Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2023 – 10:01 PM EDT

PDB ID : 4V9K
Title : 70S ribosome translocation intermediate GDPNP-I containing elongation factor EFG/GDPNP, mRNA, and tRNA bound in the pe*/E state.
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-24
Resolution : 3.50 Å(reported)

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

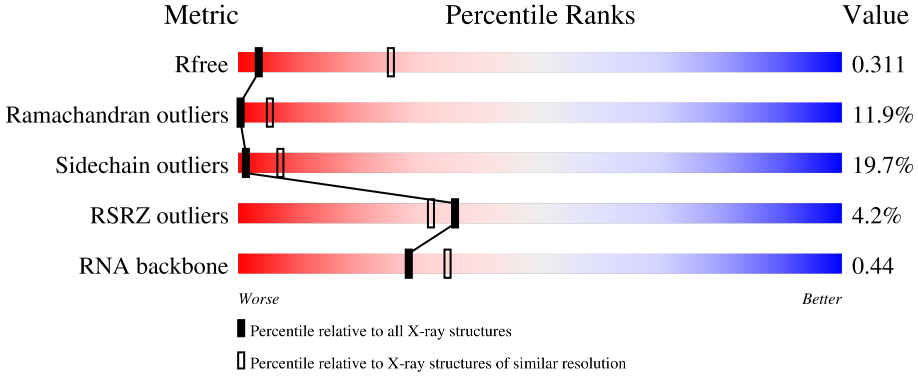
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance ⓘ

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

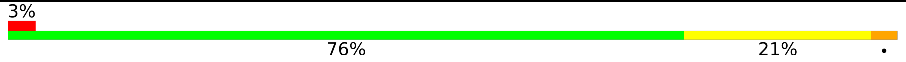
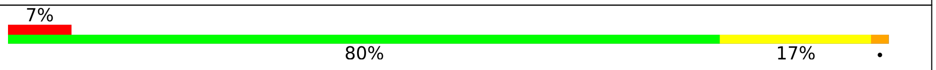
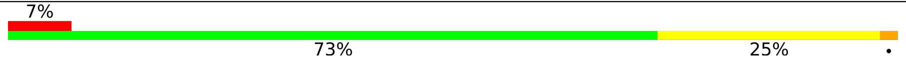
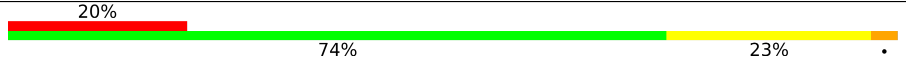
The reported resolution of this entry is 3.50 Å.

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	1659 (3.60-3.40)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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	AB	235	
1	CB	235	
2	AC	207	
2	CC	207	
3	AD	208	

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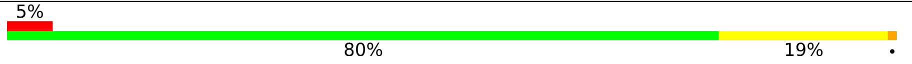
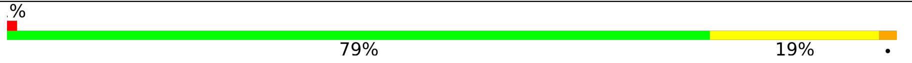
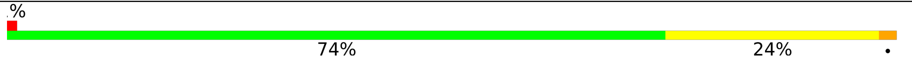
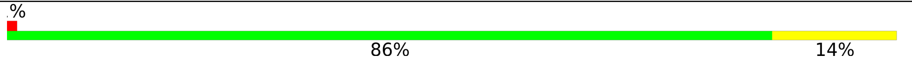
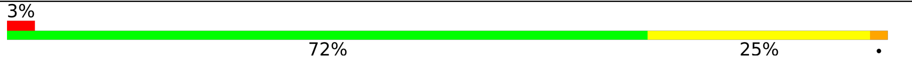
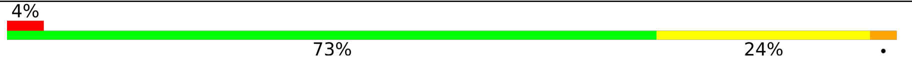
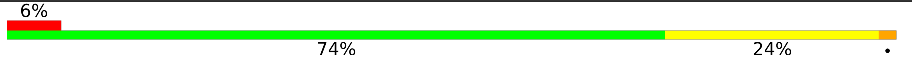
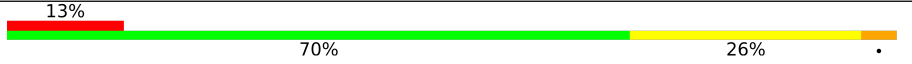
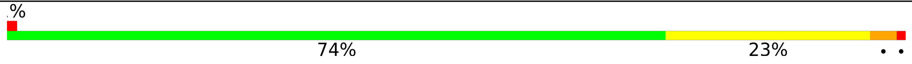
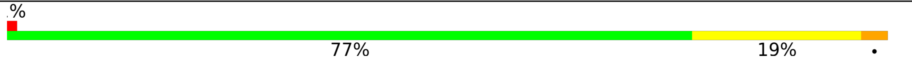
Mol	Chain	Length	Quality of chain
3	CD	208	
4	AE	151	
4	CE	151	
5	AF	101	
5	CF	101	
6	AG	155	
6	CG	155	
7	AH	138	
7	CH	138	
8	AI	127	
8	CI	127	
9	AJ	99	
9	CJ	99	
10	AK	119	
10	CK	119	
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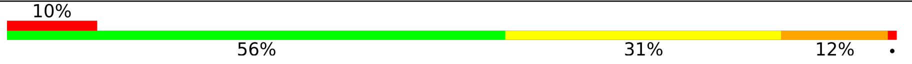
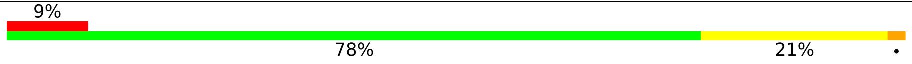
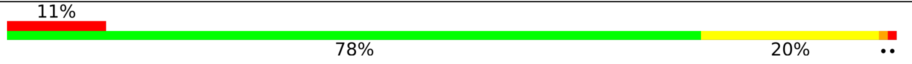
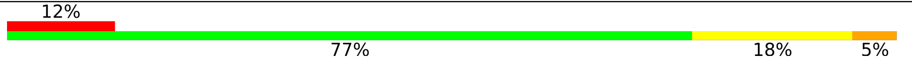
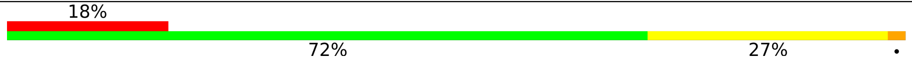
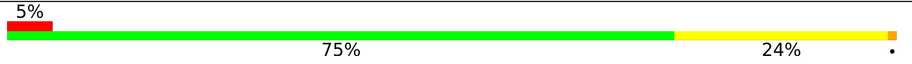
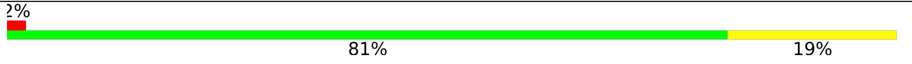
11	CL	125	
12	AM	125	
12	CM	125	
13	AN	60	
13	CN	60	
14	AO	88	
14	CO	88	
15	AP	84	
15	CP	84	

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Mol	Chain	Length	Quality of chain
16	AQ	100	6% 75% 25%
16	CQ	100	8% 76% 23% •
17	AR	70	4% 80% 20%
17	CR	70	% 80% 20%
18	AS	79	18% 77% 22% •
18	CS	79	13% 71% 25% •
19	AT	99	84% 14% •
19	CT	99	2% 85% 14% •
20	AY	687	7% 72% 25% •
20	CY	687	7% 76% 21% •
21	AA	1511	77% 22% •
21	CA	1511	78% 21% •
22	AW	77	69% 27% •
22	CW	77	73% 25% •
23	AV	23	43% 39% 17%
23	CV	23	4% 52% 30% 17%
24	AU	6	67% 33%
24	CU	6	67% 33%
25	BC	228	32% 61% 33% 5%
25	DC	228	32% 60% 36% •
26	BD	275	% 70% 28% •
26	DD	275	% 72% 27% •
27	BE	205	% 75% 21% •
27	DE	205	2% 72% 25% •
28	BF	208	7% 74% 21% 5%

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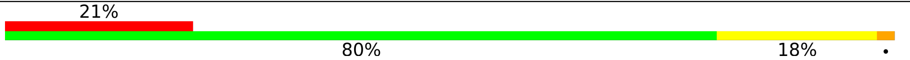
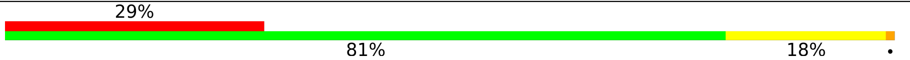
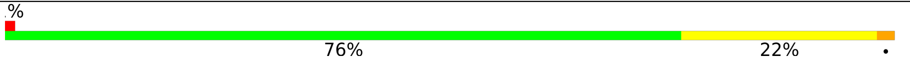
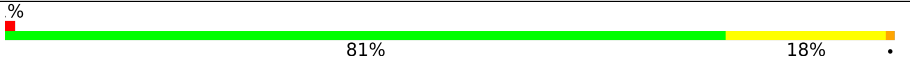
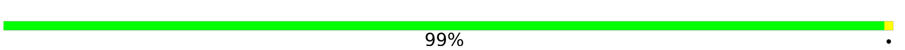
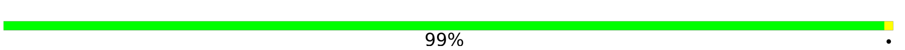
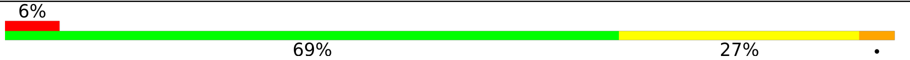
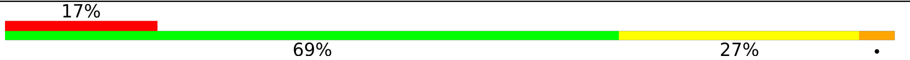
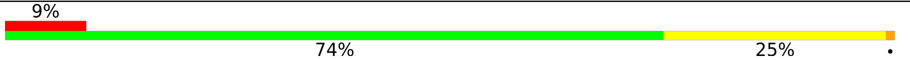
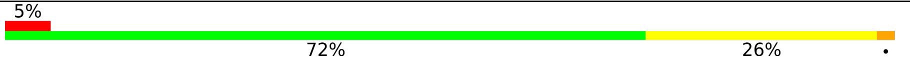
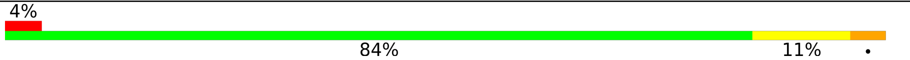
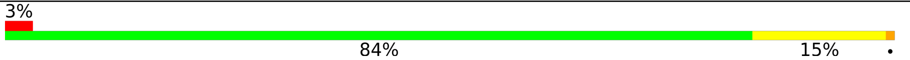
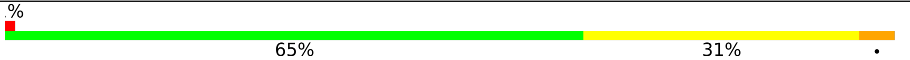
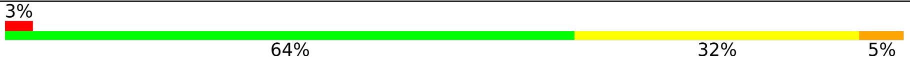
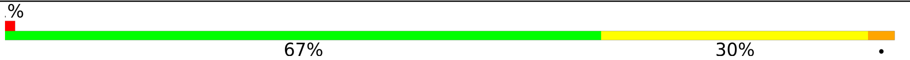
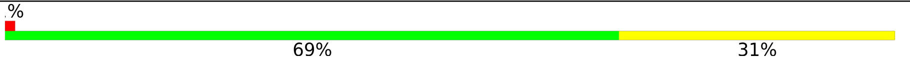
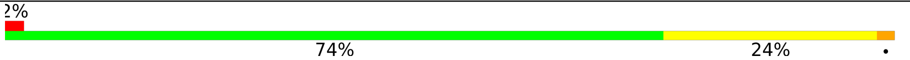
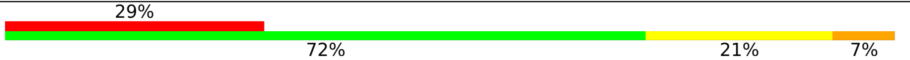
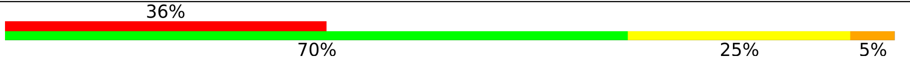
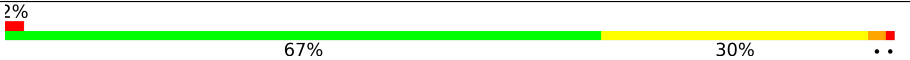
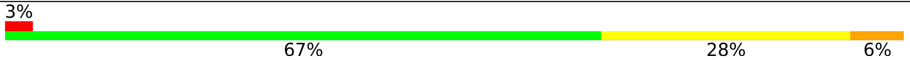
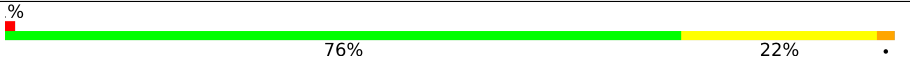
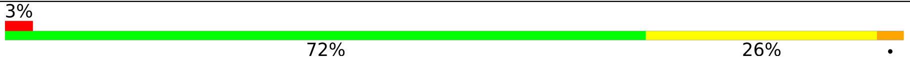
Mol	Chain	Length	Quality of chain
28	DF	208	
29	BG	181	
29	DG	181	
30	BH	167	
30	DH	167	
31	BJ	170	
31	DJ	170	
32	BK	140	
32	DK	140	
33	BN	138	
33	DN	138	
34	BO	122	
34	DO	122	
35	BP	146	
35	DP	146	
36	BQ	141	
36	DQ	141	
37	BR	117	
37	DR	117	
38	BS	99	
38	DS	99	
39	BT	138	
39	DT	138	
40	BU	117	
40	DU	117	

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Mol	Chain	Length	Quality of chain
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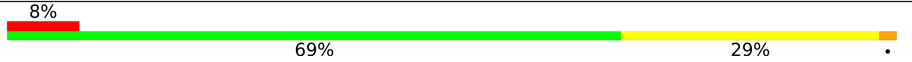
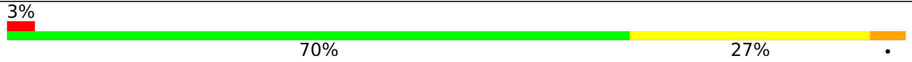
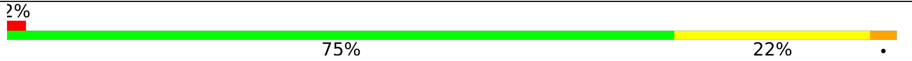
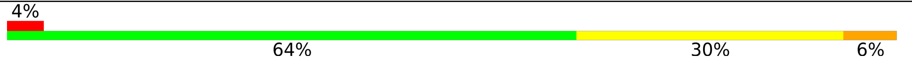
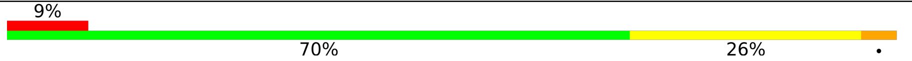
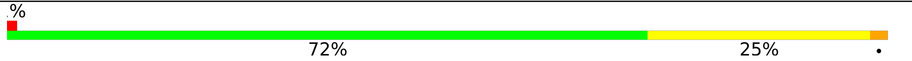
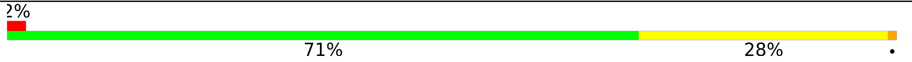
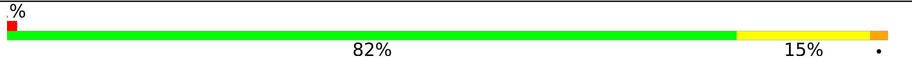
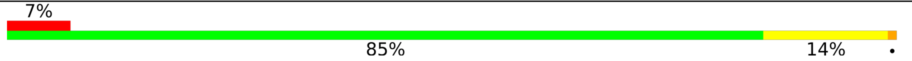
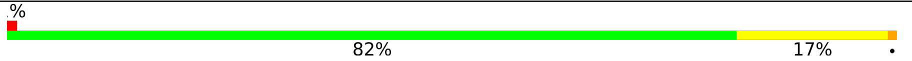
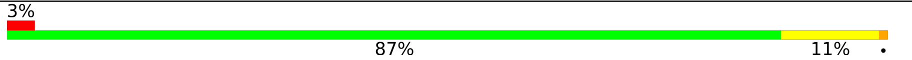
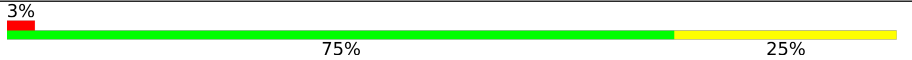
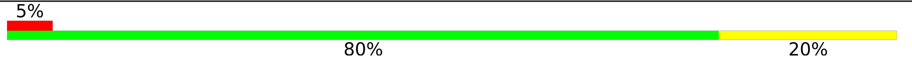
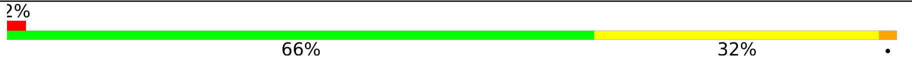
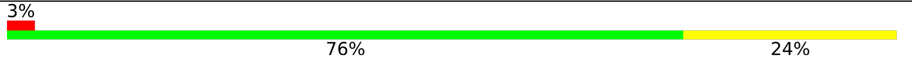
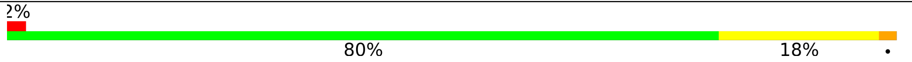
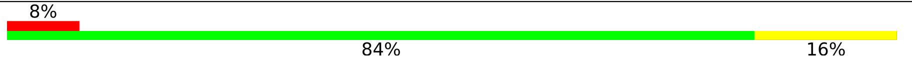
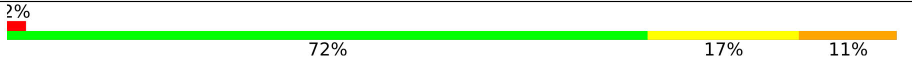
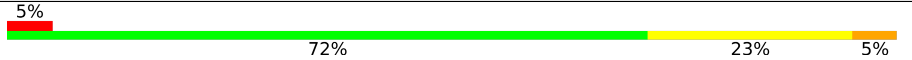
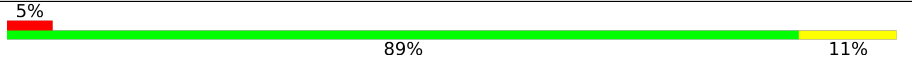
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	93	
43	DX	93	
44	BY	107	
44	DY	107	
45	BZ	185	
45	DZ	185	
46	B0	84	
46	D0	84	
47	B2	71	
47	D2	71	
48	B3	60	
48	D3	60	
49	B5	59	
49	D5	59	
50	B6	50	
50	D6	50	
51	B7	49	
51	D7	49	
52	B8	64	
52	D8	64	
53	B9	37	

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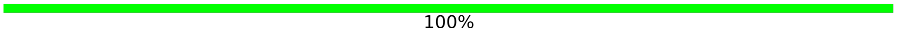
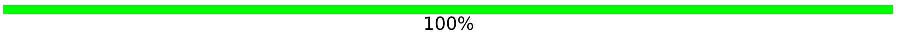
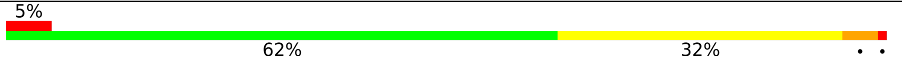
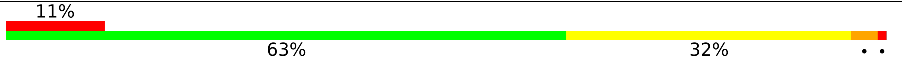
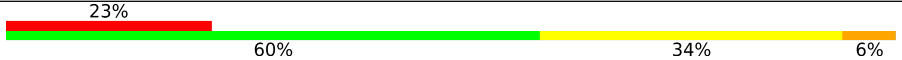
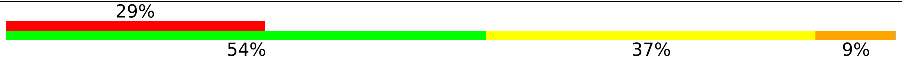
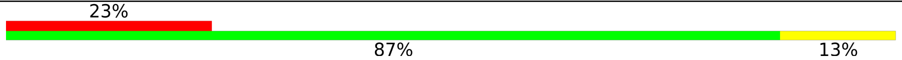
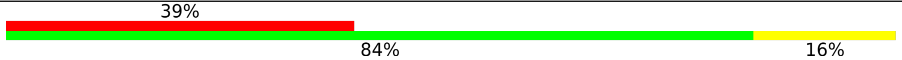
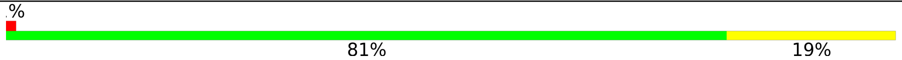
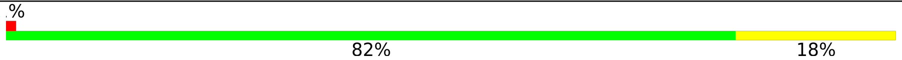
Mol	Chain	Length	Quality of chain
53	D9	37	
54	Bf	31	
54	Bg	31	
54	Df	31	
54	Dg	31	
55	Bh	30	
55	Dh	30	
56	B1	93	
56	D1	93	
57	B4	35	
57	D4	35	
58	Be	102	
58	De	102	
59	BA	2879	
59	DA	2879	
60	BB	119	
60	DB	119	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 308422 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 protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AB	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			
1	CB	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			
2	CC	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			
4	CE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	AI	127	Total C N O 1011 639 198 174	0	0	0
8	CI	127	Total C N O 1011 639 198 174	0	0	0

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	AJ	99	Total C N O S 802 504 157 140 1	0	0	0
9	CJ	99	Total C N O S 802 504 157 140 1	0	0	0

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	AL	125	Total C N O S 976 614 196 165 1	0	0	0
11	CL	125	Total C N O S 976 614 196 165 1	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	AM	125	Total C N O S 997 617 207 171 2	0	0	0
12	CM	125	Total C N O S 997 617 207 171 2	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	AP	84	Total C N O S 706 446 140 119 1	0	0	0
15	CP	84	Total C N O S 706 446 140 119 1	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	100	Total 835	C 534	N 156	O 143	S 2	0	0	0
16	CQ	100	Total 835	C 534	N 156	O 143	S 2	0	0	0

- Molecule 17 is a protein called 30S ribosomal protein S18.

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

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total 634	C 405	N 115	O 112	S 2	0	0	0
18	CS	79	Total 634	C 405	N 115	O 112	S 2	0	0	0

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	99	Total 762	C 469	N 162	O 129	S 2	0	0	0
19	CT	99	Total 762	C 469	N 162	O 129	S 2	0	0	0

- Molecule 20 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AY	687	Total 5380	C 3414	N 922	O 1024	S 20	0	0	0
20	CY	687	Total 5380	C 3414	N 922	O 1024	S 20	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	129	LYS	HIS	CONFLICT	UNP Q72I01

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Chain	Residue	Modelled	Actual	Comment	Reference
AY	226	ASN	HIS	CONFLICT	UNP Q72I01
CY	129	LYS	HIS	CONFLICT	UNP Q72I01
CY	226	ASN	HIS	CONFLICT	UNP Q72I01

- Molecule 21 is a RNA chain called ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AA	1511	Total 32474	C 14455	N 6015	O 10494	P 1510	0	0	0
21	CA	1511	Total 32474	C 14455	N 6015	O 10494	P 1510	0	0	0

- Molecule 22 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	77	Total 1635	C 732	N 291	O 536	P 76	0	0	0
22	CW	77	Total 1635	C 732	N 291	O 536	P 76	0	0	0

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AV	23	Total 503	C 227	N 106	O 148	P 22	0	0	0
23	CV	23	Total 503	C 227	N 106	O 148	P 22	0	0	0

- Molecule 24 is a protein called VIOMYCIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AU	6	Total 48	C 25	N 13	O 10	0	0	0
24	CU	6	Total 48	C 25	N 13	O 10	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L1.

