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
13	AM	126	LYS	2.7
44	DK	66	THR	2.7
44	BK	26	ALA	2.7
44	BK	105	LEU	2.7
44	DK	67	PHE	2.7
10	AJ	85	LEU	2.7
14	AN	2	ALA	2.7
41	DG	2	PRO	2.7
41	DG	149	VAL	2.7
44	BK	58	THR	2.7
24	CY	115	GLU	2.7
44	BK	6	ALA	2.7
29	D4	38	LYS	2.6
44	DK	38	VAL	2.6
42	BH	52	VAL	2.6
10	AJ	88	LEU	2.6
37	BC	14	LYS	2.6
24	CY	227	ILE	2.6
35	DA	2803	C	2.6
32	B7	48	LYS	2.6
44	BK	110	GLN	2.6
42	BH	44	VAL	2.6
44	BK	68	VAL	2.6
1	AA	1001(A)	G	2.6
44	BK	137	GLU	2.6
35	DA	654	A	2.6
13	CM	121	LYS	2.6
40	DF	2	LYS	2.6
24	CY	6	GLU	2.5
39	DE	69	LYS	2.5
35	BA	2801	A	2.5
28	B3	1	MET	2.5
44	BK	98	ARG	2.5
44	DK	45	THR	2.5
48	BP	150	ALA	2.5
35	DA	654(A)	G	2.5
31	D6	42	TRP	2.5
44	BK	74	ALA	2.5
1	AA	80	G	2.5
44	BK	54	PRO	2.5
44	DK	25	PRO	2.5
24	AY	42	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
35	BA	614(A)	U	2.5
10	AJ	25	GLU	2.5
44	DK	62	ASP	2.5
37	DC	117	THR	2.5
29	D4	22	ILE	2.5
52	DT	136	GLN	2.5
10	CJ	73	ASP	2.5
10	AJ	33	GLN	2.5
44	BK	56	GLU	2.5
2	AB	122	PHE	2.5
1	CA	83	U	2.5
51	BS	43	GLU	2.5
37	DC	113	ALA	2.5
51	DS	108	GLY	2.5
7	CG	83	ALA	2.4
35	DA	614(A)	U	2.4
9	AI	95	LYS	2.4
44	BK	19	PRO	2.4
44	BK	53	VAL	2.4
48	DP	95	VAL	2.4
44	DK	39	LYS	2.4
24	CY	204	GLU	2.4
29	B4	32	TYR	2.4
24	CY	65	ILE	2.4
42	DH	176	ALA	2.4
29	B4	53	GLU	2.4
24	CY	43	GLY	2.4
16	CP	83	GLU	2.4
42	BH	137	ASP	2.4
54	DV	101	GLY	2.4
44	DK	63	ARG	2.4
39	BE	204	ALA	2.4
42	DH	101	ARG	2.4
50	BR	2	ARG	2.4
40	BF	23	ASP	2.4
10	CJ	23	ILE	2.3
19	CS	22	LEU	2.3
25	D0	85	ALA	2.3
10	AJ	80	LYS	2.3
35	DA	1740	G	2.3
35	DA	896	A	2.3
44	DK	29	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
44	DK	48	MET	2.3
44	DK	14	ALA	2.3
18	AR	88	LYS	2.3
24	CY	445	GLU	2.3
46	DN	139	GLU	2.3
54	BV	20	LEU	2.3
13	AM	84	ILE	2.3
44	BK	57	ILE	2.3
2	AB	13	ALA	2.3
57	DY	53	PRO	2.3
48	DP	5	ASP	2.3
35	DA	884	C	2.3
42	BH	33	LEU	2.3
27	D2	72	ALA	2.3
1	AA	1037	C	2.3
33	B8	65	GLU	2.2
24	CY	97	SER	2.2
44	DK	8	VAL	2.2
19	AS	81	ARG	2.2
25	D0	81	VAL	2.2
40	DF	194	MET	2.2
46	BN	139	GLU	2.2
26	B1	85	LEU	2.2
48	BP	81	GLN	2.2
35	BA	352	G	2.2
1	AA	470	C	2.2
54	DV	1	MET	2.2
1	AA	93	G	2.2
24	CY	570	GLY	2.2
38	DD	276	LYS	2.2
52	BT	135	ALA	2.2
34	D9	1	MET	2.2
40	DF	205	ARG	2.2
44	DK	28	GLY	2.2
29	D4	58	ARG	2.2
39	BE	69	LYS	2.2
24	CY	401	SER	2.1
42	BH	175	LYS	2.1
40	DF	161	GLU	2.1
40	DF	25	PRO	2.1
57	BY	28	LYS	2.1
1	CA	1029	C	2.1

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Mol	Chain	Res	Type	RSRZ
44	DK	56	GLU	2.1
48	BP	149	GLU	2.1
42	DH	85	LYS	2.1
44	DK	23	VAL	2.1
35	BA	654(S)	G	2.1
11	AK	127	LYS	2.1
25	B0	2	ALA	2.1
44	DK	32	ALA	2.1
2	AB	14	GLY	2.1
1	AA	1005	A	2.1
35	BA	654	A	2.1
27	B2	71	ASN	2.1
25	B0	7	LEU	2.1
35	BA	1174	A	2.1
10	AJ	4	ILE	2.1
44	BK	29	GLN	2.1
28	D3	2	PRO	2.1
58	BZ	159	PRO	2.1
35	BA	156	U	2.1
44	BK	9	LYS	2.1
37	BC	131	ILE	2.1
44	DK	110	GLN	2.0
24	CY	66	THR	2.0
44	DK	42	ASN	2.0
44	BK	85	GLU	2.0
42	DH	170	ARG	2.0
40	DF	181	LEU	2.0
19	CS	21	GLU	2.0
24	AY	19	ALA	2.0
29	D4	31	ILE	2.0
37	BC	203	GLU	2.0
57	BY	107	ASP	2.0
39	BE	205	ALA	2.0
41	DG	75	LYS	2.0
37	DC	110	ASP	2.0
54	DV	14	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
22	5MU	CW	55	20/22	0.81	0.13	178,179,186,186	0
22	5MU	AW	55	20/22	0.82	0.14	161,165,168,168	0
22	5MU	AV	54	20/22	0.95	0.13	82,84,86,86	0
22	5MU	CV	54	20/22	0.97	0.11	89,92,95,96	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
59	ZN	D4	101	1/1	0.90	0.07	164,164,164,164	0
61	FUA	AY	702	37/37	0.90	0.43	98,102,110,111	0
61	FUA	CY	702	37/37	0.90	0.35	102,104,107,109	0
59	ZN	B4	101	1/1	0.91	0.12	122,122,122,122	0
62	GDP	CY	703	28/28	0.95	0.15	81,87,94,95	0
62	GDP	AY	703	28/28	0.96	0.17	78,82,83,84	0
60	MG	AY	701	1/1	0.98	0.22	30,30,30,30	0
59	ZN	CD	301	1/1	0.99	0.28	49,49,49,49	0
60	MG	CY	701	1/1	0.99	0.12	39,39,39,39	0
59	ZN	B9	101	1/1	0.99	0.15	62,62,62,62	0
59	ZN	AN	101	1/1	1.00	0.16	35,35,35,35	0
59	ZN	D9	101	1/1	1.00	0.12	86,86,86,86	0
59	ZN	AD	301	1/1	1.00	0.28	32,32,32,32	0
59	ZN	CN	101	1/1	1.00	0.16	66,66,66,66	0

6.5 Other polymers ⓘ

There are no such residues in this entry.