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	20	VAL	ILE	CONFLICT	UNP Q72GV9
BC	28	ARG	HIS	CONFLICT	UNP Q72GV9
DC	20	VAL	ILE	CONFLICT	UNP Q72GV9
DC	28	ARG	HIS	CONFLICT	UNP Q72GV9

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	205	Total 1569	C 991	N 300	O 272	S 6	0	0	0
27	DE	205	Total 1569	C 991	N 300	O 272	S 6	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	208	Total 1628	C 1037	N 304	O 284	S 3	0	0	0
28	DF	208	Total 1628	C 1037	N 304	O 284	S 3	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	2	LYS	-	INSERTION	UNP Q72I05
BF	3	GLU	-	INSERTION	UNP Q72I05
BF	4	VAL	-	INSERTION	UNP Q72I05

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Chain	Residue	Modelled	Actual	Comment	Reference
BF	5	ALA	-	INSERTION	UNP Q72I05
BF	6	VAL	-	INSERTION	UNP Q72I05
DF	2	LYS	-	INSERTION	UNP Q72I05
DF	3	GLU	-	INSERTION	UNP Q72I05
DF	4	VAL	-	INSERTION	UNP Q72I05
DF	5	ALA	-	INSERTION	UNP Q72I05
DF	6	VAL	-	INSERTION	UNP Q72I05

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	5	VAL	LEU	CONFLICT	UNP Q72I16
DG	5	VAL	LEU	CONFLICT	UNP Q72I16

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	167	Total 1274	C 806	N 238	O 229	S 1	0	0	0
30	DH	167	Total 1274	C 806	N 238	O 229	S 1	0	0	0

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L10.

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

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	BK	140	1035	659	183	188	5	0	0	0
32	DK	140	1035	659	183	188	5	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	BN	138	1104	712	206	182	4	0	0	0
33	DN	138	1104	712	206	182	4	0	0	0

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	69	ILE	VAL	CONFLICT	UNP Q72I14
DO	69	ILE	VAL	CONFLICT	UNP Q72I14

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	32	TYR	PHE	CONFLICT	UNP Q72I11
DQ	32	TYR	PHE	CONFLICT	UNP Q72I11

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
38	BS	99	775	488	155	132	0	0	0
38	DS	99	775	488	155	132	0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	BT	138	1147	713	235	198	1	0	0	0
39	DT	138	1147	713	235	198	1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	123	GLN	LYS	CONFLICT	UNP Q72JU9
BT	135	ALA	VAL	CONFLICT	UNP Q72JU9
DT	123	GLN	LYS	CONFLICT	UNP Q72JU9
DT	135	ALA	VAL	CONFLICT	UNP Q72JU9

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	BU	117	964	610	202	151	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	DU	117	964	610	202	151	1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	BW	113	900	566	177	155	2	0	0	0
42	DW	113	900	566	177	155	2	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
43	BX	93	734	477	132	125	0	0	0
43	DX	93	734	477	132	125	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	BY	107	818	524	155	134	5	0	0	0
44	DY	107	818	524	155	134	5	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BZ	185	1473	939	262	270	2	0	0	0
45	DZ	185	1473	939	262	270	2	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L27.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B0	11	ARG	LYS	CONFLICT	UNP Q72HR3
D0	11	ARG	LYS	CONFLICT	UNP Q72HR3

- Molecule 47 is a protein called 50S ribosomal protein L29.

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

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B3	60	Total 477	C 303	N 91	O 82	S 1	0	0	0
48	D3	60	Total 477	C 303	N 91	O 82	S 1	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	29	THR	ILE	CONFLICT	UNP P62652
D5	29	THR	ILE	CONFLICT	UNP P62652

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	B6	50	433	270	88	71	4	0	0	0
50	D6	50	433	270	88	71	4	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	B7	49	430	263	108	57	2	0	0	0
51	D7	49	430	263	108	57	2	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	B8	64	517	331	102	82	2	0	0	0
52	D8	64	517	331	102	82	2	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L36.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
54	Bf	31	156	93	31	32	0	0	0
54	Bg	31	156	93	31	32	0	0	0
54	Df	31	156	93	31	32	0	0	0
54	Dg	31	156	93	31	32	0	0	0

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L7/L12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
55	Bh	30	Total C N O 151 90 30 31	0	0	0
55	Dh	30	Total C N O 151 90 30 31	0	0	0

- Molecule 56 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
56	B1	93	Total C N O S 732 460 145 126 1	0	0	0
56	D1	93	Total C N O S 732 460 145 126 1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	LYS	ARG	CONFLICT	UNP Q72G84
D1	81	LYS	ARG	CONFLICT	UNP Q72G84

- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
57	B4	35	Total C N O S 271 174 44 50 3	0	0	0
57	D4	35	Total C N O S 271 174 44 50 3	0	0	0

- Molecule 58 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
58	Be	102	Total C N O 686 430 119 137	0	0	0
58	De	102	Total C N O 686 430 119 137	0	0	0

- Molecule 59 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
59	BA	2879	Total C N O P 61997 27594 11582 19943 2878	0	0	0

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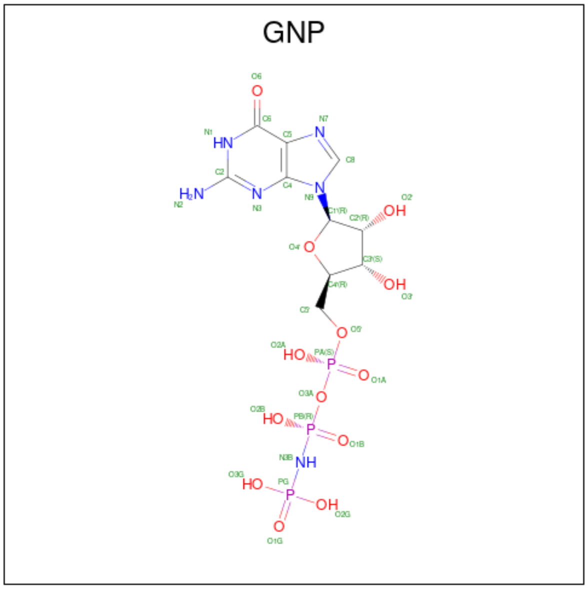
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
59	DA	2879	61997	27594	11582	19943	2878	0	0	0

- Molecule 60 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 61 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
61	AY	1	32	10	6	13	3	0	0
61	CY	1	32	10	6	13	3	0	0

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
62	AY	1	1	1	0	0

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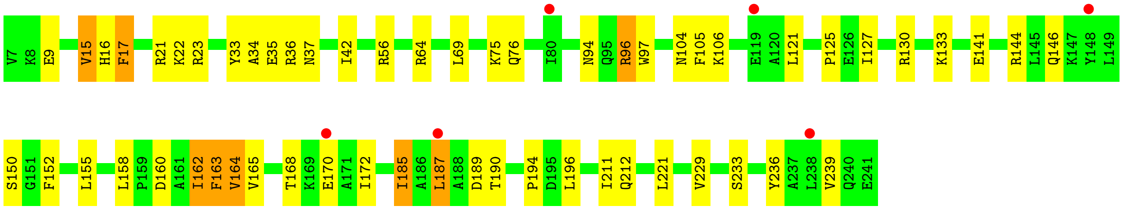
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
62	CY	1	1	1	0	0

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.

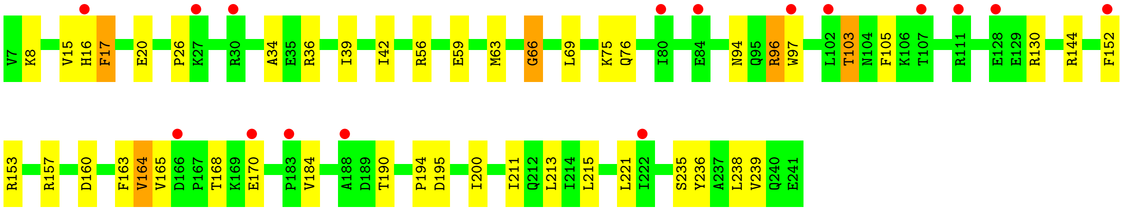
- Molecule 1: 30S ribosomal protein S2

Chain AB:



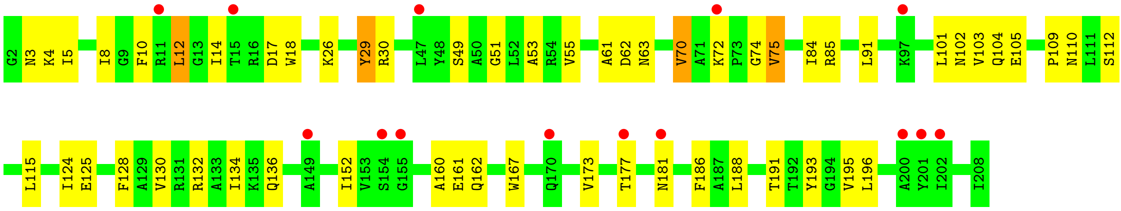
- Molecule 1: 30S ribosomal protein S2

Chain CB:



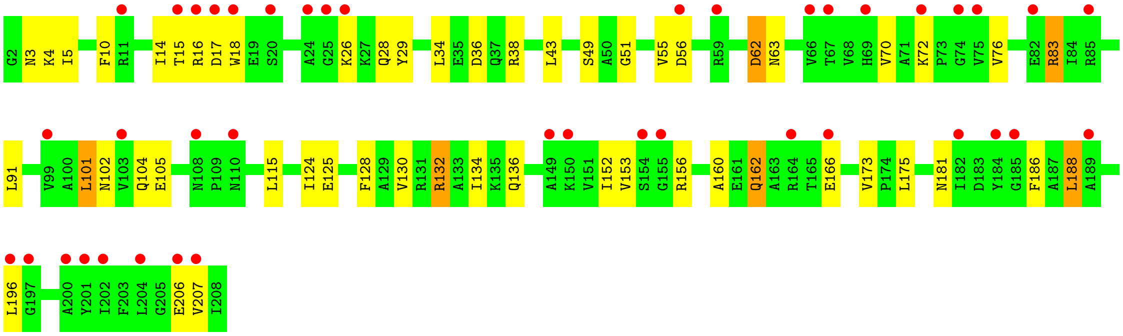
- Molecule 2: 30S ribosomal protein S3

Chain AC:



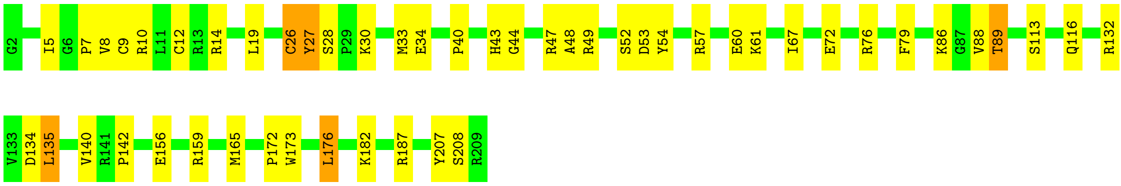
- Molecule 2: 30S ribosomal protein S3

Chain CC:



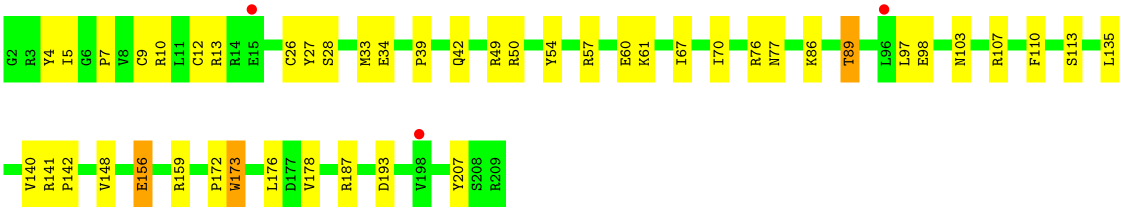
- Molecule 3: 30S ribosomal protein S4

Chain AD:



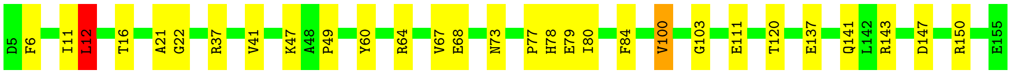
- Molecule 3: 30S ribosomal protein S4

Chain CD:



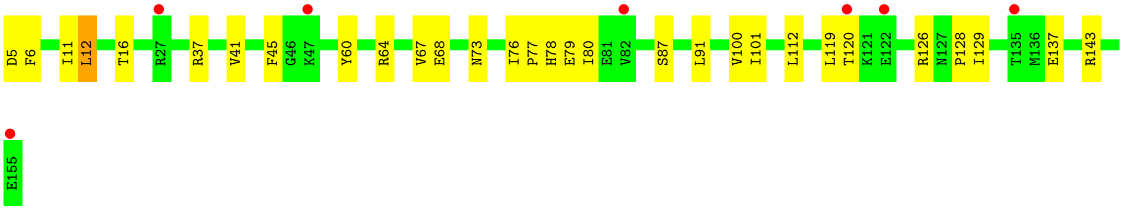
- Molecule 4: 30S ribosomal protein S5

Chain AE:

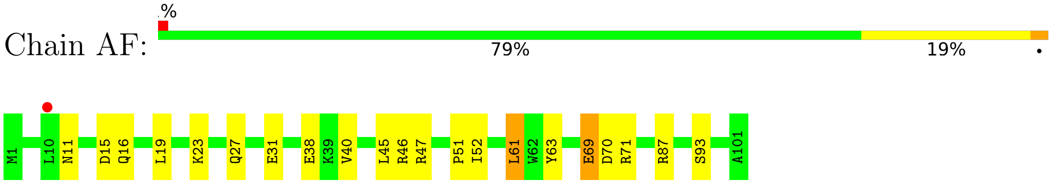


- Molecule 4: 30S ribosomal protein S5

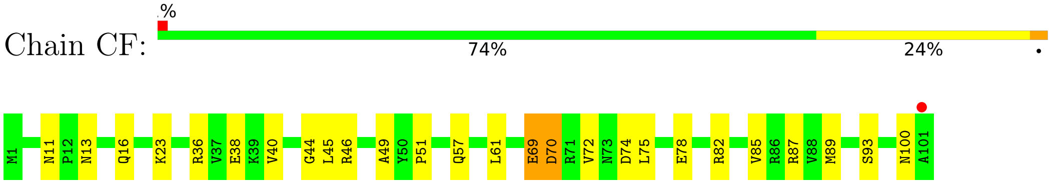
Chain CE:



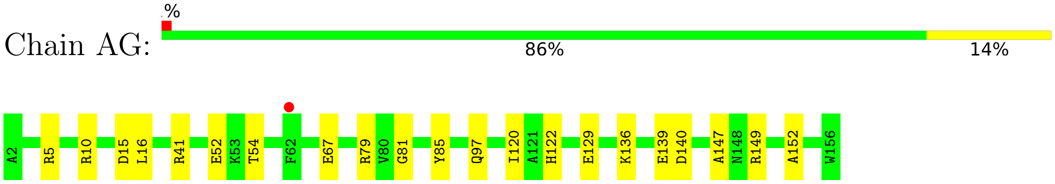
- Molecule 5: 30S ribosomal protein S6



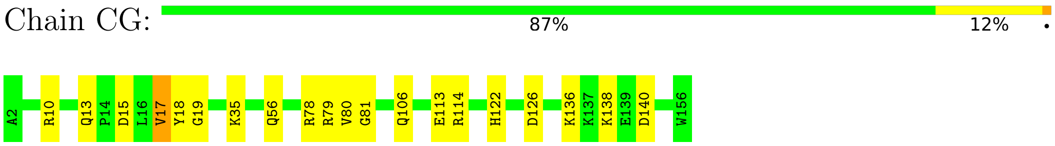
- Molecule 5: 30S ribosomal protein S6



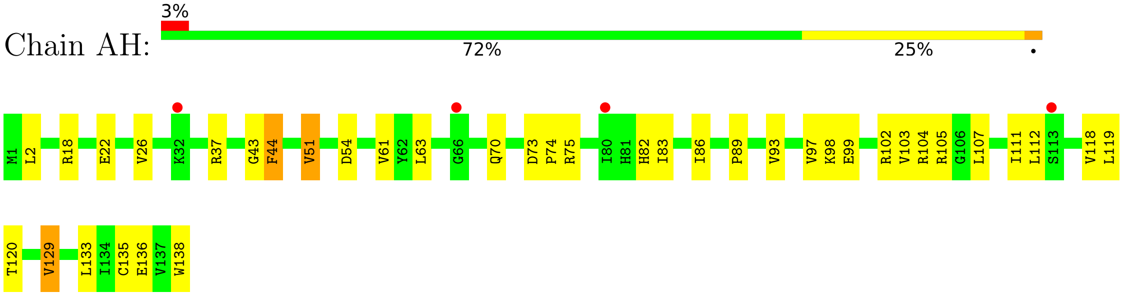
- Molecule 6: 30S ribosomal protein S7



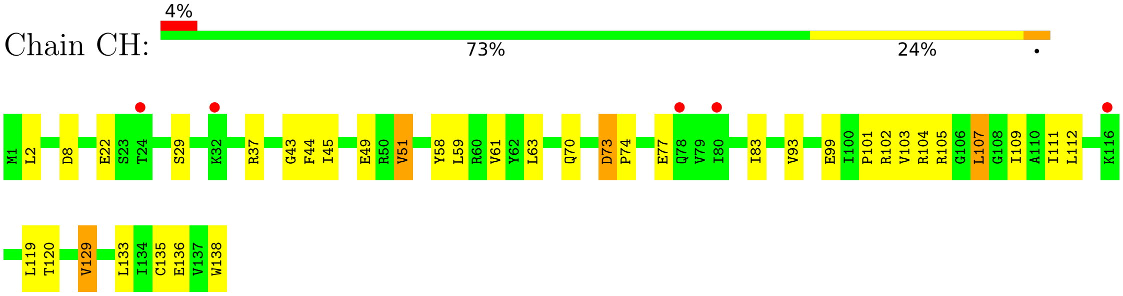
- Molecule 6: 30S ribosomal protein S7



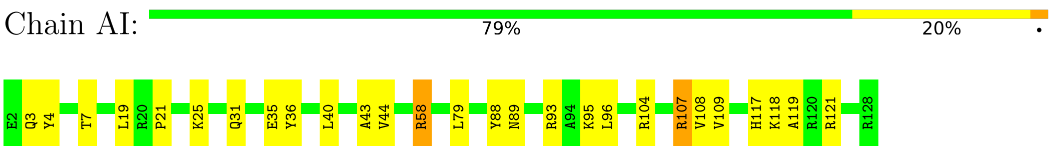
- Molecule 7: 30S ribosomal protein S8



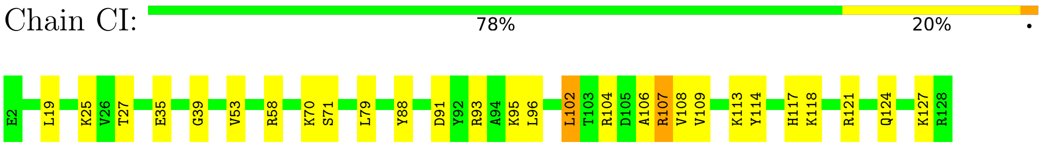
- Molecule 7: 30S ribosomal protein S8



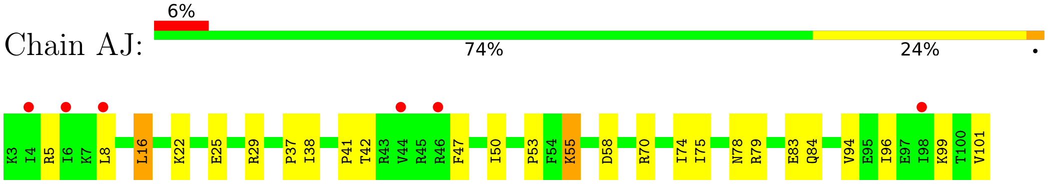
- Molecule 8: 30S ribosomal protein S9



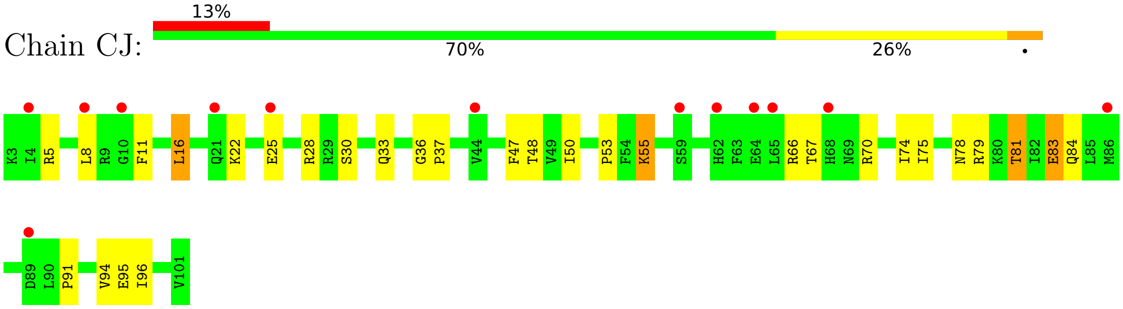
- Molecule 8: 30S ribosomal protein S9



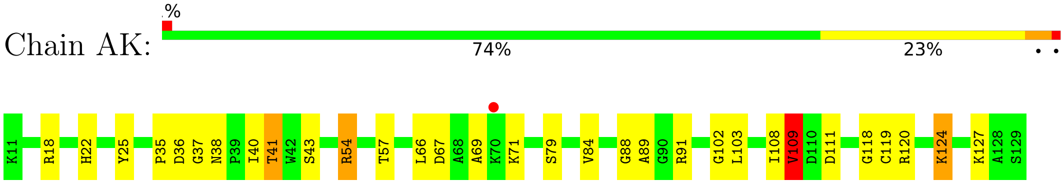
- Molecule 9: 30S ribosomal protein S10



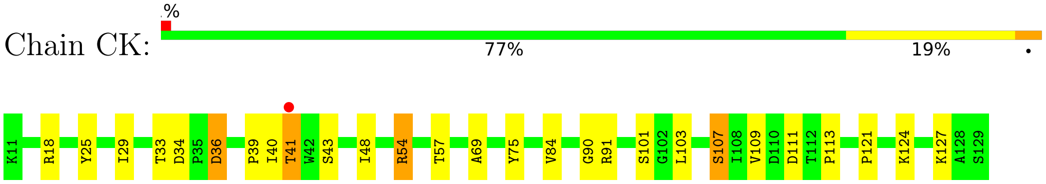
- Molecule 9: 30S ribosomal protein S10



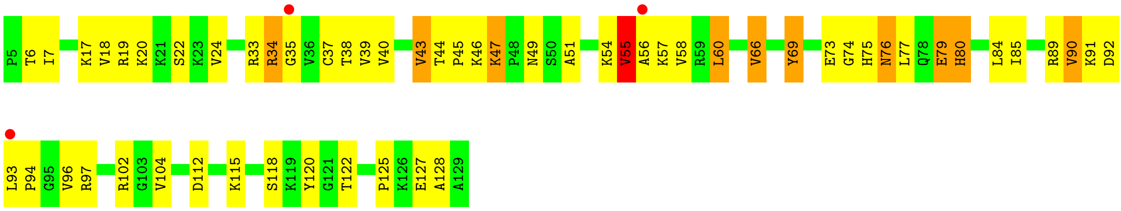
- Molecule 10: 30S ribosomal protein S11



- Molecule 10: 30S ribosomal protein S11

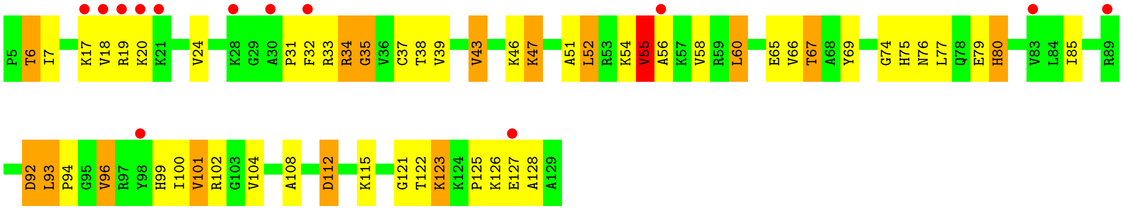


- Molecule 11: 30S ribosomal protein S12



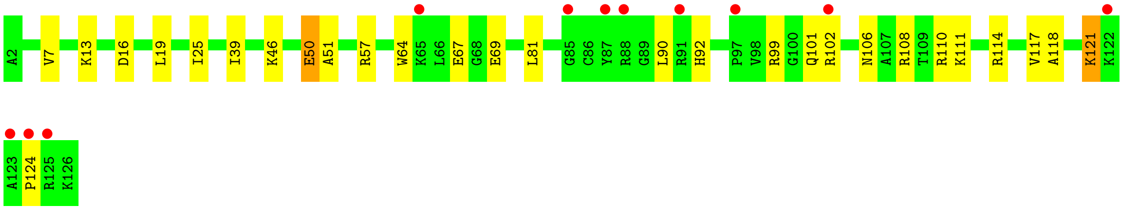
- Molecule 11: 30S ribosomal protein S12

Chain CL:



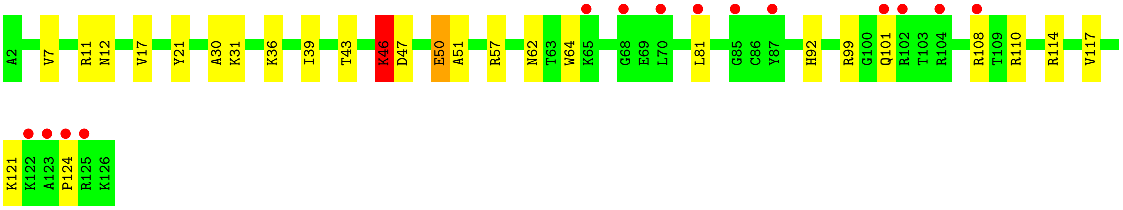
- Molecule 12: 30S ribosomal protein S13

Chain AM:



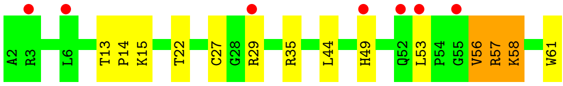
- Molecule 12: 30S ribosomal protein S13

Chain CM:



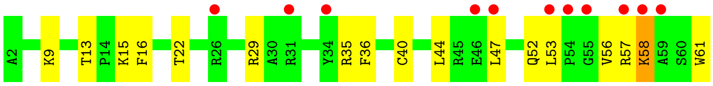
- Molecule 13: 30S ribosomal protein S14 type Z

Chain AN:



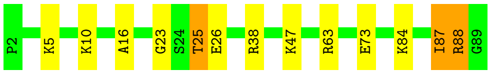
- Molecule 13: 30S ribosomal protein S14 type Z

Chain CN:



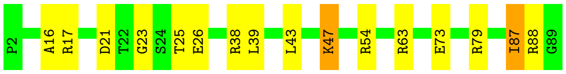
- Molecule 14: 30S ribosomal protein S15

Chain AO:



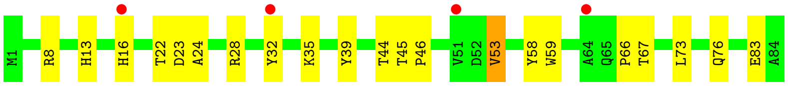
- Molecule 14: 30S ribosomal protein S15

Chain CO:



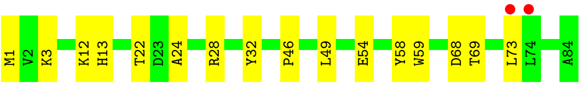
- Molecule 15: 30S ribosomal protein S16

Chain AP:



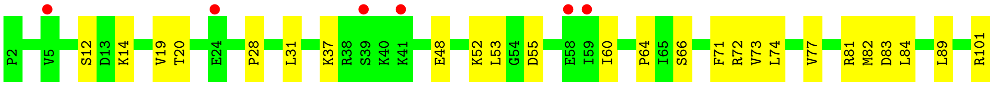
- Molecule 15: 30S ribosomal protein S16

Chain CP:



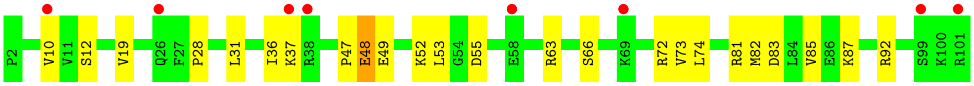
- Molecule 16: 30S ribosomal protein S17

Chain AQ:



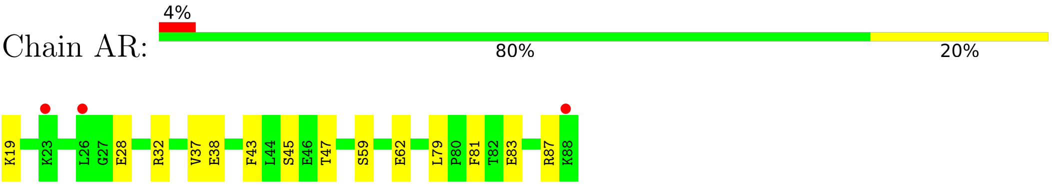
- Molecule 16: 30S ribosomal protein S17

Chain CQ:



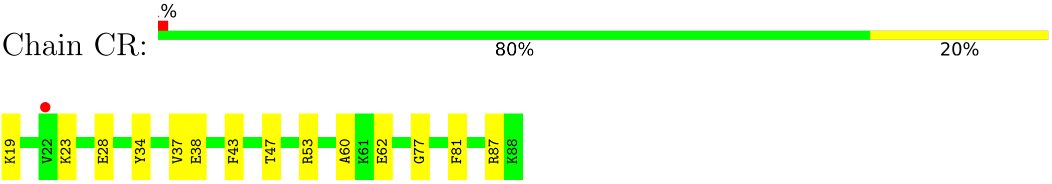
- Molecule 17: 30S ribosomal protein S18

Chain AR:



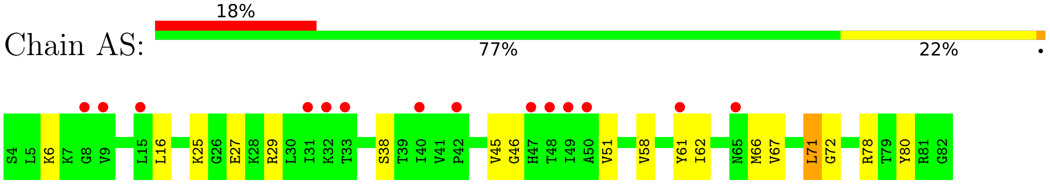
- Molecule 17: 30S ribosomal protein S18

Chain CR:



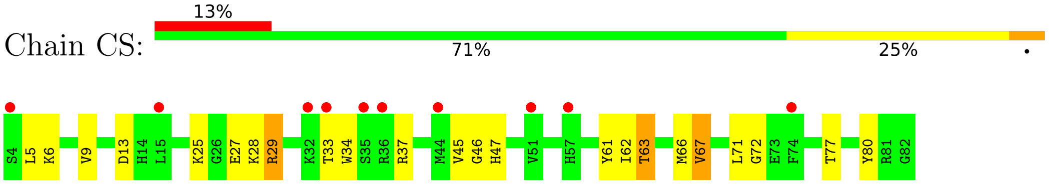
- Molecule 18: 30S ribosomal protein S19

Chain AS:



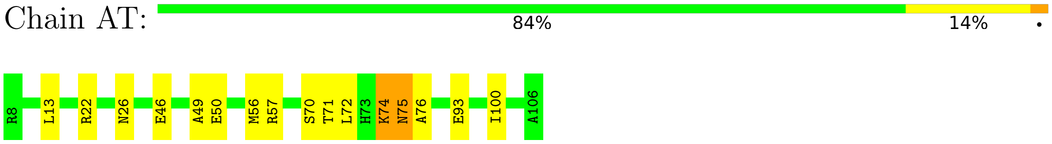
- Molecule 18: 30S ribosomal protein S19

Chain CS:



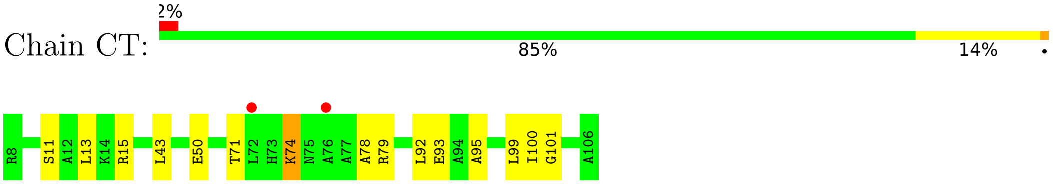
- Molecule 19: 30S ribosomal protein S20

Chain AT:



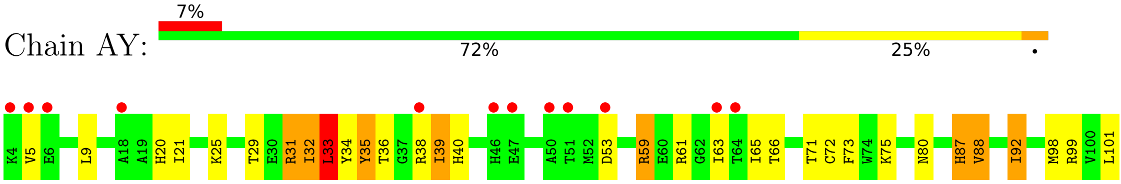
- Molecule 19: 30S ribosomal protein S20

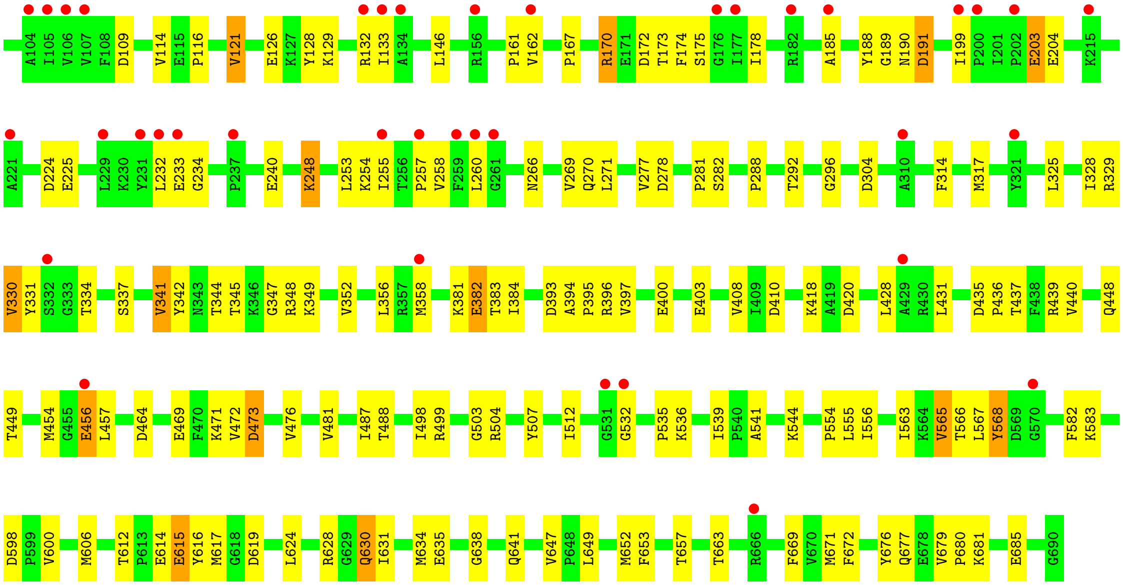
Chain CT:



- Molecule 20: Elongation factor G

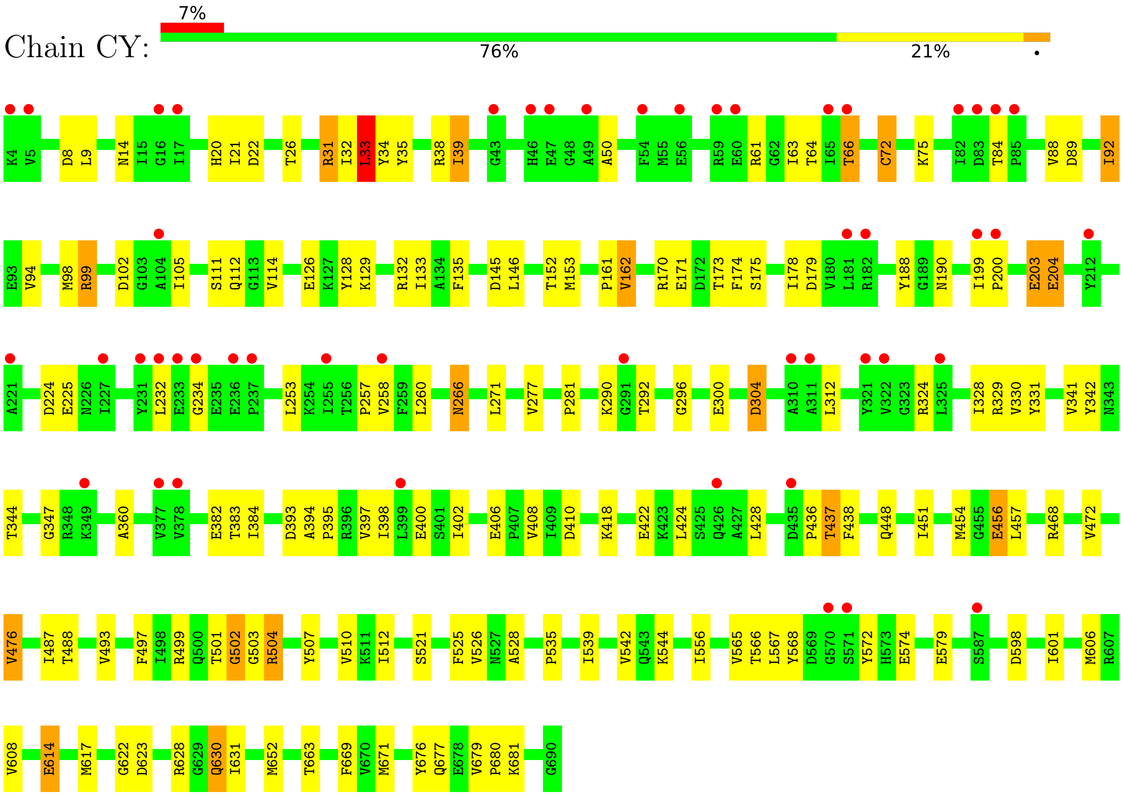
Chain AY:





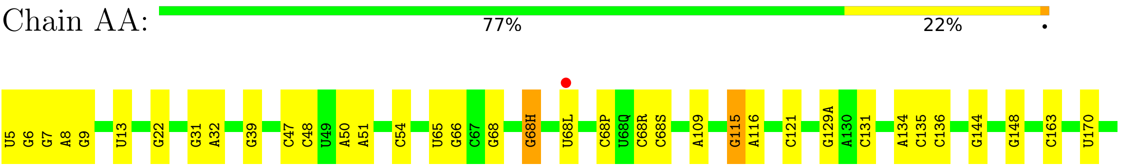
- Molecule 20: Elongation factor G

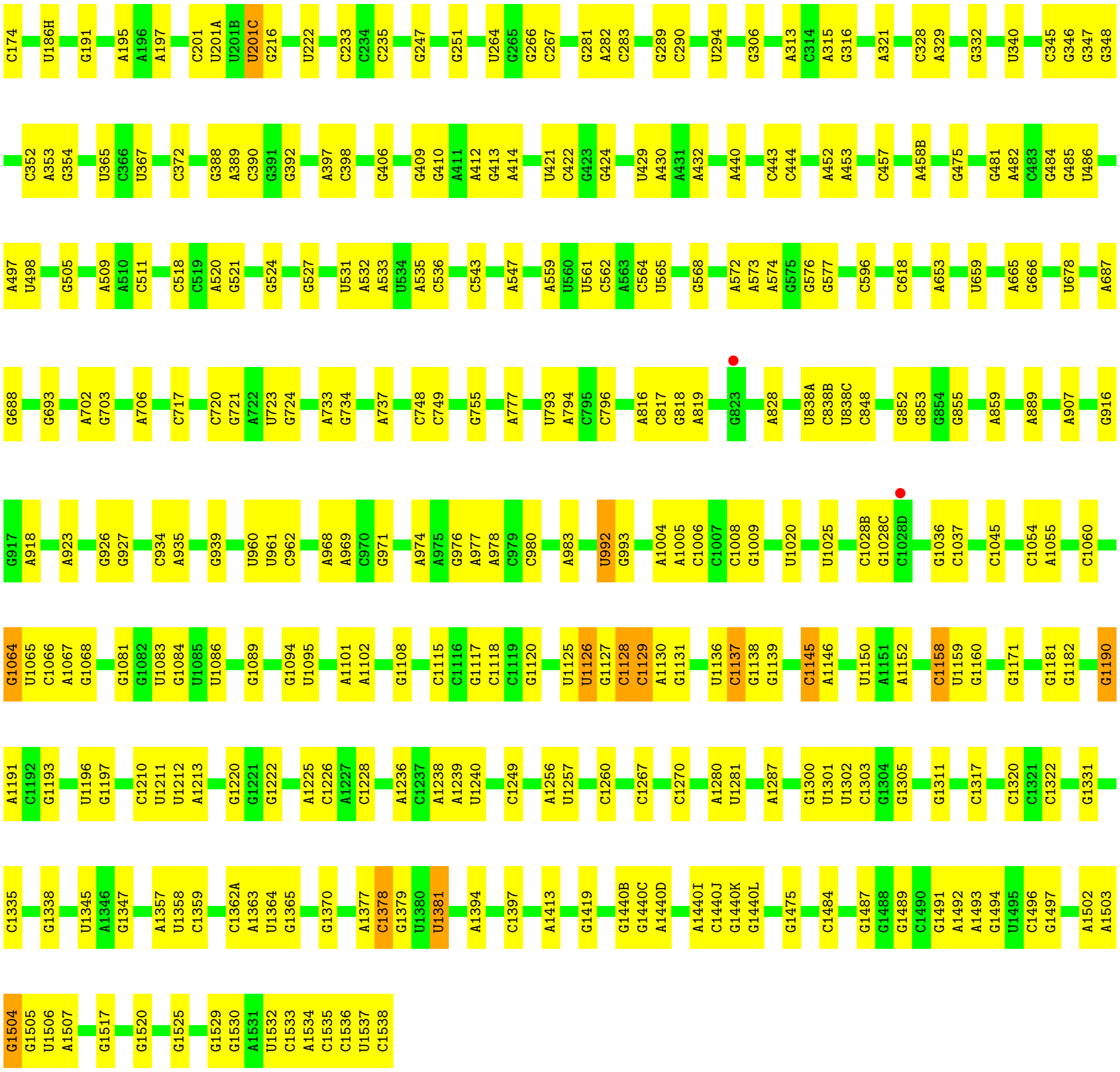
Chain CY:



- Molecule 21: ribosomal RNA 16S

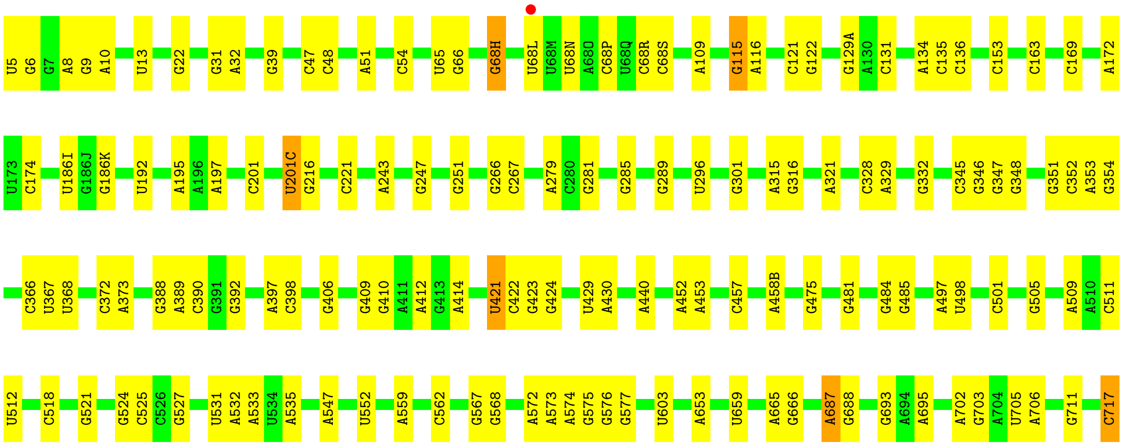
Chain AA:

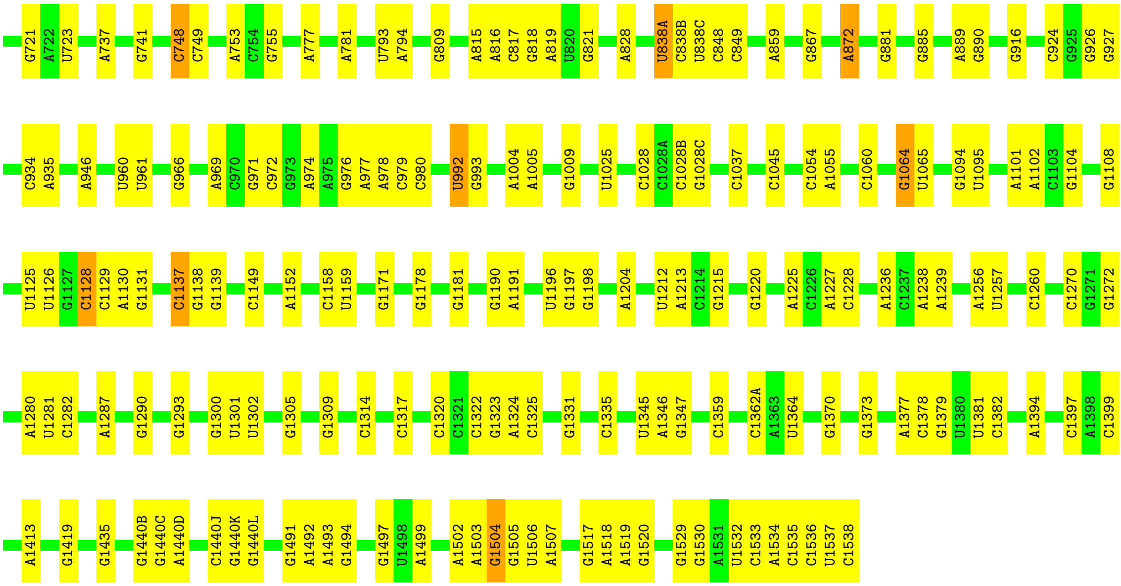




- Molecule 21: ribosomal RNA 16S

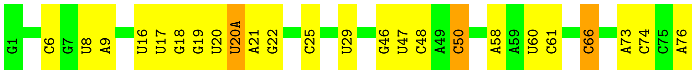
Chain CA:





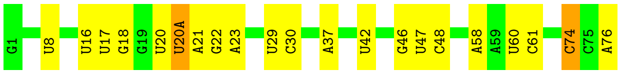
- Molecule 22: transfer RNA

Chain AW:



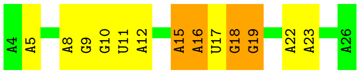
- Molecule 22: transfer RNA

Chain CW:



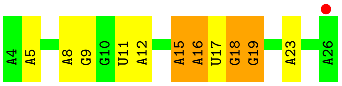
- Molecule 23: messenger RNA

Chain AV:



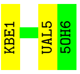
- Molecule 23: messenger RNA

Chain CV:



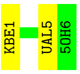
- Molecule 24: VIOMYCIN

Chain AU:



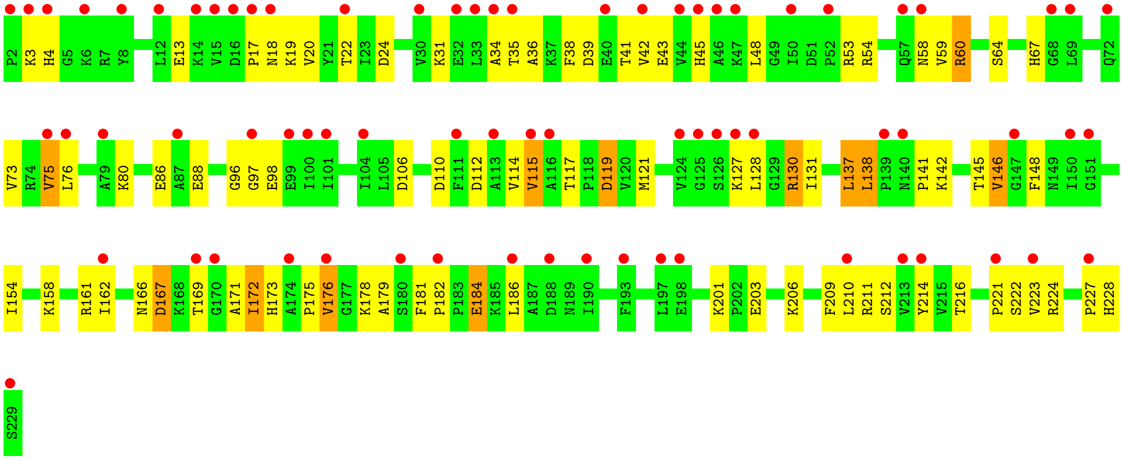
• Molecule 24: VIOMYCIN

Chain CU:



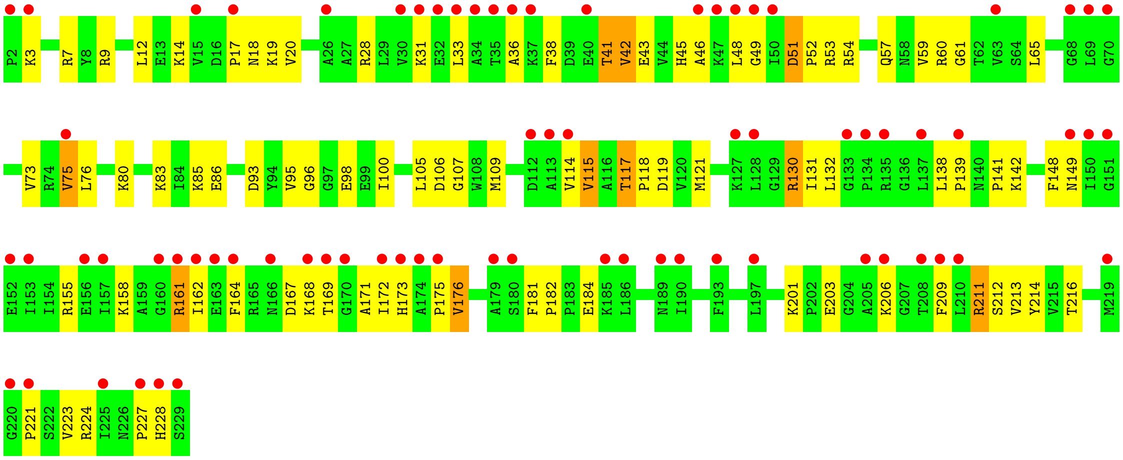
• Molecule 25: 50S ribosomal protein L1

Chain BC:



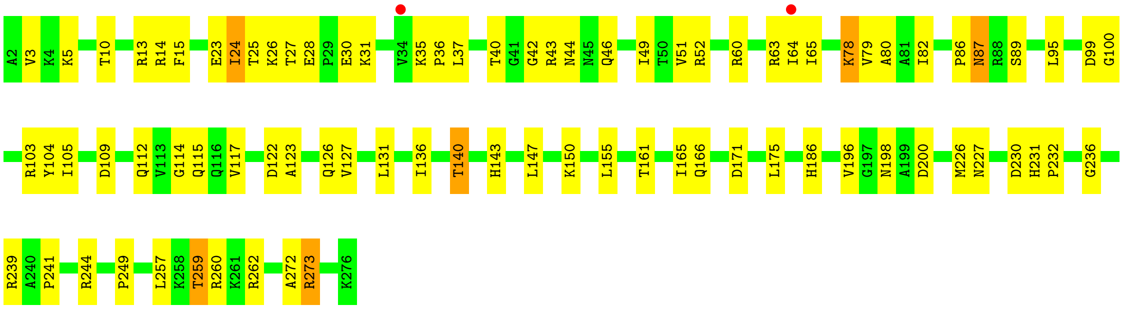
• Molecule 25: 50S ribosomal protein L1

Chain DC:



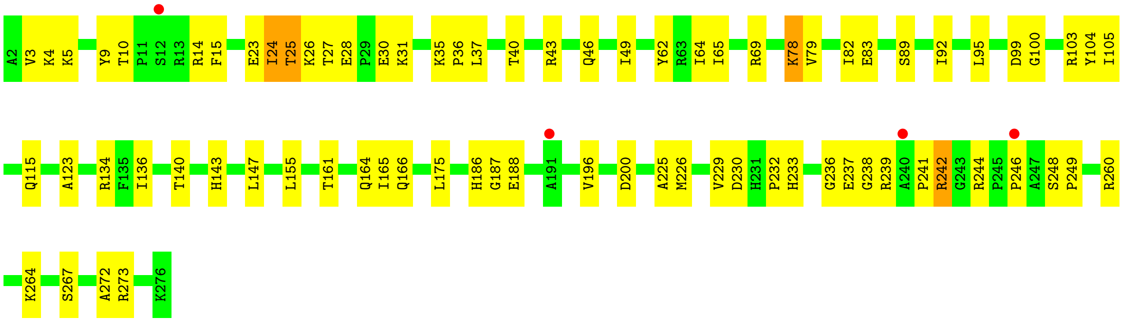
• Molecule 26: 50S ribosomal protein L2

Chain BD:



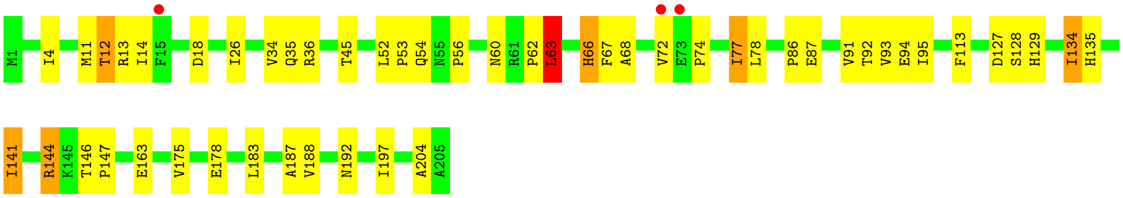
- Molecule 26: 50S ribosomal protein L2

Chain DD:



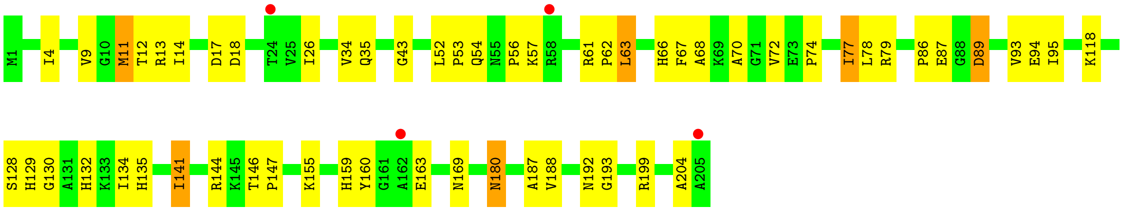
- Molecule 27: 50S ribosomal protein L3

Chain BE:



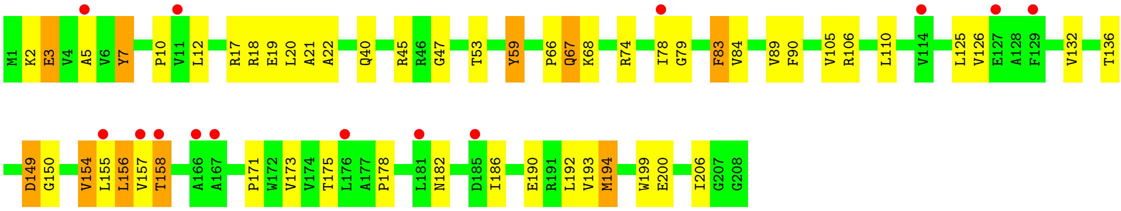
- Molecule 27: 50S ribosomal protein L3

Chain DE:



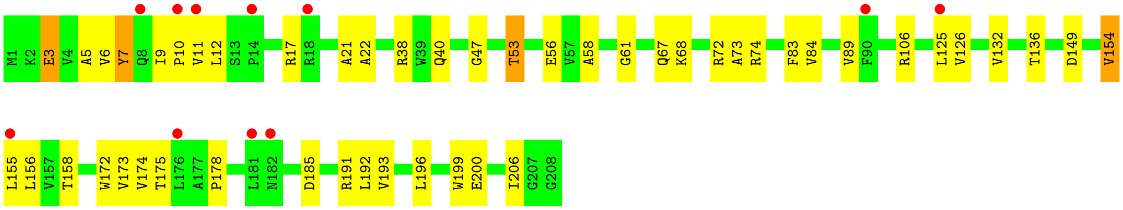
- Molecule 28: 50S ribosomal protein L4

Chain BF:



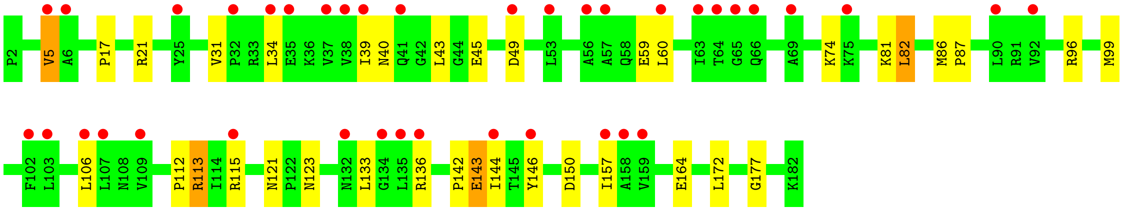
- Molecule 28: 50S ribosomal protein L4

Chain DF:



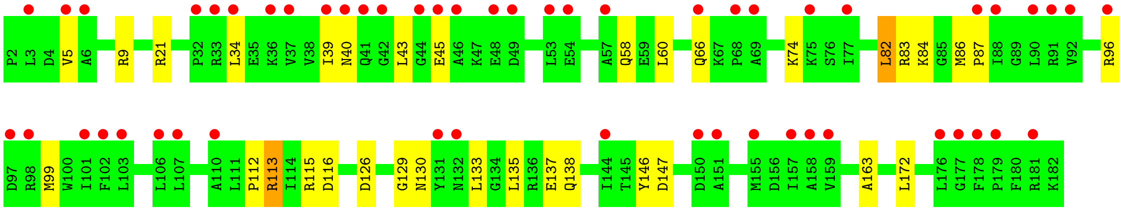
- Molecule 29: 50S ribosomal protein L5

Chain BG:



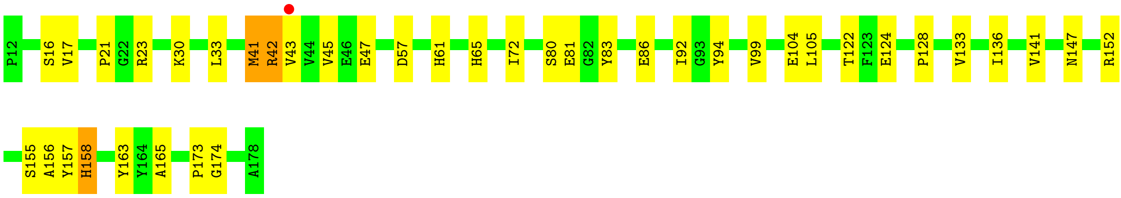
- Molecule 29: 50S ribosomal protein L5

Chain DG:



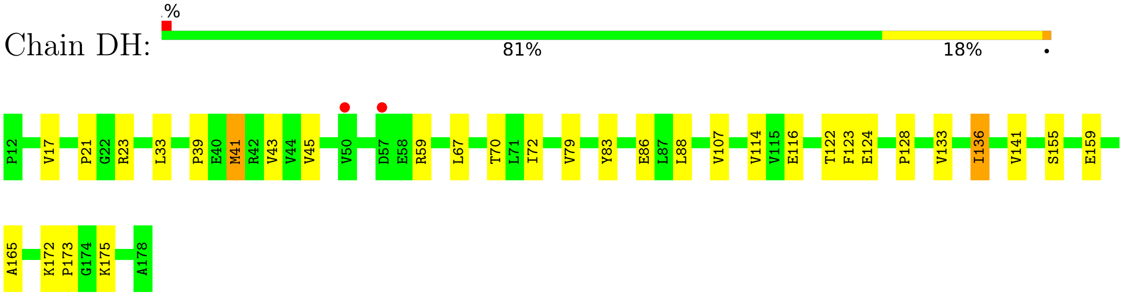
- Molecule 30: 50S ribosomal protein L6

Chain BH:



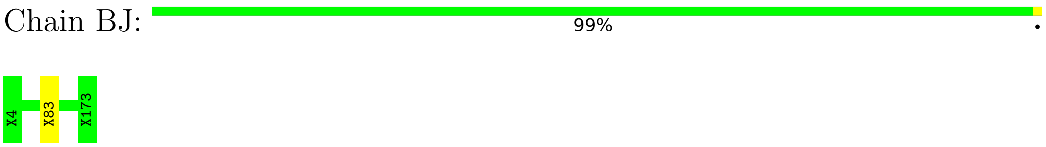
- Molecule 30: 50S ribosomal protein L6

Chain DH:



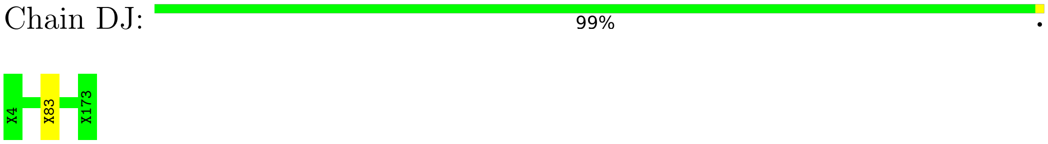
- Molecule 31: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



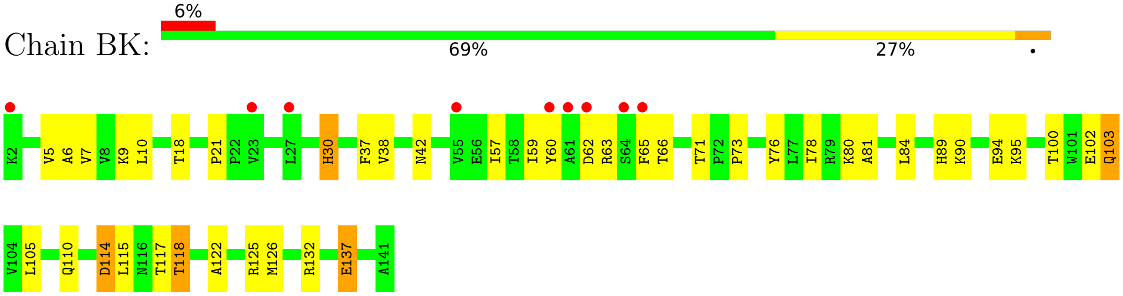
- Molecule 31: 50S RIBOSOMAL PROTEIN L10

Chain DJ:



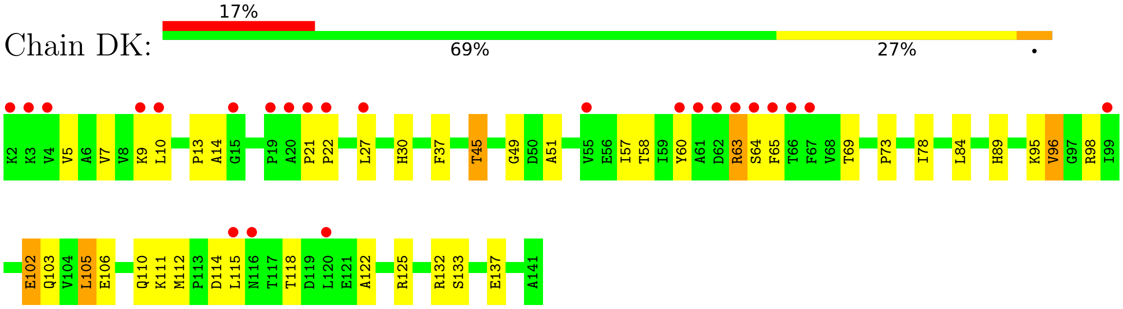
- Molecule 32: 50S ribosomal protein L11

Chain BK:



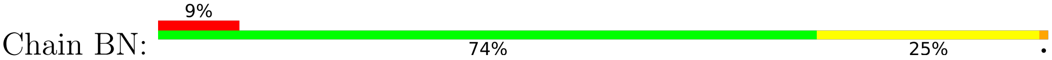
- Molecule 32: 50S ribosomal protein L11

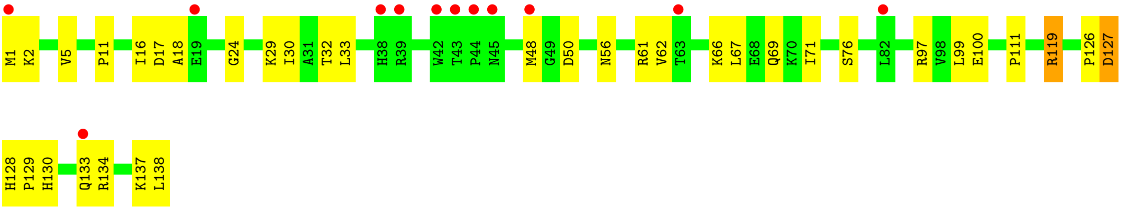
Chain DK:



- Molecule 33: 50S ribosomal protein L13

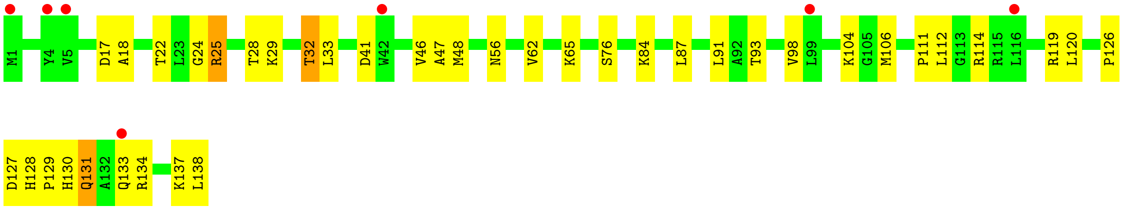
Chain BN:





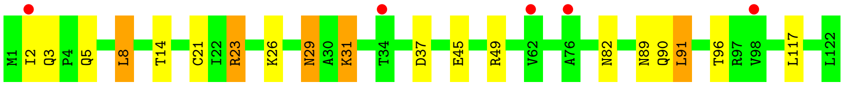
- Molecule 33: 50S ribosomal protein L13

Chain DN:



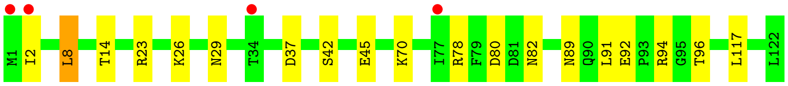
- Molecule 34: 50S ribosomal protein L14

Chain BO:



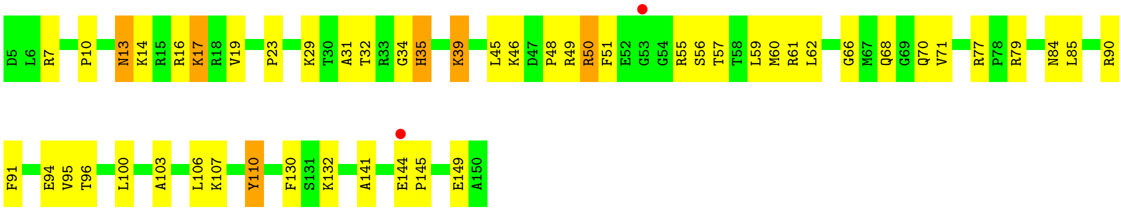
- Molecule 34: 50S ribosomal protein L14

Chain DO:



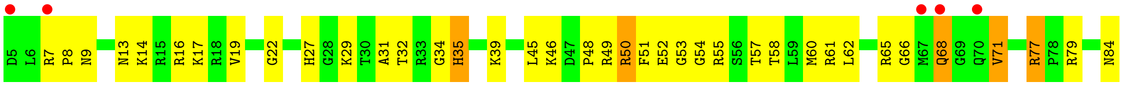
- Molecule 35: 50S ribosomal protein L15

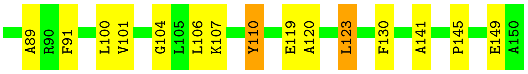
Chain BP:



- Molecule 35: 50S ribosomal protein L15

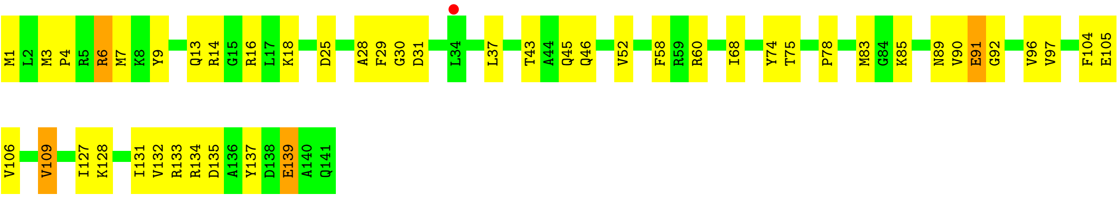
Chain DP:





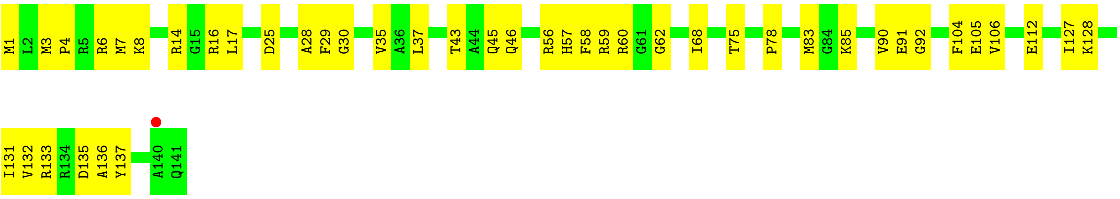
- Molecule 36: 50S ribosomal protein L16

Chain BQ:



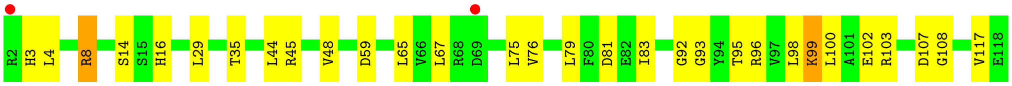
- Molecule 36: 50S ribosomal protein L16

Chain DQ:



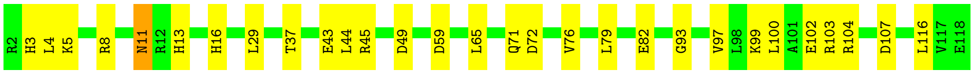
- Molecule 37: 50S ribosomal protein L17

Chain BR:



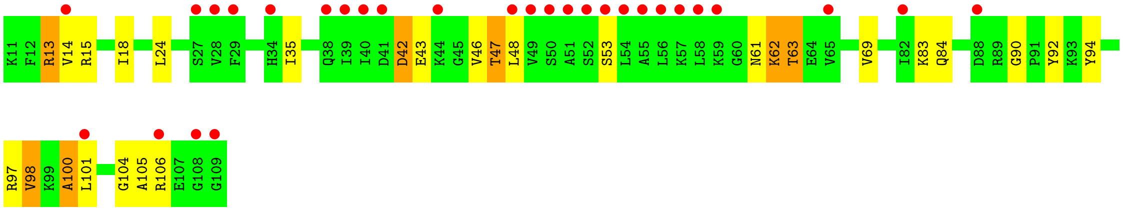
- Molecule 37: 50S ribosomal protein L17

Chain DR:

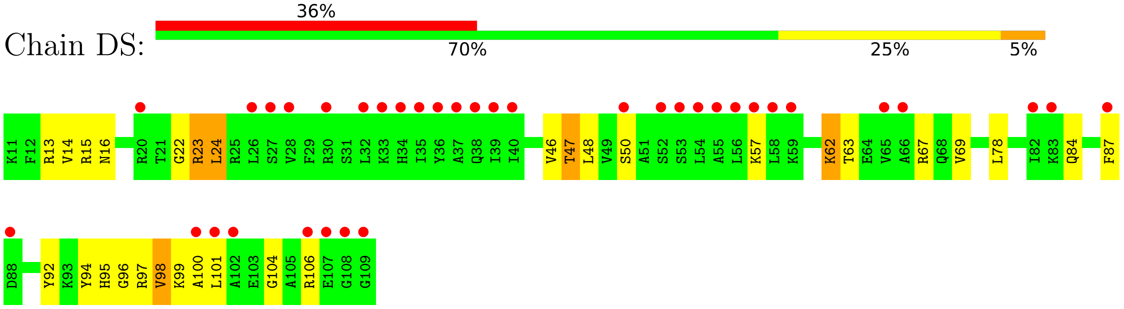


- Molecule 38: 50S ribosomal protein L18

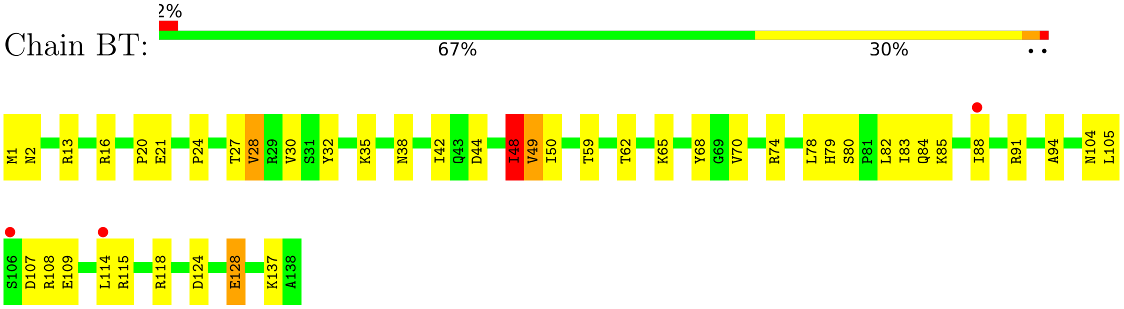
Chain BS:



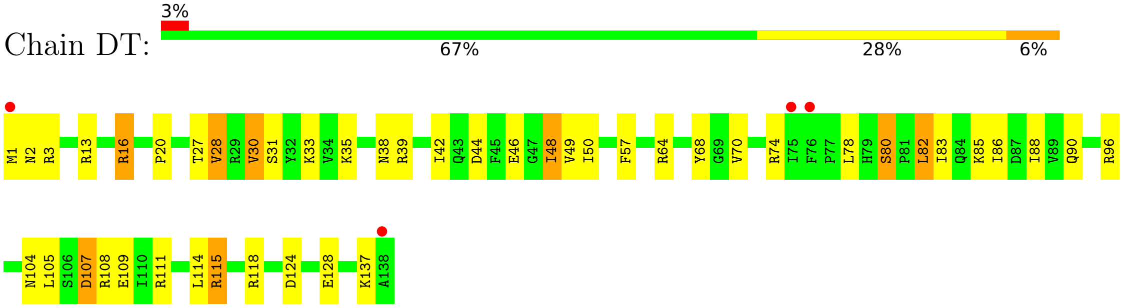
- Molecule 38: 50S ribosomal protein L18



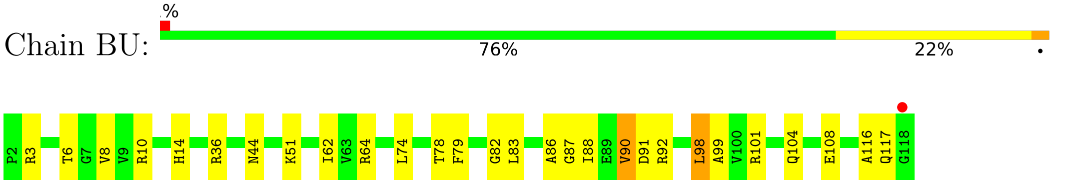
- Molecule 39: 50S ribosomal protein L19



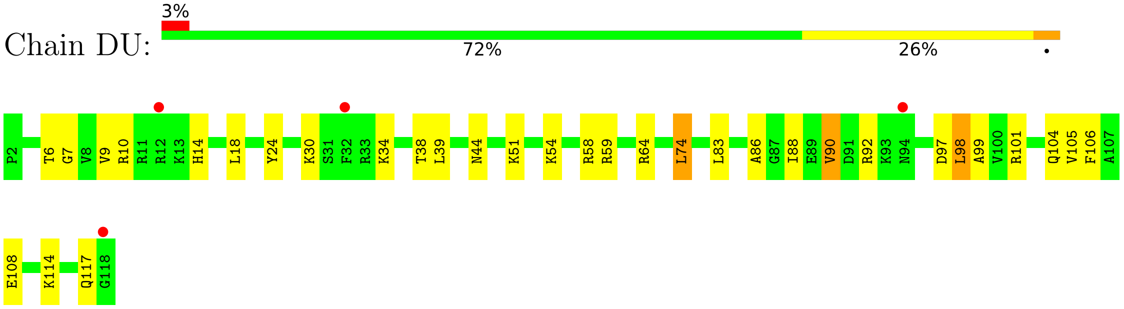
- Molecule 39: 50S ribosomal protein L19



- Molecule 40: 50S ribosomal protein L20

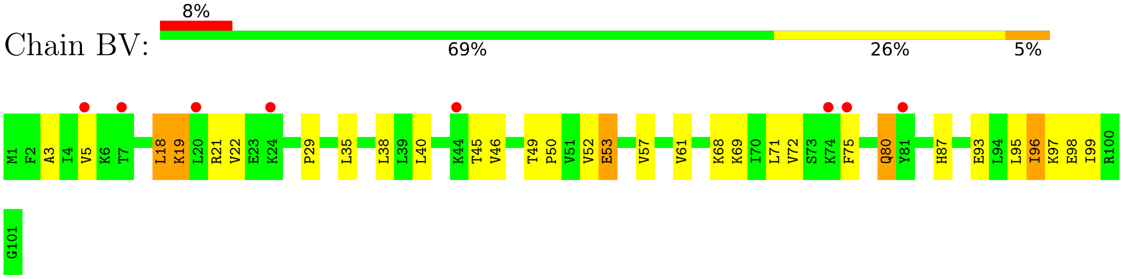


- Molecule 40: 50S ribosomal protein L20



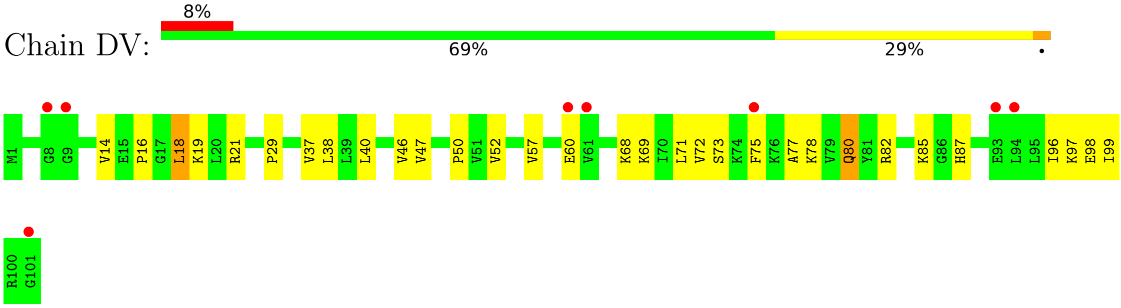
- Molecule 41: 50S ribosomal protein L21

Chain BV:



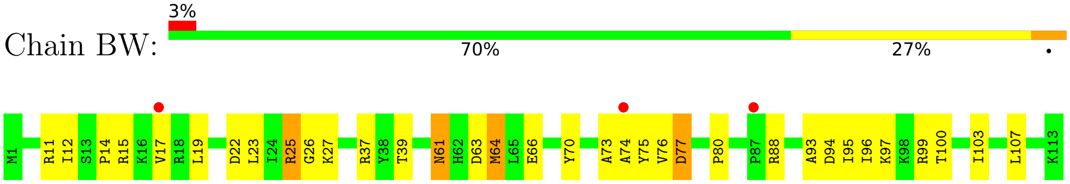
- Molecule 41: 50S ribosomal protein L21

Chain DV:



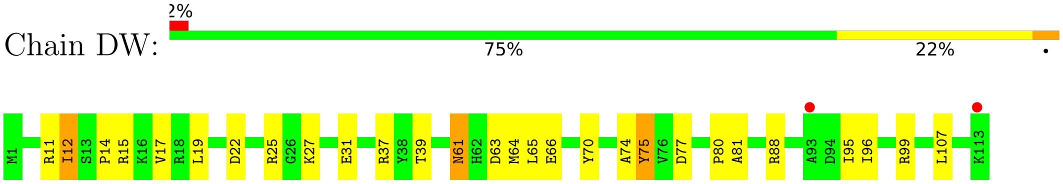
- Molecule 42: 50S ribosomal protein L22

Chain BW:



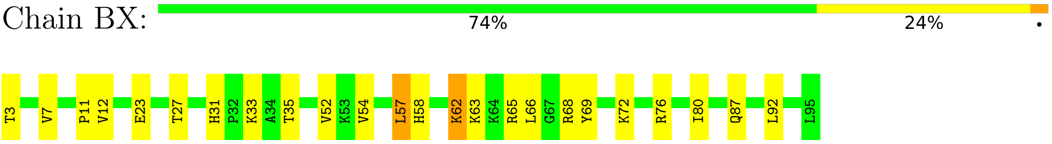
- Molecule 42: 50S ribosomal protein L22

Chain DW:



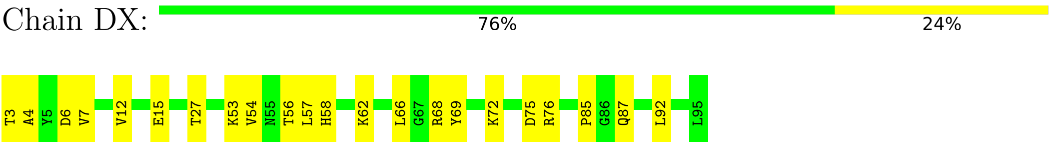
- Molecule 43: 50S ribosomal protein L23

Chain BX:



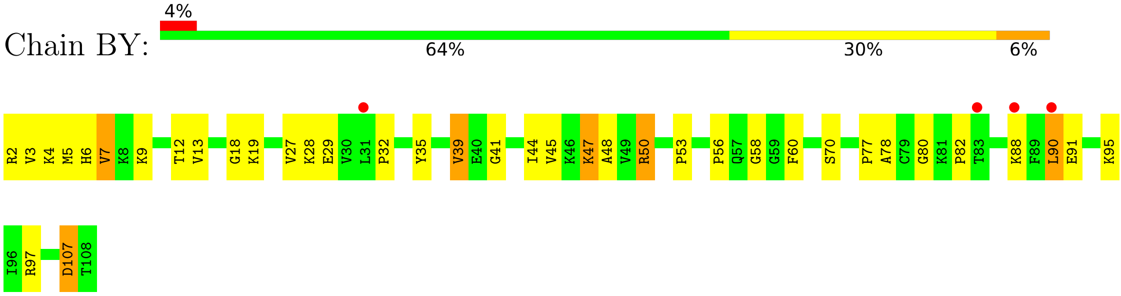
- Molecule 43: 50S ribosomal protein L23

Chain DX:



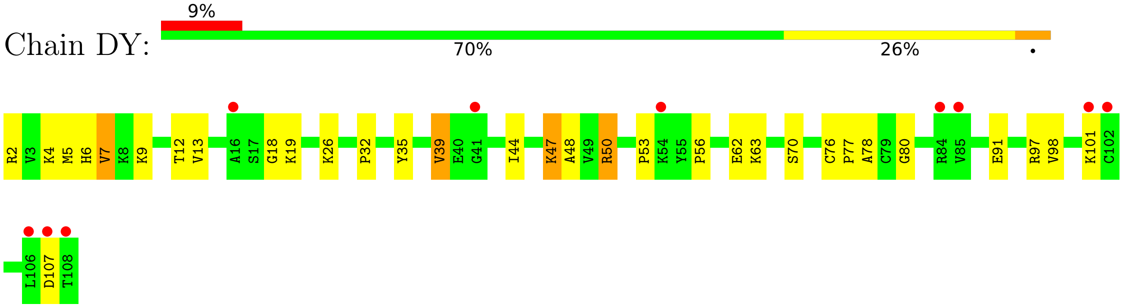
- Molecule 44: 50S ribosomal protein L24

Chain BY:



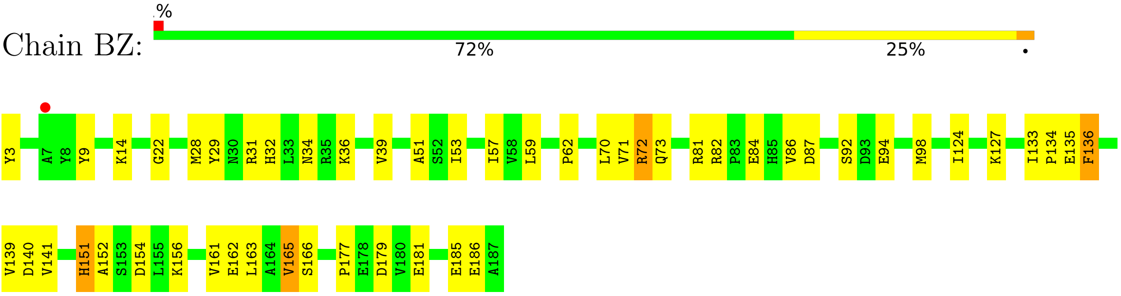
- Molecule 44: 50S ribosomal protein L24

Chain DY:



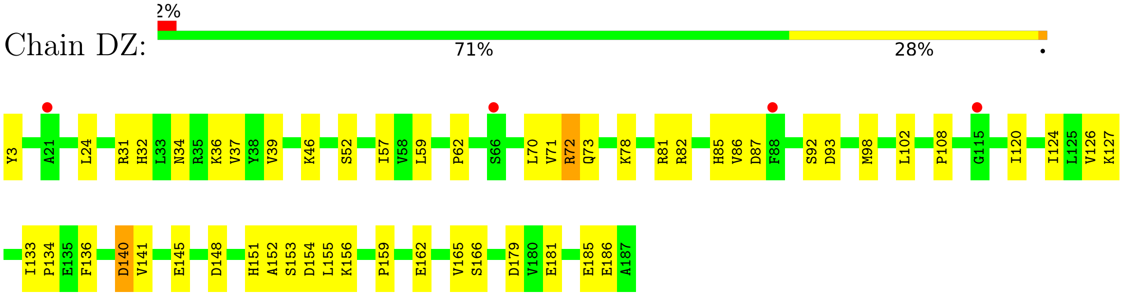
- Molecule 45: 50S ribosomal protein L25

Chain BZ:



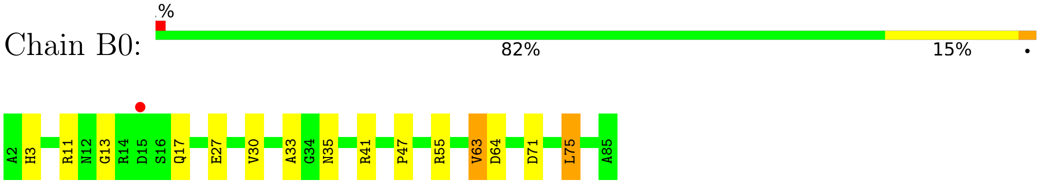
- Molecule 45: 50S ribosomal protein L25

Chain DZ:

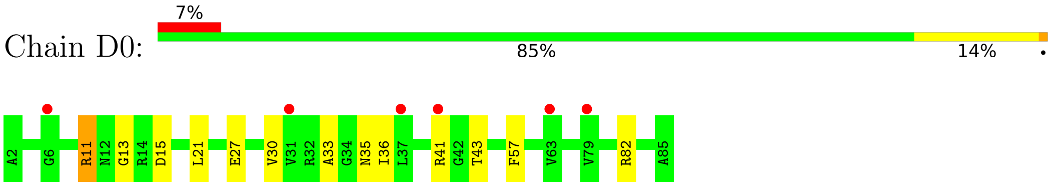


- Molecule 46: 50S ribosomal protein L27

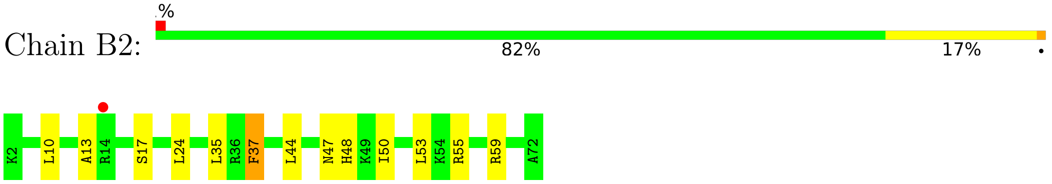
Chain B0:



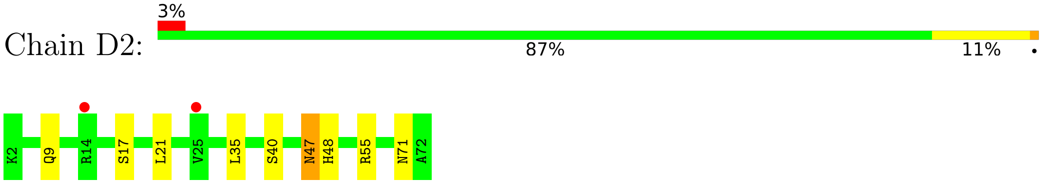
- Molecule 46: 50S ribosomal protein L27



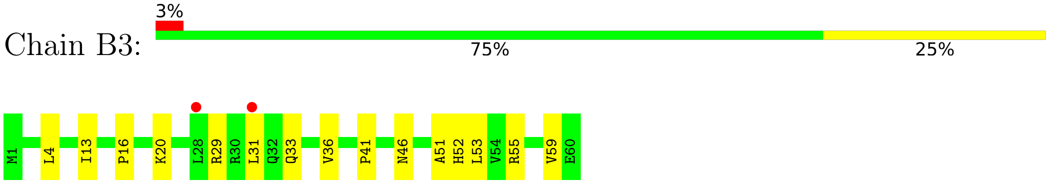
- Molecule 47: 50S ribosomal protein L29



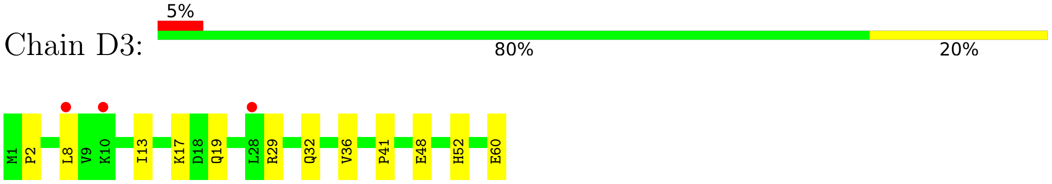
- Molecule 47: 50S ribosomal protein L29



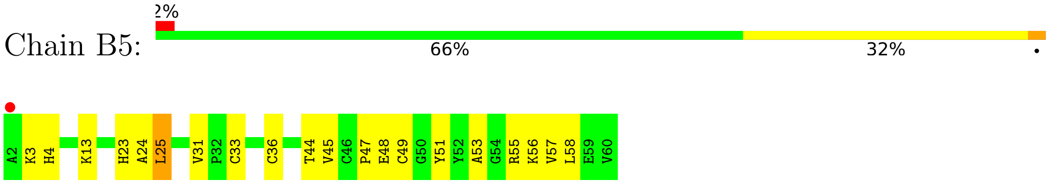
- Molecule 48: 50S ribosomal protein L30



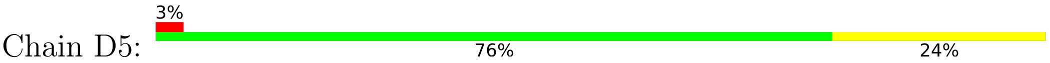
- Molecule 48: 50S ribosomal protein L30

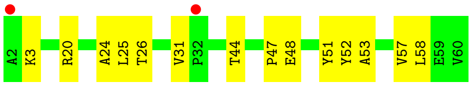


- Molecule 49: 50S ribosomal protein L32



- Molecule 49: 50S ribosomal protein L32



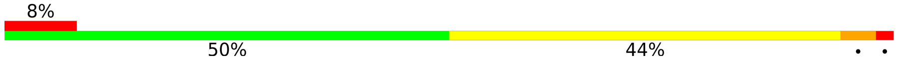


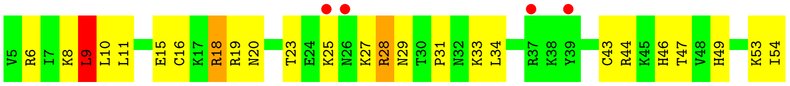
- Molecule 50: 50S ribosomal protein L33

Chain B6:

- Molecule 50: 50S ribosomal protein L33

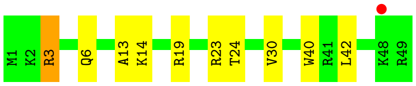
Chain D6:





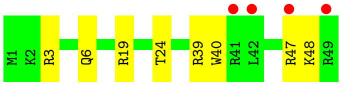
- Molecule 51: 50S ribosomal protein L34

Chain B7:



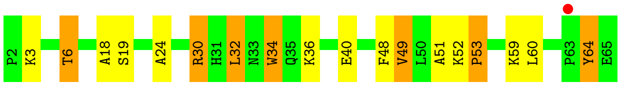
- Molecule 51: 50S ribosomal protein L34

Chain D7:



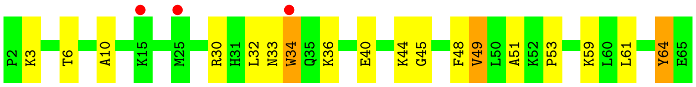
- Molecule 52: 50S ribosomal protein L35

Chain B8:



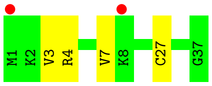
- Molecule 52: 50S ribosomal protein L35

Chain D8:



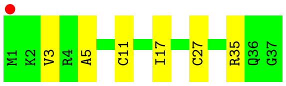
- Molecule 53: 50S ribosomal protein L36

Chain B9:



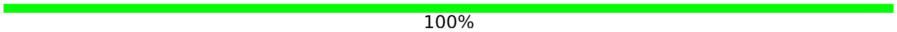
- Molecule 53: 50S ribosomal protein L36

Chain D9:



- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bf:



There are no outlier residues recorded for this chain.

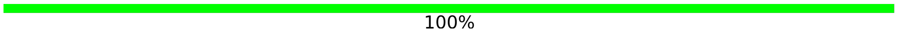
- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bg:

There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Df:



There are no outlier residues recorded for this chain.

- Molecule 54: 50S RIBOSOMAL PROTEIN L7/L12

Chain Dg:

There are no outlier residues recorded for this chain.

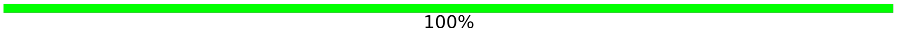
- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

Chain Bh:

There are no outlier residues recorded for this chain.

- Molecule 55: 50S RIBOSOMAL PROTEIN L7/L12

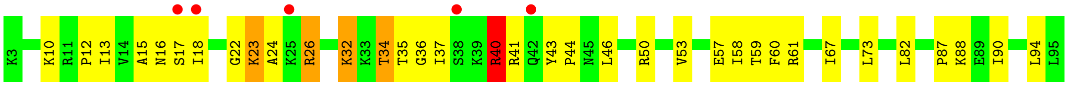
Chain Dh:



There are no outlier residues recorded for this chain.

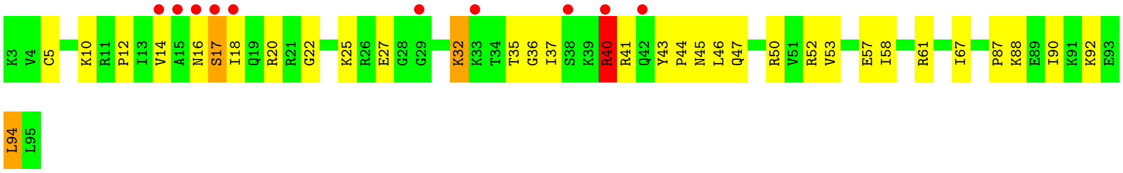
- Molecule 56: 50S ribosomal protein L28

Chain B1:



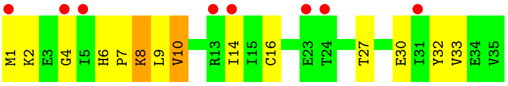
- Molecule 56: 50S ribosomal protein L28

Chain D1:



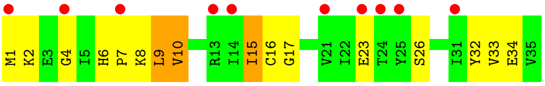
- Molecule 57: 50S ribosomal protein L31

Chain B4:



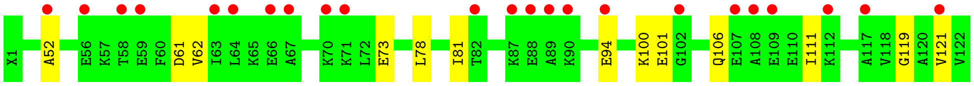
- Molecule 57: 50S ribosomal protein L31

Chain D4:



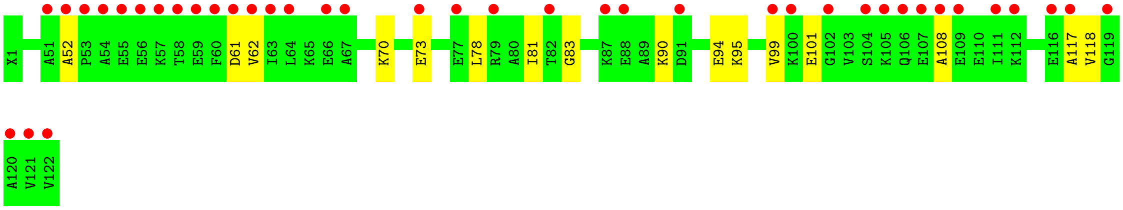
- Molecule 58: 50S ribosomal protein L7/L12

Chain Be:



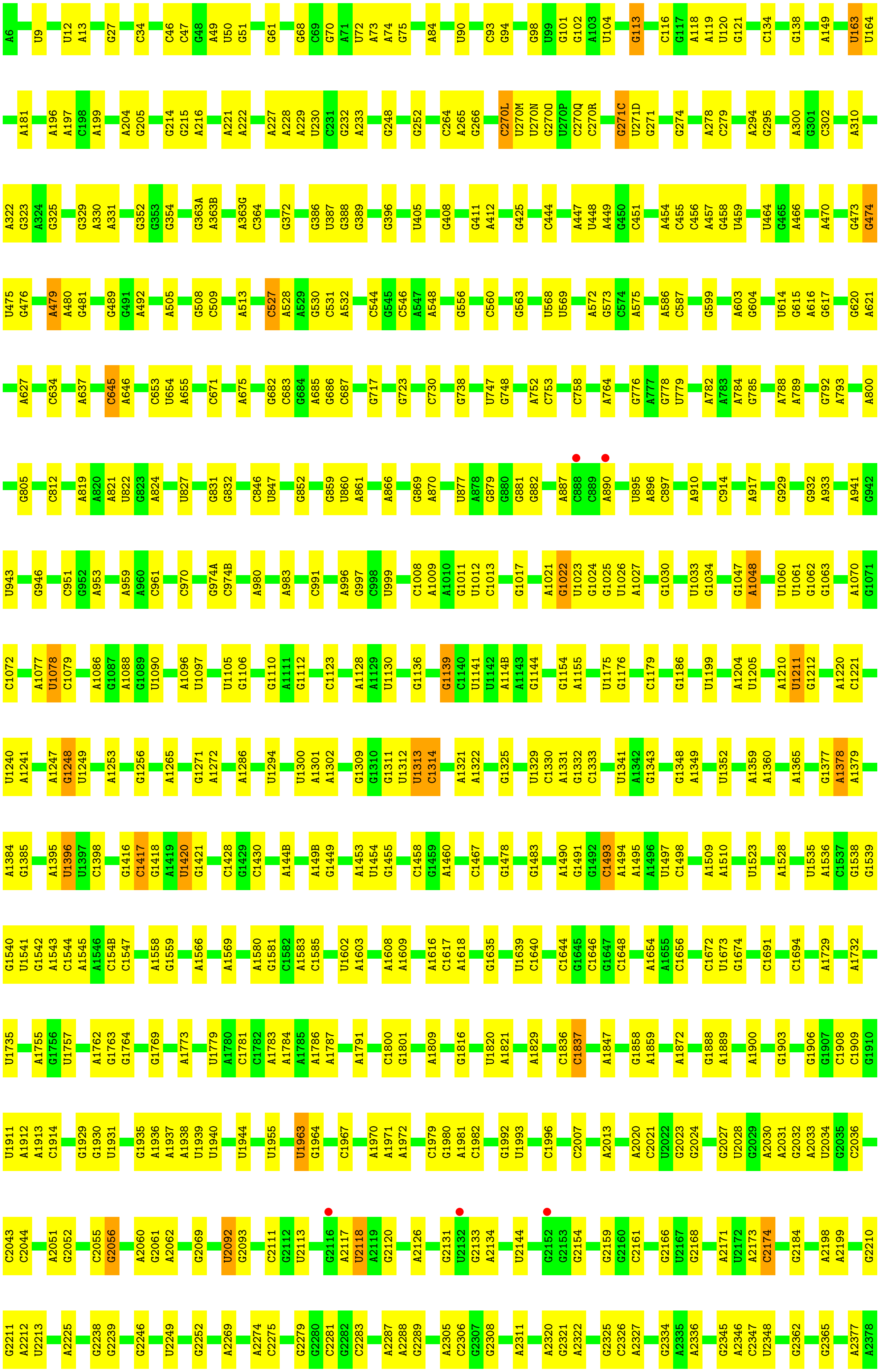
- Molecule 58: 50S ribosomal protein L7/L12

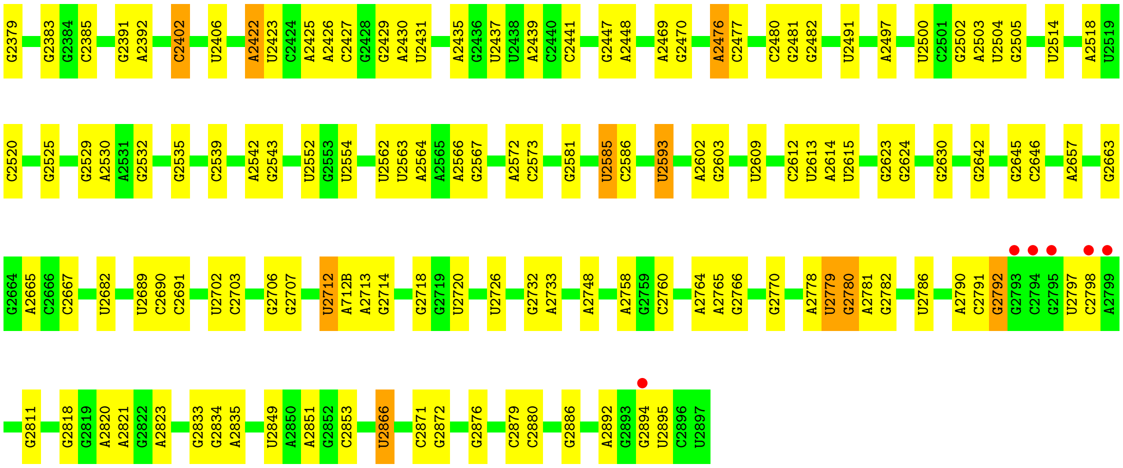
Chain De:



- Molecule 59: 23S ribosomal RNA

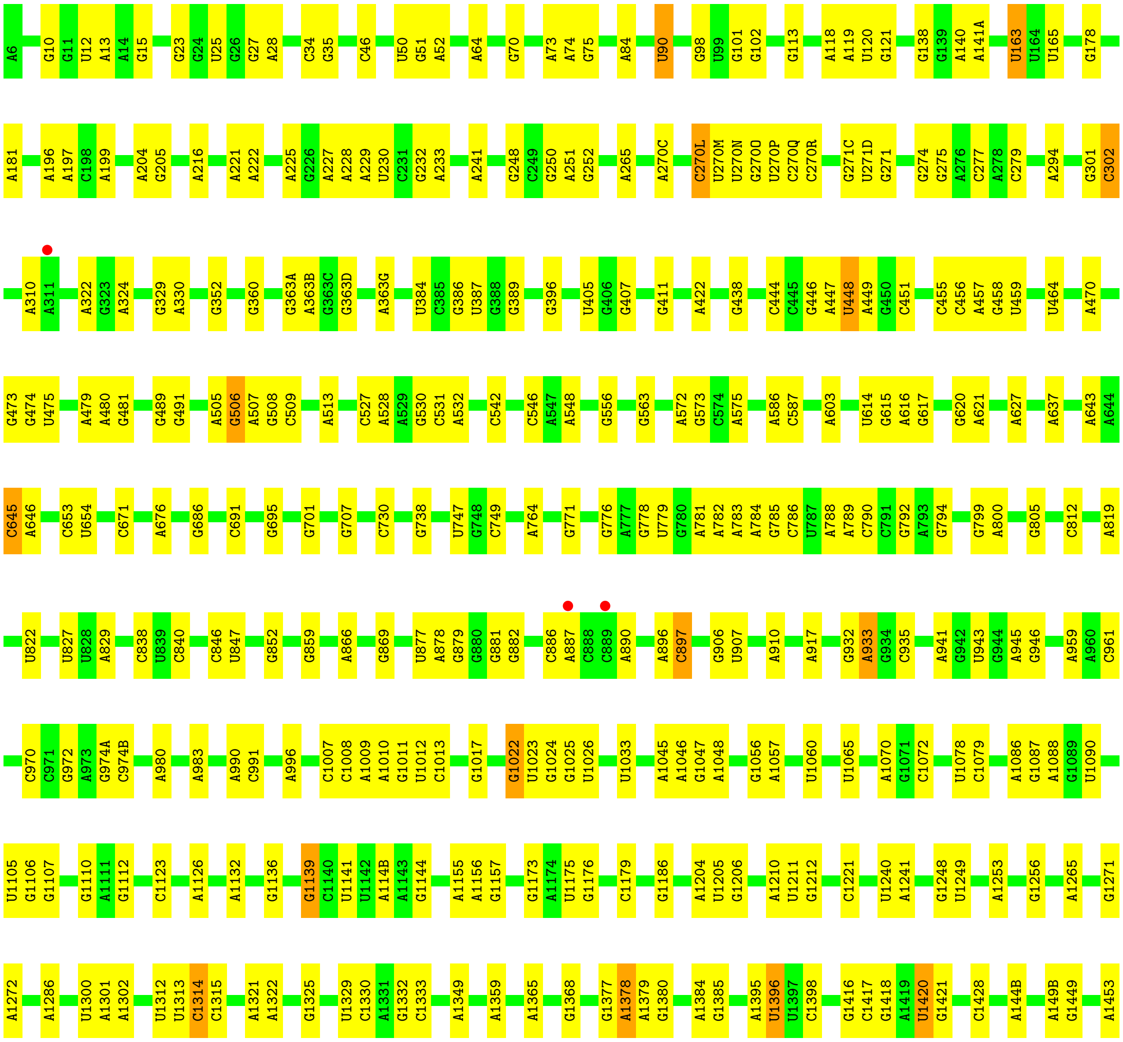
Chain BA:

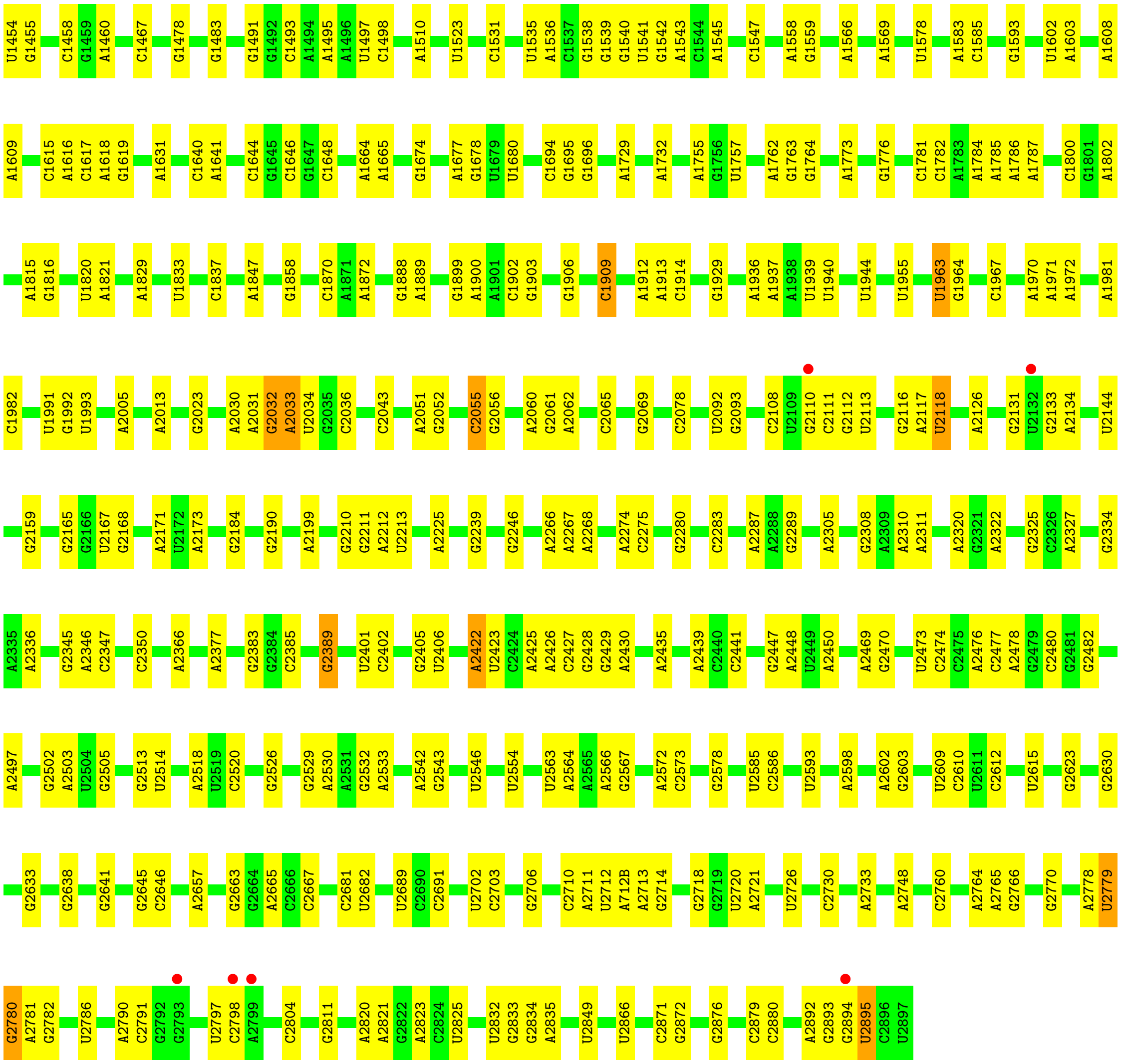

A6 U9 U12 A13 G27 C34 C46 C47 G48 A49 U50 G51 G61 G68 C69 G70 A71 U72 A73 A74 G75 A84 U90 C93 G94 G98 U99 G101 G102 A103 U104 G113 C116 G117 A118 A119 U120 G121 C134 G138 A149 U163 U164
A181 A196 A197 C198 A199 A204 G205 G214 G215 A216 A221 A222 A227 A228 A229 U230 C231 G232 A233 G248 G252 C264 A265 G266 C270L U270M U270N G270O U270P C270Q C270R G271C U271D G271 G274 A278 C279 A294 G295 A300 G301 C302 A310
A322 G323 A324 G325 G329 A330 A331 G352 G353 G354 G363A A363B A363G C364 G372 G386 U387 G388 G389 G396 U405 G408 G411 A412 G425 C444 A447 U448 A449 G450 C451 A454 C455 C456 A457 G458 U459 U464 G465 A466 A470 G473 G474
U475 G476 A479 A480 G481 G489 G491 A492 A505 G508 C509 A513 C527 A528 A529 G530 C531 A532 C544 G545 C546 A547 A548 G556 C560 G563 U568 U569 A572 G573 C574 A575 A586 C587 G599 A603 G604 U614 G615 A616 G617 G620 A621
A627 C634 A637 C645 A646 C653 U654 A655 C671 A675 G682 C683 G684 A685 G686 C687 G717 G723 C730 G738 U747 G748 A752 C753 C758 A764 G776 A777 G778 U779 A782 A783 A784 G785 A788 A789 G792 A793 A800
G805 C812 A819 A820 A821 U822 G823 A824 U827 G831 G832 C846 U847 G852 G859 U860 A861 A866 G869 A870 U877 A878 G879 G880 G881 G882 A887 C888 C889 A890 U895 A896 C897 A910 C914 A917 G929 G932 A933 A941 G942
U943 G946 C951 G952 A953 A959 A960 C961 C970 G974A C974B A980 A983 C991 A996 G997 C998 U999 C1008 A1009 A1010 G1011 U1012 C1013 G1017 A1021 G1022 U1023 G1024 G1025 U1026 A1027 G1030 U1033 G1034 G1047 A1048 U1060 U1061 G1062 G1063 A1070 G1071
C1072 A1077 U1078 C1079 A1086 G1087 A1088 G1089 U1090 A1096 U1097 U1105 G1106 G1110 A1111 G1112 C1123 A1128 A1129 U1130 G1136 G1139 C1140 U1141 U1142 A114B A1143 G1144 G1154 A1155 U1175 G1176 C1179 G1186 U1199 A1204 U1205 A1210 U1211 G1212 A1220 C1221
U1240 A1241 A1247 G1248 U1249 A1253 G1256 A1265 G1271 A1272 A1286 U1294 U1300 A1301 A1302 G1309 G1310 G1311 U1312 U1313 C1314 A1321 A1322 G1325 U1329 C1330 A1331 G1332 C1333 U1341 A1342 G1343 G1348 A1349 U1352 A1359 A1360 A1365 G1377 A1378 A1379
A1384 G1385 A1395 U1396 U1397 C1398 G1416 C1417 G1418 A1419 U1420 G1421 C1428 G1429 C1430 A144B A149B G1449 A1453 U1454 G1455 C1458 G1459 A1460 C1467 G1478 G1483 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1498 A1509 A1510 U1523 A1528 U1535 A1536 C1537 G1538 G1539
G1540 U1541 G1542 A1543 C1544 A1545 A1546 C154B C1547 A1558 G1559 A1566 A1569 A1580 G1581 C1582 A1583 C1585 U1602 A1603 A1608 A1609 A1616 C1617 A1618 G1635 U1639 C1640 C1644 G1645 C1646 G1647 C1648 A1654 A1655 C1656 C1672 U1673 G1674 C1691 C1694 A1729 A1732
U1735 A1755 G1756 U1757 A1762 G1763 G1764 G1769 A1773 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 A1791 C1800 G1801 A1809 G1816 U1820 A1821 A1829 C1836 C1837 A1847 G1858 A1859 A1872 G1888 A1889 A1900 G1903 G1906 G1907 C1908 C1909 G1910
U1911 A1912 A1913 C1914 G1929 G1930 U1931 G1935 A1936 A1937 A1938 U1939 U1940 U1944 U1955 U1963 G1964 C1967 A1970 A1971 A1972 C1979 G1980 A1981 C1982 G1992 U1993 C1996 C2007 A2013 A2020 C2021 U2022 G2023 G2024 G2027 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036
C2043 C2044 A2051 G2052 C2055 G2056 A2060 G2061 A2062 G2069 U2092 G2093 C2111 G2112 U2113 G2116 A2117 U2118 A2119 G2120 A2126 G2131 U2132 G2133 A2134 U2144 G2152 G2153 G2154 G2159 G2160 C2161 G2166 U2167 G2168 A2171 U2172 A2173 C2174 G2184 A2198 A2199 G2210
G2211 A2212 U2213 A2225 G2238 G2239 G2246 U2249 G2252 A2269 A2274 C2275 G2279 G2280 C2281 G2282 C2283 A2287 A2288 G2289 A2305 C2306 G2307 G2308 A2311 A2320 G2321 A2322 G2325 C2326 A2327 G2334 A2335 A2336 G2345 A2346 C2347 U2348 G2362 G2365 A2377 A2378



- Molecule 59: 23S ribosomal RNA

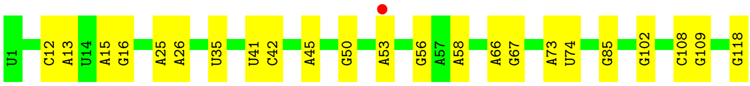
Chain DA:





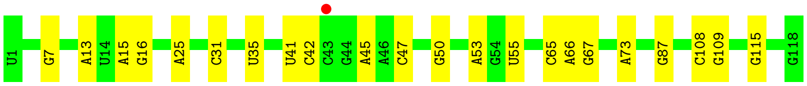
- Molecule 60: 5S ribosomal RNA

Chain BB:



- Molecule 60: 5S ribosomal RNA

Chain DB:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	306.01Å 673.49Å 351.98Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 131.34 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 74.9 (131.34-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.262 , 0.309 0.270 , 0.311	Depositor DCC
R_{free} test set	38188 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	80.5	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 85.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.26$, $< L^2 > = 0.11$	Xtriage
Estimated twinning fraction	0.247 for h,-k,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	308422	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: MG, KBE, 5OH, UAL, DPP, GNP

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	AB	0.42	0/1945	0.73	4/2621 (0.2%)
1	CB	0.40	0/1945	0.69	1/2621 (0.0%)
2	AC	0.35	0/1645	0.60	0/2216
2	CC	0.33	0/1645	0.58	1/2216 (0.0%)
3	AD	0.37	0/1733	0.60	0/2318
3	CD	0.34	0/1733	0.61	0/2318
4	AE	0.35	0/1172	0.63	1/1576 (0.1%)
4	CE	0.34	0/1172	0.63	1/1576 (0.1%)
5	AF	0.38	0/856	0.67	2/1154 (0.2%)
5	CF	0.35	0/856	0.64	1/1154 (0.1%)
6	AG	0.34	0/1276	0.58	0/1709
6	CG	0.35	0/1276	0.58	0/1709
7	AH	0.34	0/1136	0.58	0/1527
7	CH	0.33	0/1136	0.57	0/1527
8	AI	0.36	0/1029	0.63	1/1378 (0.1%)
8	CI	0.36	0/1029	0.61	1/1378 (0.1%)
9	AJ	0.37	0/815	0.64	1/1095 (0.1%)
9	CJ	0.33	0/815	0.65	1/1095 (0.1%)
10	AK	0.40	0/900	0.65	0/1213
10	CK	0.37	0/900	0.63	0/1213
11	AL	0.47	0/992	0.89	3/1327 (0.2%)
11	CL	0.47	0/992	0.88	4/1327 (0.3%)
12	AM	0.33	0/1008	0.61	0/1347
12	CM	0.32	0/1008	0.58	0/1347
13	AN	0.37	0/501	0.57	0/664
13	CN	0.35	0/501	0.57	0/664
14	AO	0.39	0/745	0.62	0/992
14	CO	0.35	0/745	0.59	0/992
15	AP	0.34	0/722	0.58	0/970
15	CP	0.33	0/722	0.56	0/970
16	AQ	0.45	0/848	0.75	0/1131
16	CQ	0.42	0/848	0.71	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AR	0.33	0/579	0.59	0/768
17	CR	0.31	0/579	0.57	0/768
18	AS	0.32	0/647	0.59	0/870
18	CS	0.31	0/647	0.56	0/870
19	AT	0.36	0/764	0.57	0/1006
19	CT	0.37	0/764	0.62	0/1006
20	AY	0.47	6/5481 (0.1%)	0.72	5/7418 (0.1%)
20	CY	0.52	7/5481 (0.1%)	0.76	12/7418 (0.2%)
21	AA	0.39	0/36351	0.97	36/56736 (0.1%)
21	CA	0.38	0/36351	0.95	35/56736 (0.1%)
22	AW	0.40	0/1827	1.06	9/2845 (0.3%)
22	CW	0.41	1/1827 (0.1%)	1.06	9/2845 (0.3%)
23	AV	0.78	1/568 (0.2%)	1.49	16/886 (1.8%)
23	CV	0.95	3/568 (0.5%)	1.74	19/886 (2.1%)
24	AU	1.05	0/11	1.28	0/13
24	CU	1.06	0/11	1.28	0/13
25	BC	0.44	0/1774	0.74	1/2391 (0.0%)
25	DC	0.50	1/1774 (0.1%)	0.76	0/2391
26	BD	0.38	0/2195	0.65	0/2955
26	DD	0.38	0/2195	0.67	0/2955
27	BE	0.39	0/1602	0.69	1/2160 (0.0%)
27	DE	0.35	0/1602	0.67	1/2160 (0.0%)
28	BF	0.41	0/1663	0.80	5/2249 (0.2%)
28	DF	0.41	0/1663	0.79	4/2249 (0.2%)
29	BG	0.57	1/1499 (0.1%)	0.60	0/2016
29	DG	0.59	1/1499 (0.1%)	0.67	3/2016 (0.1%)
30	BH	0.34	0/1298	0.59	0/1751
30	DH	0.34	0/1298	0.62	0/1751
32	BK	0.34	0/1054	0.60	0/1427
32	DK	0.34	0/1054	0.56	1/1427 (0.1%)
33	BN	0.58	0/1131	0.85	0/1525
33	DN	0.54	0/1131	0.80	0/1525
34	BO	0.36	0/943	0.65	1/1269 (0.1%)
34	DO	0.36	0/943	0.64	1/1269 (0.1%)
35	BP	0.34	0/1131	0.71	0/1504
35	DP	0.34	0/1131	0.71	0/1504
36	BQ	0.37	0/1143	0.64	0/1527
36	DQ	0.36	0/1143	0.60	0/1527
37	BR	0.38	0/974	0.65	0/1302
37	DR	0.34	0/974	0.62	1/1302 (0.1%)
38	BS	0.40	0/783	0.76	0/1041
38	DS	0.40	0/783	0.75	0/1041
39	BT	0.39	0/1161	0.76	3/1549 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	DT	0.37	0/1161	0.67	0/1549
40	BU	0.39	0/982	0.67	1/1306 (0.1%)
40	DU	0.42	0/982	0.68	1/1306 (0.1%)
41	BV	0.37	0/790	0.66	0/1057
41	DV	0.38	0/790	0.71	0/1057
42	BW	0.38	0/911	0.65	0/1220
42	DW	0.37	0/911	0.65	0/1220
43	BX	0.35	0/748	0.59	1/1004 (0.1%)
43	DX	0.35	0/748	0.60	0/1004
44	BY	0.35	0/831	0.65	0/1108
44	DY	0.34	0/831	0.60	0/1108
45	BZ	0.33	0/1505	0.60	0/2042
45	DZ	0.32	0/1505	0.59	0/2042
46	B0	0.33	0/671	0.55	0/892
46	D0	0.31	0/671	0.56	0/892
47	B2	0.37	0/600	0.65	1/793 (0.1%)
47	D2	0.34	0/600	0.60	0/793
48	B3	0.34	0/482	0.63	0/646
48	D3	0.31	0/482	0.58	0/646
49	B5	0.33	0/473	0.58	0/639
49	D5	0.34	0/473	0.60	0/639
50	B6	0.38	0/440	0.81	0/586
50	D6	0.35	0/440	0.79	1/586 (0.2%)
51	B7	0.38	0/438	0.62	0/575
51	D7	0.48	0/438	0.69	0/575
52	B8	0.37	0/525	0.67	0/691
52	D8	0.36	0/525	0.64	0/691
53	B9	0.32	0/310	0.55	0/407
53	D9	0.29	0/310	0.55	0/407
56	B1	0.53	0/739	0.83	1/981 (0.1%)
56	D1	0.54	0/739	0.84	2/981 (0.2%)
57	B4	0.40	0/276	0.65	0/372
57	D4	0.45	0/276	0.66	0/372
58	Be	0.36	0/538	0.55	0/715
58	De	0.35	0/538	0.61	0/715
59	BA	0.41	2/69437 (0.0%)	0.99	82/108401 (0.1%)
59	DA	0.40	1/69437 (0.0%)	0.97	72/108401 (0.1%)
60	BB	0.34	0/2853	0.93	0/4451
60	DB	0.34	0/2853	0.90	1/4451 (0.0%)
All	All	0.40	24/330902 (0.0%)	0.90	348/492664 (0.1%)

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	AB	0	2
1	CB	0	1
10	AK	0	1
11	AL	0	1
11	CL	0	1
20	AY	0	3
20	CY	0	8
25	BC	0	3
25	DC	0	2
26	DD	0	1
28	BF	0	2
28	DF	0	2
29	BG	0	1
29	DG	0	1
31	BJ	0	1
31	DJ	0	1
38	BS	0	2
38	DS	0	2
39	BT	0	2
39	DT	0	1
42	DW	0	1
56	B1	0	2
56	D1	0	3
All	All	0	44

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	CY	502	GLY	C-O	18.54	1.53	1.23
29	DG	112	PRO	CA-C	17.59	1.88	1.52
29	BG	112	PRO	CA-C	17.54	1.88	1.52
23	CV	16	A	O3'-P	-10.50	1.48	1.61
20	AY	499	ARG	C-N	9.84	1.56	1.34
20	CY	504	ARG	C-N	8.54	1.48	1.33
22	CW	37	A	O3'-P	-8.36	1.51	1.61
23	CV	15	A	N9-C4	-7.84	1.33	1.37
59	BA	2780	G	N7-C5	-6.61	1.35	1.39
20	CY	499	ARG	C-N	6.39	1.48	1.34
25	DC	46	ALA	CA-CB	6.31	1.65	1.52
23	AV	16	A	N9-C4	6.21	1.41	1.37
59	DA	2780	G	N7-C5	-6.19	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CV	16	A	N9-C4	6.18	1.41	1.37
20	CY	31	ARG	C-O	6.18	1.35	1.23
20	AY	61	ARG	N-CA	6.13	1.58	1.46
20	AY	72	CYS	CB-SG	5.78	1.92	1.82
59	BA	2780	G	N9-C8	-5.77	1.33	1.37
20	AY	61	ARG	C-N	-5.72	1.22	1.33
20	CY	72	CYS	CA-CB	-5.62	1.41	1.53
20	AY	59	ARG	C-N	5.57	1.46	1.34
20	CY	33	LEU	CA-C	-5.30	1.39	1.52
20	CY	33	LEU	N-CA	5.27	1.56	1.46
20	AY	31	ARG	C-O	5.13	1.33	1.23

All (348) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	CW	37	A	P-O3'-C3'	19.49	143.09	119.70
23	CV	16	A	P-O3'-C3'	18.93	142.41	119.70
20	CY	502	GLY	O-C-N	-12.85	101.35	123.20
20	CY	502	GLY	CA-C-N	12.59	141.38	116.20
20	CY	502	GLY	C-N-CA	11.35	146.14	122.30
23	CV	15	A	N1-C6-N6	-10.80	112.12	118.60
23	CV	16	A	O3'-P-O5'	-10.76	83.56	104.00
29	DG	116	ASP	O-C-N	-10.28	106.25	122.70
28	DF	193	VAL	N-CA-C	-10.27	83.28	111.00
23	CV	18	G	C8-N9-C4	-9.98	102.41	106.40
59	DA	645	C	C2-N1-C1'	9.76	129.54	118.80
59	BA	645	C	C2-N1-C1'	9.30	129.03	118.80
23	CV	15	A	C8-N9-C4	9.20	109.48	105.80
22	CW	74	C	C2-N1-C1'	9.09	128.80	118.80
23	AV	15	A	N1-C6-N6	-9.09	113.15	118.60
23	AV	15	A	C2-N3-C4	9.02	115.11	110.60
21	CA	1137	C	C2-N1-C1'	8.93	128.62	118.80
59	BA	163	U	C2-N1-C1'	8.85	128.32	117.70
22	AW	74	C	N1-C2-O2	8.78	124.17	118.90
20	CY	503	GLY	O-C-N	-8.59	108.95	122.70
23	CV	18	G	C2'-C3'-O3'	8.53	128.28	109.50
23	CV	15	A	C4-C5-C6	-8.47	112.76	117.00
59	BA	1493	C	N1-C2-O2	8.39	123.93	118.90
23	CV	16	A	OP1-P-O3'	8.38	123.64	105.20
20	CY	33	LEU	CA-CB-CG	8.38	134.57	115.30
23	AV	15	A	C4-C5-C6	-8.30	112.85	117.00
59	DA	645	C	N1-C2-O2	8.29	123.88	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AW	74	C	C2-N1-C1'	8.28	127.91	118.80
21	CA	723	U	C2-N1-C1'	8.20	127.54	117.70
59	BA	1493	C	C2-N1-C1'	8.19	127.81	118.80
23	AV	15	A	N1-C2-N3	-8.16	125.22	129.30
23	CV	15	A	C5-C6-N1	8.16	121.78	117.70
28	BF	193	VAL	N-CA-C	-8.14	89.03	111.00
20	CY	72	CYS	CB-CA-C	-8.07	94.26	110.40
21	CA	1158	C	C2-N1-C1'	7.97	127.57	118.80
21	AA	1158	C	C2-N1-C1'	7.95	127.54	118.80
21	CA	1137	C	N1-C2-O2	7.94	123.67	118.90
59	BA	2779	U	OP1-P-O3'	-7.89	87.85	105.20
20	AY	33	LEU	CA-CB-CG	7.82	133.28	115.30
59	BA	2780	G	O5'-P-OP1	-7.75	98.72	105.70
21	CA	201(C)	U	C2-N1-C1'	7.71	126.95	117.70
23	AV	18	G	C6-N1-C2	7.60	129.66	125.10
22	CW	74	C	N1-C2-O2	7.38	123.33	118.90
59	BA	527	C	C6-N1-C2	-7.35	117.36	120.30
23	CV	15	A	C6-C5-N7	7.32	137.42	132.30
59	DA	270(L)	C	N1-C2-O2	7.29	123.28	118.90
59	DA	645	C	C6-N1-C1'	-7.26	112.08	120.80
59	BA	2780	G	O4'-C1'-N9	7.24	114.00	108.20
21	AA	421	U	C2-N1-C1'	7.23	126.37	117.70
22	CW	37	A	OP1-P-O3'	7.18	121.01	105.20
59	DA	1022	G	N3-C4-C5	-7.15	125.02	128.60
59	BA	2593	U	C6-N1-C2	-7.14	116.72	121.00
21	AA	1137	C	C2-N1-C1'	7.08	126.59	118.80
59	BA	645	C	C6-N1-C2	-7.06	117.47	120.30
39	BT	48	ILE	CB-CA-C	-7.06	97.48	111.60
20	CY	72	CYS	CA-CB-SG	-7.05	101.30	114.00
21	AA	201(C)	U	C2-N1-C1'	7.05	126.16	117.70
59	DA	163	U	C2-N1-C1'	7.05	126.16	117.70
21	CA	1158	C	N1-C2-O2	7.05	123.13	118.90
23	AV	18	G	C2'-C3'-O3'	7.03	124.96	109.50
29	DG	116	ASP	CA-C-N	7.01	132.63	117.20
59	DA	1963	U	C2-N1-C1'	6.94	126.03	117.70
28	DF	155	LEU	N-CA-C	-6.90	92.38	111.00
23	AV	18	G	C4'-C3'-O3'	6.89	126.77	113.00
28	BF	155	LEU	N-CA-C	-6.86	92.48	111.00
21	CA	1137	C	C6-N1-C1'	-6.85	112.58	120.80
20	CY	72	CYS	N-CA-CB	-6.80	98.36	110.60
22	AW	74	C	N3-C2-O2	-6.80	117.14	121.90
59	DA	1963	U	N1-C2-O2	6.79	127.56	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BA	2402	C	N1-C2-O2	6.78	122.97	118.90
59	BA	1396	U	C2-N1-C1'	6.77	125.82	117.70
59	BA	645	C	N1-C2-O2	6.74	122.95	118.90
59	BA	645	C	C5-C6-N1	6.74	124.37	121.00
23	CV	15	A	N7-C8-N9	-6.73	110.43	113.80
28	BF	156	LEU	CA-CB-CG	6.73	130.78	115.30
22	AW	73	A	C8-N9-C4	-6.72	103.11	105.80
23	AV	19	G	C4-N9-C1'	6.72	135.24	126.50
8	AI	58	ARG	NE-CZ-NH1	6.71	123.65	120.30
59	BA	2585	U	C2-N1-C1'	6.70	125.74	117.70
21	AA	1378	C	C2-N1-C1'	6.70	126.17	118.80
8	CI	58	ARG	NE-CZ-NH1	6.69	123.65	120.30
23	AV	15	A	C5-C6-N1	6.68	121.04	117.70
20	CY	503	GLY	C-N-CA	6.66	138.36	121.70
21	AA	962	C	C6-N1-C2	-6.65	117.64	120.30
59	BA	2780	G	C4-C5-C6	6.65	122.79	118.80
21	AA	1267	C	C6-N1-C2	-6.64	117.64	120.30
21	AA	1145	C	C6-N1-C2	-6.62	117.65	120.30
59	BA	2866	U	C2-N1-C1'	6.59	125.61	117.70
59	DA	2780	G	O5'-P-OP1	-6.55	99.80	105.70
59	DA	448	U	N1-C2-O2	6.55	127.38	122.80
59	BA	1314	C	C2-N1-C1'	6.54	126.00	118.80
23	CV	18	G	N7-C8-N9	6.54	116.37	113.10
59	BA	1139	G	O5'-P-OP2	-6.53	99.82	105.70
59	BA	1211	U	C2-N1-C1'	6.52	125.53	117.70
21	CA	748	C	P-O3'-C3'	6.52	127.53	119.70
59	DA	2780	G	C4-C5-C6	6.51	122.71	118.80
21	CA	924	C	C6-N1-C2	-6.46	117.72	120.30
59	BA	1963	U	C2-N1-C1'	6.46	125.45	117.70
59	DA	1396	U	C2-N1-C1'	6.44	125.43	117.70
1	AB	163	PHE	N-CA-C	-6.41	93.70	111.00
22	CW	74	C	C6-N1-C1'	-6.40	113.12	120.80
23	AV	17	U	N3-C4-O4	6.39	123.87	119.40
11	CL	55	VAL	CB-CA-C	-6.38	99.28	111.40
20	CY	72	CYS	N-CA-C	6.38	128.22	111.00
59	DA	2780	G	N1-C6-O6	6.35	123.71	119.90
40	DU	98	LEU	CA-CB-CG	6.35	129.90	115.30
23	AV	16	A	O5'-P-OP2	6.30	118.26	110.70
21	CA	1128	C	C2-N1-C1'	6.29	125.72	118.80
59	BA	270(L)	C	N1-C2-O2	6.29	122.67	118.90
21	CA	1158	C	C6-N1-C1'	-6.29	113.26	120.80
59	BA	1963	U	N1-C2-O2	6.27	127.19	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BA	1979	C	C6-N1-C2	-6.26	117.79	120.30
59	DA	1420	U	C2-N1-C1'	6.21	125.15	117.70
59	DA	448	U	N3-C2-O2	-6.21	117.85	122.20
59	BA	2585	U	N1-C2-O2	6.21	127.14	122.80
59	BA	645	C	C6-N1-C1'	-6.20	113.36	120.80
59	DA	1314	C	C2-N1-C1'	6.20	125.62	118.80
4	CE	12	LEU	CA-CB-CG	6.19	129.54	115.30
4	AE	12	LEU	CA-CB-CG	6.19	129.53	115.30
23	CV	18	G	N3-C4-C5	-6.18	125.51	128.60
21	CA	881	G	C8-N9-C4	-6.17	103.93	106.40
11	CL	60	LEU	CA-CB-CG	6.17	129.50	115.30
21	AA	723	U	C2-N1-C1'	6.17	125.10	117.70
20	CY	503	GLY	CA-C-N	6.16	130.76	117.20
59	DA	676	A	O4'-C1'-N9	6.16	113.13	108.20
21	AA	1158	C	C6-N1-C1'	-6.14	113.43	120.80
59	BA	2690	C	C6-N1-C2	6.14	122.75	120.30
59	DA	1909	C	C2-N1-C1'	6.12	125.54	118.80
22	AW	74	C	C6-N1-C1'	-6.12	113.45	120.80
59	BA	2476	A	O4'-C1'-N9	6.11	113.09	108.20
22	CW	20(A)	U	P-O3'-C3'	6.11	127.03	119.70
59	DA	2585	U	C2-N1-C1'	6.11	125.03	117.70
59	DA	1313	U	C2-N1-C1'	6.09	125.00	117.70
59	BA	758	C	N3-C2-O2	-6.06	117.66	121.90
59	BA	1493	C	C6-N1-C1'	-6.02	113.58	120.80
22	CW	74	C	N3-C2-O2	-6.01	117.69	121.90
59	DA	270(L)	C	N3-C2-O2	-6.00	117.70	121.90
21	AA	421	U	N1-C2-O2	5.98	126.99	122.80
21	AA	543	C	C6-N1-C2	-5.97	117.91	120.30
1	AB	187	LEU	CA-CB-CG	5.97	129.02	115.30
23	CV	19	G	C4-N9-C1'	5.96	134.25	126.50
59	DA	2780	G	C6-C5-N7	-5.96	126.82	130.40
21	CA	872	A	O4'-C1'-N9	5.95	112.96	108.20
59	BA	687	C	N3-C2-O2	-5.94	117.74	121.90
39	BT	78	LEU	CA-CB-CG	5.93	128.95	115.30
56	B1	40	ARG	N-CA-C	5.92	126.98	111.00
59	BA	1313	U	C2-N1-C1'	5.91	124.79	117.70
40	BU	98	LEU	CA-CB-CG	5.89	128.85	115.30
11	AL	34	ARG	N-CA-C	5.87	126.85	111.00
59	DA	2780	G	N3-C4-N9	5.86	129.52	126.00
59	DA	645	C	N3-C2-O2	-5.86	117.80	121.90
59	BA	1396	U	N1-C2-O2	5.85	126.89	122.80
27	DE	63	LEU	CA-CB-CG	5.84	128.74	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AA	1158	C	N1-C2-O2	5.84	122.40	118.90
20	AY	503	GLY	O-C-N	-5.83	113.38	122.70
59	BA	163	U	C5-C6-N1	5.82	125.61	122.70
59	DA	2585	U	N1-C2-O2	5.82	126.87	122.80
21	AA	1009	G	O4'-C1'-N9	5.81	112.84	108.20
59	BA	1248	G	P-O3'-C3'	5.80	126.66	119.70
59	BA	1396	U	N3-C2-O2	-5.80	118.14	122.20
59	DA	2779	U	OP2-P-O3'	5.77	117.89	105.20
59	BA	163	U	C6-N1-C1'	-5.76	113.13	121.20
50	D6	9	LEU	CA-CB-CG	5.76	128.56	115.30
21	AA	115	G	P-O3'-C3'	5.75	126.60	119.70
20	CY	33	LEU	CA-C-N	-5.75	104.55	117.20
21	AA	421	U	N3-C2-O2	-5.75	118.18	122.20
59	BA	466	A	O5'-P-OP1	-5.74	100.53	105.70
59	BA	1493	C	N3-C2-O2	-5.74	117.89	121.90
21	CA	723	U	C6-N1-C1'	-5.74	113.17	121.20
5	AF	19	LEU	CA-CB-CG	5.72	128.47	115.30
23	CV	16	A	C5'-C4'-C3'	5.72	125.16	116.00
59	BA	1314	C	C6-N1-C1'	-5.72	113.94	120.80
21	CA	1504	G	P-O3'-C3'	5.72	126.56	119.70
21	AA	201(C)	U	N1-C2-O2	5.71	126.80	122.80
59	BA	2306	C	C6-N1-C2	-5.70	118.02	120.30
21	CA	201(C)	U	C5-C6-N1	5.70	125.55	122.70
59	DA	2779	U	OP1-P-O3'	-5.68	92.70	105.20
59	DA	270(L)	C	C2-N1-C1'	5.68	125.04	118.80
23	CV	18	G	C4'-C3'-O3'	5.67	124.34	113.00
21	CA	1128	C	N1-C2-O2	5.66	122.30	118.90
23	AV	17	U	N3-C2-O2	5.66	126.16	122.20
59	BA	1417	C	C6-N1-C2	-5.64	118.04	120.30
21	CA	1137	C	N3-C2-O2	-5.64	117.95	121.90
59	DA	1315	C	N1-C2-O2	5.64	122.29	118.90
21	AA	1137	C	C6-N1-C2	-5.64	118.04	120.30
59	BA	1048	A	N1-C6-N6	5.64	121.98	118.60
59	BA	474	G	P-O3'-C3'	5.64	126.47	119.70
59	BA	1779	U	C2-N1-C1'	5.63	124.46	117.70
25	BC	138	LEU	CA-CB-CG	5.63	128.25	115.30
21	CA	723	U	N1-C2-O2	5.62	126.74	122.80
21	CA	201(C)	U	N1-C2-O2	5.62	126.73	122.80
56	D1	40	ARG	N-CA-C	5.62	126.17	111.00
21	AA	992	U	P-O3'-C3'	5.62	126.44	119.70
59	BA	1420	U	N1-C2-O2	5.62	126.73	122.80
47	B2	24	LEU	CA-CB-CG	5.61	128.20	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	DA	90	U	C2-N1-C1'	5.60	124.42	117.70
59	BA	2780	G	C4-C5-N7	-5.60	108.56	110.80
22	AW	20(A)	U	P-O3'-C3'	5.60	126.42	119.70
21	CA	992	U	P-O3'-C3'	5.59	126.41	119.70
59	DA	2895	U	C2-N1-C1'	5.59	124.41	117.70
21	AA	1129	C	N1-C2-O2	5.59	122.25	118.90
59	BA	163	U	N1-C2-O2	5.59	126.71	122.80
59	BA	2402	C	N3-C2-O2	-5.58	117.99	121.90
22	CW	74	C	C6-N1-C2	-5.58	118.07	120.30
22	AW	66	C	C6-N1-C2	-5.57	118.07	120.30
27	BE	63	LEU	CA-CB-CG	5.57	128.12	115.30
59	DA	1396	U	N1-C2-O2	5.57	126.70	122.80
5	AF	61	LEU	CA-CB-CG	5.56	128.09	115.30
59	BA	2021	C	C6-N1-C2	5.55	122.52	120.30
21	AA	1381	U	O4'-C1'-N1	5.54	112.64	108.20
23	AV	16	A	N9-C4-C5	-5.53	103.59	105.80
59	BA	2007	C	C6-N1-C2	-5.53	118.09	120.30
28	DF	156	LEU	CA-CB-CG	5.52	128.00	115.30
23	CV	16	A	N9-C4-C5	-5.52	103.59	105.80
59	DA	2111	C	C6-N1-C2	-5.51	118.09	120.30
20	AY	61	ARG	C-N-CA	-5.51	110.73	122.30
11	AL	55	VAL	CB-CA-C	-5.51	100.94	111.40
59	BA	2866	U	C5-C6-N1	5.50	125.45	122.70
59	BA	1022	G	P-O3'-C3'	5.50	126.30	119.70
23	CV	17	U	C6-N1-C2	-5.50	117.70	121.00
59	BA	1378	A	O4'-C1'-N9	5.49	112.59	108.20
59	DA	2710	C	C6-N1-C2	-5.48	118.11	120.30
21	AA	1137	C	N1-C2-O2	5.47	122.18	118.90
21	CA	421	U	C2-N1-C1'	5.47	124.26	117.70
59	BA	2780	G	N1-C2-N3	5.46	127.18	123.90
59	DA	645	C	C5-C6-N1	5.46	123.73	121.00
59	BA	758	C	N1-C2-O2	5.45	122.17	118.90
60	DB	31	C	C6-N1-C2	-5.45	118.12	120.30
21	AA	1126	U	C2-N1-C1'	5.44	124.23	117.70
59	BA	2092	U	N1-C2-O2	5.43	126.60	122.80
11	AL	60	LEU	CA-CB-CG	5.43	127.79	115.30
59	BA	113	G	C4-N9-C1'	5.43	133.55	126.50
1	AB	162	ILE	CB-CA-C	5.42	122.44	111.60
20	AY	32	ILE	CB-CA-C	5.41	122.41	111.60
59	DA	2804	C	C6-N1-C2	-5.41	118.14	120.30
59	DA	448	U	C2-N1-C1'	5.40	124.18	117.70
21	AA	1064	G	P-O3'-C3'	5.38	126.16	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	DA	1396	U	N3-C2-O2	-5.38	118.43	122.20
23	AV	19	G	C8-N9-C1'	-5.38	120.01	127.00
2	CC	188	LEU	CA-CB-CG	5.37	127.65	115.30
23	CV	19	G	C8-N9-C1'	-5.37	120.02	127.00
23	AV	18	G	N1-C2-N3	-5.37	120.68	123.90
59	DA	2033	A	N9-C4-C5	5.36	107.94	105.80
59	DA	2033	A	C8-N9-C4	-5.35	103.66	105.80
59	BA	687	C	N1-C2-O2	5.34	122.11	118.90
21	CA	68(H)	G	N1-C6-O6	-5.34	116.70	119.90
34	DO	8	LEU	CA-CB-CG	5.34	127.58	115.30
11	CL	35	GLY	N-CA-C	5.33	126.43	113.10
21	AA	365	U	C2-N1-C1'	5.32	124.08	117.70
28	DF	174	VAL	N-CA-C	-5.31	96.65	111.00
21	AA	1128	C	C2-N1-C1'	5.31	124.64	118.80
22	CW	30	C	C6-N1-C2	-5.31	118.18	120.30
59	BA	271(C)	G	P-O3'-C3'	5.31	126.07	119.70
59	DA	2118	U	C2-N1-C1'	5.31	124.07	117.70
21	CA	1064	G	P-O3'-C3'	5.30	126.06	119.70
21	CA	201(C)	U	N3-C2-O2	-5.30	118.49	122.20
59	BA	1420	U	C2-N1-C1'	5.30	124.06	117.70
9	CJ	16	LEU	CA-CB-CG	5.29	127.47	115.30
59	DA	1680	U	C2-N1-C1'	-5.29	111.35	117.70
21	CA	748	C	OP2-P-O3'	5.29	116.83	105.20
59	DA	1664	A	C8-N9-C4	-5.28	103.69	105.80
59	DA	933	A	O4'-C1'-N9	5.28	112.42	108.20
21	CA	838(A)	U	C2-N1-C1'	5.27	124.02	117.70
21	CA	421	U	N3-C2-O2	-5.26	118.52	122.20
21	AA	1378	C	N1-C2-O2	5.26	122.06	118.90
59	BA	1837	C	C2-N1-C1'	5.26	124.59	118.80
59	DA	165	U	O4'-C1'-N1	5.26	112.41	108.20
59	BA	2174	C	C6-N1-C2	-5.25	118.20	120.30
59	DA	935	C	C2-N1-C1'	5.25	124.57	118.80
59	BA	1420	U	N3-C2-O2	-5.23	118.54	122.20
59	DA	2032	G	C8-N9-C4	-5.23	104.31	106.40
21	AA	1086	U	C2-N1-C1'	5.23	123.98	117.70
59	DA	1963	U	N3-C2-O2	-5.23	118.54	122.20
59	DA	2598	A	N1-C6-N6	5.22	121.73	118.60
59	DA	1139	G	O5'-P-OP2	-5.22	101.00	105.70
21	CA	421	U	N1-C2-O2	5.22	126.45	122.80
59	BA	270(L)	C	N3-C2-O2	-5.21	118.25	121.90
59	DA	840	C	C6-N1-C2	-5.21	118.22	120.30
20	AY	503	GLY	C-N-CA	5.21	134.72	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	DA	1776	G	C6-C5-N7	-5.21	127.28	130.40
59	BA	2792	G	C8-N9-C4	-5.20	104.32	106.40
21	CA	351	G	N3-C4-C5	-5.20	126.00	128.60
59	DA	2730	C	C2-N1-C1'	5.20	124.52	118.80
59	BA	2092	U	N3-C2-O2	-5.20	118.56	122.20
21	CA	351	G	C8-N9-C4	-5.20	104.32	106.40
59	DA	2055	C	C6-N1-C2	-5.20	118.22	120.30
59	DA	165	U	C2-N1-C1'	5.19	123.93	117.70
59	BA	1673	U	O4'-C1'-N1	5.18	112.35	108.20
56	D1	17	SER	N-CA-C	-5.18	97.02	111.00
28	BF	156	LEU	C-N-CA	-5.17	108.77	121.70
59	BA	1078	U	C2-N1-C1'	5.17	123.91	117.70
1	CB	66	GLY	N-CA-C	5.17	126.03	113.10
59	DA	1909	C	C6-N1-C1'	-5.17	114.59	120.80
22	AW	73	A	N7-C8-N9	5.17	116.38	113.80
21	AA	962	C	C5-C6-N1	5.17	123.58	121.00
59	DA	1314	C	C6-N1-C2	-5.16	118.23	120.30
28	BF	157	VAL	CB-CA-C	5.16	121.20	111.40
59	BA	2866	U	N1-C2-O2	5.16	126.41	122.80
21	AA	235	C	C6-N1-C2	5.16	122.36	120.30
23	AV	17	U	N3-C4-C5	-5.15	111.51	114.60
5	CF	75	LEU	CA-CB-CG	5.15	127.15	115.30
37	DR	116	LEU	CA-CB-CG	5.15	127.15	115.30
59	DA	2780	G	C5-N7-C8	5.15	106.88	104.30
21	AA	1128	C	N1-C2-O2	5.13	121.98	118.90
43	BX	57	LEU	CA-CB-CG	5.13	127.10	115.30
59	BA	2422	A	OP1-P-O3'	5.13	116.48	105.20
22	AW	50	C	C2-N1-C1'	-5.12	113.16	118.80
59	DA	1776	G	C4-N9-C1'	5.11	133.15	126.50
34	BO	8	LEU	CA-CB-CG	5.11	127.05	115.30
32	DK	105	LEU	CA-CB-CG	5.10	127.04	115.30
21	AA	1083	U	O4'-C1'-N1	5.10	112.28	108.20
21	AA	1190	G	C4-N9-C1'	5.10	133.12	126.50
11	CL	34	ARG	N-CA-C	5.10	124.76	111.00
59	DA	1313	U	C5-C6-N1	5.09	125.25	122.70
39	BT	79	HIS	N-CA-C	5.09	124.74	111.00
21	AA	443	C	N1-C2-O2	5.08	121.95	118.90
59	BA	2581	G	N3-C4-N9	5.08	129.05	126.00
59	DA	270(L)	C	C6-N1-C2	-5.08	118.27	120.30
21	AA	1504	G	P-O3'-C3'	5.08	125.79	119.70
21	CA	1009	G	O4'-C1'-N9	5.08	112.26	108.20
59	BA	1872	A	N1-C6-N6	5.07	121.64	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	DA	1378	A	O4'-C1'-N9	5.07	112.25	108.20
59	DA	1776	G	C4-C5-N7	5.06	112.83	110.80
59	DA	1909	C	N1-C2-O2	5.06	121.94	118.90
59	DA	897	C	C2-N1-C1'	5.06	124.37	118.80
59	BA	1493	C	C5-C6-N1	5.06	123.53	121.00
59	BA	2712	U	N3-C2-O2	-5.05	118.66	122.20
21	AA	68(H)	G	O4'-C1'-N9	5.04	112.23	108.20
59	DA	691	C	C6-N1-C2	-5.04	118.28	120.30
59	BA	2118	U	C2-N1-C1'	5.03	123.74	117.70
59	DA	302	C	O4'-C1'-N1	5.03	112.23	108.20
9	AJ	16	LEU	CA-CB-CG	5.03	126.87	115.30
59	BA	1314	C	N1-C2-O2	5.03	121.92	118.90
59	DA	2389	G	N3-C4-N9	-5.03	122.98	126.00
21	CA	687	A	P-O3'-C3'	5.03	125.73	119.70
29	DG	116	ASP	C-N-CA	5.03	134.27	121.70
1	AB	185	ILE	O-C-N	5.03	130.74	122.70
59	DA	2473	U	C2-N1-C1'	5.03	123.73	117.70
59	BA	2585	U	N3-C2-O2	-5.02	118.69	122.20
59	DA	506	G	O4'-C1'-N9	5.02	112.22	108.20
59	DA	2422	A	P-O3'-C3'	5.02	125.72	119.70
21	CA	717	C	C2-N1-C1'	5.01	124.31	118.80
59	BA	2422	A	C8-N9-C4	-5.01	103.80	105.80
21	CA	115	G	P-O3'-C3'	5.01	125.71	119.70
59	BA	2056	G	C4-C5-N7	5.00	112.80	110.80
59	BA	476	G	C8-N9-C4	-5.00	104.40	106.40
59	BA	479	A	N1-C6-N6	-5.00	115.60	118.60
59	DA	935	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	162	ILE	Peptide
1	AB	163	PHE	Peptide
10	AK	109	VAL	Peptide
11	AL	57	LYS	Peptide
20	AY	31	ARG	Peptide
20	AY	34	TYR	Peptide
20	AY	630	GLN	Peptide
56	B1	16	ASN	Peptide
56	B1	17	SER	Peptide
25	BC	171	ALA	Peptide

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Mol	Chain	Res	Type	Group
25	BC	60	ARG	Peptide
25	BC	88	GLU	Peptide
28	BF	154	VAL	Peptide
28	BF	173	VAL	Peptide
29	BG	113	ARG	Peptide
31	BJ	83	UNK	Peptide
38	BS	100	ALA	Peptide
38	BS	46	VAL	Peptide
39	BT	28	VAL	Peptide
39	BT	48	ILE	Peptide
1	CB	163	PHE	Peptide
11	CL	32	PHE	Peptide
20	CY	162	VAL	Peptide
20	CY	31	ARG	Peptide
20	CY	32	ILE	Peptide
20	CY	329	ARG	Peptide
20	CY	34	TYR	Peptide
20	CY	502	GLY	Peptide,Mainchain
20	CY	630	GLN	Peptide
56	D1	16	ASN	Peptide
56	D1	17	SER	Peptide
56	D1	18	ILE	Peptide
25	DC	171	ALA	Peptide
25	DC	211	ARG	Peptide
26	DD	78	LYS	Peptide
28	DF	154	VAL	Peptide
28	DF	173	VAL	Peptide
29	DG	113	ARG	Peptide
31	DJ	83	UNK	Peptide
38	DS	100	ALA	Peptide
38	DS	46	VAL	Peptide
39	DT	28	VAL	Peptide
42	DW	75	TYR	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	233/235 (99%)	173 (74%)	40 (17%)	20 (9%)	1	9
1	CB	233/235 (99%)	174 (75%)	36 (16%)	23 (10%)	0	7
2	AC	205/207 (99%)	137 (67%)	44 (22%)	24 (12%)	0	5
2	CC	205/207 (99%)	152 (74%)	34 (17%)	19 (9%)	0	8
3	AD	206/208 (99%)	146 (71%)	42 (20%)	18 (9%)	1	9
3	CD	206/208 (99%)	149 (72%)	46 (22%)	11 (5%)	2	17
4	AE	149/151 (99%)	107 (72%)	31 (21%)	11 (7%)	1	11
4	CE	149/151 (99%)	116 (78%)	24 (16%)	9 (6%)	1	15
5	AF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1	12
5	CF	99/101 (98%)	81 (82%)	7 (7%)	11 (11%)	0	6
6	AG	153/155 (99%)	120 (78%)	27 (18%)	6 (4%)	3	25
6	CG	153/155 (99%)	119 (78%)	27 (18%)	7 (5%)	2	21
7	AH	136/138 (99%)	98 (72%)	22 (16%)	16 (12%)	0	5
7	CH	136/138 (99%)	102 (75%)	21 (15%)	13 (10%)	0	8
8	AI	125/127 (98%)	88 (70%)	26 (21%)	11 (9%)	1	8
8	CI	125/127 (98%)	92 (74%)	25 (20%)	8 (6%)	1	14
9	AJ	97/99 (98%)	71 (73%)	17 (18%)	9 (9%)	0	8
9	CJ	97/99 (98%)	71 (73%)	16 (16%)	10 (10%)	0	7
10	AK	117/119 (98%)	74 (63%)	25 (21%)	18 (15%)	0	3
10	CK	117/119 (98%)	78 (67%)	26 (22%)	13 (11%)	0	6
11	AL	123/125 (98%)	42 (34%)	46 (37%)	35 (28%)	0	0
11	CL	123/125 (98%)	39 (32%)	44 (36%)	40 (32%)	0	0
12	AM	123/125 (98%)	86 (70%)	24 (20%)	13 (11%)	0	7
12	CM	123/125 (98%)	91 (74%)	18 (15%)	14 (11%)	0	6
13	AN	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	CN	58/60 (97%)	40 (69%)	14 (24%)	4 (7%)	1	12
14	AO	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	9
14	CO	86/88 (98%)	66 (77%)	15 (17%)	5 (6%)	1	16
15	AP	82/84 (98%)	55 (67%)	18 (22%)	9 (11%)	0	6
15	CP	82/84 (98%)	59 (72%)	18 (22%)	5 (6%)	1	15
16	AQ	98/100 (98%)	68 (69%)	18 (18%)	12 (12%)	0	5
16	CQ	98/100 (98%)	68 (69%)	20 (20%)	10 (10%)	0	7
17	AR	68/70 (97%)	50 (74%)	12 (18%)	6 (9%)	1	8
17	CR	68/70 (97%)	52 (76%)	10 (15%)	6 (9%)	1	8
18	AS	77/79 (98%)	51 (66%)	18 (23%)	8 (10%)	0	7
18	CS	77/79 (98%)	56 (73%)	12 (16%)	9 (12%)	0	5
19	AT	97/99 (98%)	72 (74%)	17 (18%)	8 (8%)	1	9
19	CT	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	9
20	AY	685/687 (100%)	431 (63%)	168 (24%)	86 (13%)	0	5
20	CY	685/687 (100%)	457 (67%)	156 (23%)	72 (10%)	0	7
24	AU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
24	CU	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
25	BC	226/228 (99%)	108 (48%)	70 (31%)	48 (21%)	0	1
25	DC	226/228 (99%)	105 (46%)	75 (33%)	46 (20%)	0	1
26	BD	273/275 (99%)	180 (66%)	54 (20%)	39 (14%)	0	3
26	DD	273/275 (99%)	188 (69%)	47 (17%)	38 (14%)	0	3
27	BE	203/205 (99%)	130 (64%)	43 (21%)	30 (15%)	0	3
27	DE	203/205 (99%)	133 (66%)	36 (18%)	34 (17%)	0	2
28	BF	206/208 (99%)	126 (61%)	54 (26%)	26 (13%)	0	5
28	DF	206/208 (99%)	137 (66%)	47 (23%)	22 (11%)	0	6
29	BG	179/181 (99%)	120 (67%)	46 (26%)	13 (7%)	1	11
29	DG	179/181 (99%)	127 (71%)	44 (25%)	8 (4%)	2	21
30	BH	165/167 (99%)	118 (72%)	29 (18%)	18 (11%)	0	6
30	DH	165/167 (99%)	118 (72%)	32 (19%)	15 (9%)	1	8
32	BK	138/140 (99%)	88 (64%)	33 (24%)	17 (12%)	0	5
32	DK	138/140 (99%)	86 (62%)	33 (24%)	19 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	BN	136/138 (99%)	93 (68%)	24 (18%)	19 (14%)	0	3
33	DN	136/138 (99%)	91 (67%)	27 (20%)	18 (13%)	0	4
34	BO	120/122 (98%)	92 (77%)	20 (17%)	8 (7%)	1	13
34	DO	120/122 (98%)	95 (79%)	20 (17%)	5 (4%)	3	23
35	BP	144/146 (99%)	81 (56%)	36 (25%)	27 (19%)	0	2
35	DP	144/146 (99%)	76 (53%)	35 (24%)	33 (23%)	0	1
36	BQ	139/141 (99%)	87 (63%)	32 (23%)	20 (14%)	0	3
36	DQ	139/141 (99%)	91 (66%)	31 (22%)	17 (12%)	0	5
37	BR	115/117 (98%)	83 (72%)	21 (18%)	11 (10%)	0	8
37	DR	115/117 (98%)	91 (79%)	17 (15%)	7 (6%)	1	15
38	BS	97/99 (98%)	56 (58%)	25 (26%)	16 (16%)	0	2
38	DS	97/99 (98%)	57 (59%)	25 (26%)	15 (16%)	0	3
39	BT	136/138 (99%)	76 (56%)	41 (30%)	19 (14%)	0	3
39	DT	136/138 (99%)	82 (60%)	28 (21%)	26 (19%)	0	2
40	BU	115/117 (98%)	79 (69%)	25 (22%)	11 (10%)	0	8
40	DU	115/117 (98%)	80 (70%)	23 (20%)	12 (10%)	0	7
41	BV	99/101 (98%)	57 (58%)	28 (28%)	14 (14%)	0	3
41	DV	99/101 (98%)	64 (65%)	22 (22%)	13 (13%)	0	4
42	BW	111/113 (98%)	82 (74%)	14 (13%)	15 (14%)	0	4
42	DW	111/113 (98%)	81 (73%)	16 (14%)	14 (13%)	0	5
43	BX	91/93 (98%)	73 (80%)	12 (13%)	6 (7%)	1	13
43	DX	91/93 (98%)	70 (77%)	16 (18%)	5 (6%)	2	17
44	BY	105/107 (98%)	50 (48%)	30 (29%)	25 (24%)	0	0
44	DY	105/107 (98%)	50 (48%)	34 (32%)	21 (20%)	0	1
45	BZ	183/185 (99%)	116 (63%)	46 (25%)	21 (12%)	0	6
45	DZ	183/185 (99%)	121 (66%)	44 (24%)	18 (10%)	0	7
46	B0	82/84 (98%)	59 (72%)	16 (20%)	7 (8%)	1	9
46	D0	82/84 (98%)	65 (79%)	13 (16%)	4 (5%)	2	19
47	B2	69/71 (97%)	49 (71%)	14 (20%)	6 (9%)	1	9
47	D2	69/71 (97%)	50 (72%)	17 (25%)	2 (3%)	4	31
48	B3	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	D3	58/60 (97%)	44 (76%)	9 (16%)	5 (9%)	1	9
49	B5	57/59 (97%)	44 (77%)	4 (7%)	9 (16%)	0	2
49	D5	57/59 (97%)	42 (74%)	11 (19%)	4 (7%)	1	12
50	B6	48/50 (96%)	28 (58%)	9 (19%)	11 (23%)	0	1
50	D6	48/50 (96%)	27 (56%)	8 (17%)	13 (27%)	0	0
51	B7	47/49 (96%)	30 (64%)	13 (28%)	4 (8%)	1	9
51	D7	47/49 (96%)	34 (72%)	11 (23%)	2 (4%)	2	22
52	B8	62/64 (97%)	42 (68%)	7 (11%)	13 (21%)	0	1
52	D8	62/64 (97%)	40 (64%)	11 (18%)	11 (18%)	0	2
53	B9	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	16
53	D9	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	16
56	B1	91/93 (98%)	56 (62%)	17 (19%)	18 (20%)	0	1
56	D1	91/93 (98%)	59 (65%)	18 (20%)	14 (15%)	0	3
57	B4	33/35 (94%)	15 (46%)	11 (33%)	7 (21%)	0	1
57	D4	33/35 (94%)	15 (46%)	9 (27%)	9 (27%)	0	0
58	Be	70/102 (69%)	36 (51%)	29 (41%)	5 (7%)	1	12
58	De	70/102 (69%)	40 (57%)	22 (31%)	8 (11%)	0	6
All	All	13304/13576 (98%)	8904 (67%)	2822 (21%)	1578 (12%)	0	5

All (1578) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	17	PHE
1	AB	22	LYS
1	AB	35	GLU
1	AB	75	LYS
1	AB	76	GLN
1	AB	96	ARG
1	AB	160	ASP
2	AC	5	ILE
2	AC	10	PHE
2	AC	29	TYR
2	AC	49	SER
2	AC	161	GLU
3	AD	34	GLU
3	AD	89	THR

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Mol	Chain	Res	Type
3	AD	134	ASP
3	AD	172	PRO
3	AD	176	LEU
4	AE	6	PHE
4	AE	12	LEU
4	AE	77	PRO
4	AE	79	GLU
5	AF	69	GLU
5	AF	70	ASP
5	AF	93	SER
6	AG	15	ASP
6	AG	81	GLY
7	AH	22	GLU
8	AI	89	ASN
8	AI	107	ARG
8	AI	118	LYS
9	AJ	38	ILE
9	AJ	55	LYS
9	AJ	75	ILE
10	AK	36	ASP
10	AK	41	THR
10	AK	43	SER
10	AK	109	VAL
11	AL	7	ILE
11	AL	34	ARG
11	AL	39	VAL
11	AL	43	VAL
11	AL	46	LYS
11	AL	66	VAL
11	AL	80	HIS
11	AL	94	PRO
11	AL	122	THR
12	AM	50	GLU
12	AM	106	ASN
12	AM	118	ALA
13	AN	15	LYS
15	AP	35	LYS
16	AQ	12	SER
16	AQ	14	LYS
16	AQ	72	ARG
16	AQ	74	LEU
16	AQ	83	ASP

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Mol	Chain	Res	Type
18	AS	67	VAL
18	AS	72	GLY
19	AT	50	GLU
19	AT	74	LYS
19	AT	75	ASN
19	AT	76	ALA
19	AT	100	ILE
20	AY	33	LEU
20	AY	35	TYR
20	AY	36	THR
20	AY	39	ILE
20	AY	75	LYS
20	AY	88	VAL
20	AY	92	ILE
20	AY	203	GLU
20	AY	204	GLU
20	AY	266	ASN
20	AY	330	VAL
20	AY	331	TYR
20	AY	349	LYS
20	AY	393	ASP
20	AY	395	PRO
20	AY	400	GLU
20	AY	418	LYS
20	AY	456	GLU
20	AY	544	LYS
20	AY	555	LEU
20	AY	566	THR
20	AY	567	LEU
20	AY	615	GLU
20	AY	628	ARG
20	AY	631	ILE
20	AY	680	PRO
25	BC	3	LYS
25	BC	17	PRO
25	BC	35	THR
25	BC	41	THR
25	BC	60	ARG
25	BC	80	LYS
25	BC	114	VAL
25	BC	115	VAL
25	BC	119	ASP

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Mol	Chain	Res	Type
25	BC	141	PRO
25	BC	172	ILE
25	BC	182	PRO
25	BC	184	GLU
25	BC	211	ARG
25	BC	212	SER
25	BC	223	VAL
25	BC	227	PRO
25	BC	228	HIS
26	BD	49	ILE
26	BD	79	VAL
26	BD	87	ASN
26	BD	89	SER
26	BD	99	ASP
26	BD	127	VAL
26	BD	166	GLN
26	BD	231	HIS
26	BD	273	ARG
27	BE	11	MET
27	BE	12	THR
27	BE	14	ILE
27	BE	34	VAL
27	BE	54	GLN
27	BE	56	PRO
27	BE	60	ASN
27	BE	62	PRO
27	BE	63	LEU
27	BE	67	PHE
27	BE	68	ALA
27	BE	74	PRO
27	BE	77	ILE
27	BE	94	GLU
27	BE	128	SER
27	BE	144	ARG
27	BE	147	PRO
27	BE	188	VAL
27	BE	204	ALA
28	BF	7	TYR
28	BF	10	PRO
28	BF	22	ALA
28	BF	47	GLY
28	BF	59	TYR

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Mol	Chain	Res	Type
28	BF	67	GLN
28	BF	84	VAL
28	BF	89	VAL
28	BF	149	ASP
28	BF	192	LEU
29	BG	87	PRO
29	BG	96	ARG
30	BH	30	LYS
30	BH	41	MET
30	BH	94	TYR
30	BH	124	GLU
30	BH	155	SER
30	BH	158	HIS
30	BH	173	PRO
32	BK	5	VAL
32	BK	62	ASP
32	BK	102	GLU
32	BK	103	GLN
32	BK	114	ASP
32	BK	118	THR
33	BN	17	ASP
33	BN	18	ALA
33	BN	50	ASP
33	BN	56	ASN
33	BN	66	LYS
33	BN	111	PRO
33	BN	126	PRO
33	BN	128	HIS
33	BN	130	HIS
33	BN	133	GLN
34	BO	23	ARG
35	BP	14	LYS
35	BP	17	LYS
35	BP	39	LYS
35	BP	45	LEU
35	BP	57	THR
35	BP	71	VAL
35	BP	141	ALA
36	BQ	18	LYS
36	BQ	83	MET
36	BQ	85	LYS
36	BQ	91	GLU

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Mol	Chain	Res	Type
37	BR	14	SER
38	BS	47	THR
38	BS	48	LEU
38	BS	62	LYS
38	BS	63	THR
38	BS	98	VAL
38	BS	101	LEU
38	BS	104	GLY
38	BS	106	ARG
39	BT	30	VAL
39	BT	49	VAL
39	BT	50	ILE
39	BT	68	TYR
39	BT	94	ALA
39	BT	104	ASN
39	BT	128	GLU
40	BU	86	ALA
40	BU	88	ILE
40	BU	91	ASP
41	BV	46	VAL
41	BV	96	ILE
42	BW	12	ILE
42	BW	75	TYR
42	BW	76	VAL
43	BX	7	VAL
43	BX	12	VAL
44	BY	32	PRO
44	BY	53	PRO
44	BY	95	LYS
44	BY	107	ASP
45	BZ	71	VAL
45	BZ	72	ARG
45	BZ	73	GLN
45	BZ	134	PRO
45	BZ	140	ASP
45	BZ	152	ALA
48	B3	52	HIS
50	B6	9	LEU
50	B6	15	GLU
50	B6	20	ASN
52	B8	6	THR
52	B8	32	LEU

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Mol	Chain	Res	Type
52	B8	34	TRP
52	B8	49	VAL
56	B1	12	PRO
56	B1	26	ARG
56	B1	35	THR
56	B1	87	PRO
57	B4	16	CYS
58	Be	62	VAL
58	Be	121	VAL
1	CB	17	PHE
1	CB	66	GLY
1	CB	75	LYS
1	CB	76	GLN
1	CB	96	ARG
1	CB	160	ASP
1	CB	235	SER
1	CB	236	TYR
2	CC	3	ASN
2	CC	4	LYS
2	CC	5	ILE
2	CC	14	ILE
2	CC	62	ASP
2	CC	63	ASN
2	CC	207	VAL
3	CD	4	TYR
3	CD	7	PRO
4	CE	6	PHE
4	CE	79	GLU
5	CF	44	GLY
5	CF	69	GLU
5	CF	70	ASP
6	CG	15	ASP
6	CG	17	VAL
6	CG	35	LYS
7	CH	22	GLU
9	CJ	75	ILE
10	CK	41	THR
10	CK	43	SER
10	CK	109	VAL
10	CK	111	ASP
11	CL	6	THR
11	CL	7	ILE

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Mol	Chain	Res	Type
11	CL	34	ARG
11	CL	39	VAL
11	CL	43	VAL
11	CL	46	LYS
11	CL	51	ALA
11	CL	66	VAL
11	CL	67	THR
11	CL	80	HIS
11	CL	94	PRO
11	CL	100	ILE
11	CL	108	ALA
12	CM	7	VAL
12	CM	12	ASN
12	CM	50	GLU
12	CM	51	ALA
14	CO	47	LYS
15	CP	46	PRO
16	CQ	12	SER
16	CQ	72	ARG
16	CQ	74	LEU
17	CR	28	GLU
17	CR	37	VAL
18	CS	28	LYS
18	CS	67	VAL
19	CT	50	GLU
19	CT	95	ALA
19	CT	100	ILE
20	CY	39	ILE
20	CY	88	VAL
20	CY	92	ILE
20	CY	111	SER
20	CY	146	LEU
20	CY	161	PRO
20	CY	204	GLU
20	CY	257	PRO
20	CY	266	ASN
20	CY	330	VAL
20	CY	331	TYR
20	CY	400	GLU
20	CY	418	LYS
20	CY	476	VAL
20	CY	544	LYS

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Mol	Chain	Res	Type
20	CY	566	THR
20	CY	567	LEU
20	CY	631	ILE
20	CY	680	PRO
25	DC	17	PRO
25	DC	41	THR
25	DC	42	VAL
25	DC	43	GLU
25	DC	52	PRO
25	DC	80	LYS
25	DC	96	GLY
25	DC	115	VAL
25	DC	141	PRO
25	DC	142	LYS
25	DC	162	ILE
25	DC	176	VAL
25	DC	182	PRO
25	DC	184	GLU
25	DC	212	SER
25	DC	223	VAL
25	DC	227	PRO
25	DC	228	HIS
26	DD	3	VAL
26	DD	27	THR
26	DD	36	PRO
26	DD	46	GLN
26	DD	49	ILE
26	DD	79	VAL
26	DD	89	SER
26	DD	165	ILE
26	DD	166	GLN
26	DD	187	GLY
26	DD	200	ASP
26	DD	273	ARG
27	DE	11	MET
27	DE	12	THR
27	DE	13	ARG
27	DE	56	PRO
27	DE	62	PRO
27	DE	63	LEU
27	DE	67	PHE
27	DE	68	ALA

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Mol	Chain	Res	Type
27	DE	72	VAL
27	DE	77	ILE
27	DE	128	SER
27	DE	129	HIS
27	DE	144	ARG
27	DE	187	ALA
28	DF	3	GLU
28	DF	7	TYR
28	DF	10	PRO
28	DF	21	ALA
28	DF	84	VAL
28	DF	89	VAL
28	DF	192	LEU
29	DG	87	PRO
29	DG	130	ASN
29	DG	137	GLU
30	DH	124	GLU
30	DH	141	VAL
30	DH	155	SER
30	DH	165	ALA
30	DH	172	LYS
30	DH	173	PRO
32	DK	45	THR
32	DK	96	VAL
32	DK	137	GLU
33	DN	17	ASP
33	DN	18	ALA
33	DN	25	ARG
33	DN	126	PRO
33	DN	128	HIS
33	DN	130	HIS
33	DN	133	GLN
34	DO	14	THR
34	DO	23	ARG
35	DP	9	ASN
35	DP	22	GLY
35	DP	45	LEU
35	DP	57	THR
35	DP	71	VAL
35	DP	110	TYR
35	DP	120	ALA
35	DP	141	ALA

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Mol	Chain	Res	Type
35	DP	149	GLU
36	DQ	29	PHE
36	DQ	83	MET
36	DQ	85	LYS
36	DQ	92	GLY
36	DQ	133	ARG
36	DQ	136	ALA
37	DR	103	ARG
38	DS	22	GLY
38	DS	47	THR
38	DS	48	LEU
38	DS	62	LYS
38	DS	98	VAL
38	DS	101	LEU
38	DS	104	GLY
38	DS	106	ARG
39	DT	3	ARG
39	DT	30	VAL
39	DT	49	VAL
39	DT	80	SER
39	DT	86	ILE
39	DT	104	ASN
39	DT	137	LYS
40	DU	24	TYR
40	DU	88	ILE
40	DU	90	VAL
41	DV	29	PRO
41	DV	46	VAL
41	DV	50	PRO
41	DV	78	LYS
41	DV	96	ILE
41	DV	97	LYS
42	DW	12	ILE
42	DW	14	PRO
42	DW	15	ARG
42	DW	61	ASN
42	DW	74	ALA
42	DW	75	TYR
42	DW	77	ASP
42	DW	81	ALA
43	DX	7	VAL
43	DX	12	VAL

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Mol	Chain	Res	Type
44	DY	32	PRO
44	DY	39	VAL
44	DY	53	PRO
44	DY	56	PRO
44	DY	77	PRO
45	DZ	71	VAL
45	DZ	72	ARG
45	DZ	92	SER
45	DZ	140	ASP
45	DZ	152	ALA
46	D0	15	ASP
47	D2	47	ASN
47	D2	48	HIS
48	D3	41	PRO
50	D6	8	LYS
50	D6	9	LEU
50	D6	15	GLU
50	D6	20	ASN
50	D6	27	LYS
50	D6	29	ASN
52	D8	32	LEU
52	D8	49	VAL
56	D1	12	PRO
56	D1	35	THR
56	D1	87	PRO
56	D1	94	LEU
57	D4	16	CYS
58	De	52	ALA
1	AB	97	TRP
1	AB	164	VAL
1	AB	165	VAL
1	AB	236	TYR
2	AC	4	LYS
2	AC	51	GLY
2	AC	61	ALA
2	AC	74	GLY
2	AC	102	ASN
2	AC	110	ASN
2	AC	160	ALA
2	AC	181	ASN
3	AD	7	PRO
3	AD	27	TYR

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Mol	Chain	Res	Type
3	AD	44	GLY
3	AD	88	VAL
4	AE	67	VAL
5	AF	15	ASP
5	AF	38	GLU
7	AH	93	VAL
8	AI	35	GLU
8	AI	117	HIS
9	AJ	53	PRO
10	AK	69	ALA
10	AK	88	GLY
10	AK	89	ALA
10	AK	91	ARG
10	AK	111	ASP
10	AK	119	CYS
10	AK	120	ARG
11	AL	6	THR
11	AL	19	ARG
11	AL	35	GLY
11	AL	51	ALA
11	AL	56	ALA
11	AL	69	TYR
11	AL	76	ASN
11	AL	90	VAL
11	AL	96	VAL
11	AL	97	ARG
11	AL	104	VAL
12	AM	46	LYS
12	AM	51	ALA
12	AM	121	LYS
13	AN	13	THR
13	AN	56	VAL
14	AO	47	LYS
14	AO	73	GLU
14	AO	88	ARG
15	AP	24	ALA
15	AP	28	ARG
16	AQ	28	PRO
16	AQ	71	PHE
16	AQ	73	VAL
16	AQ	82	MET
17	AR	37	VAL

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Mol	Chain	Res	Type
17	AR	59	SER
19	AT	72	LEU
20	AY	21	ILE
20	AY	25	LYS
20	AY	32	ILE
20	AY	146	LEU
20	AY	161	PRO
20	AY	162	VAL
20	AY	224	ASP
20	AY	233	GLU
20	AY	257	PRO
20	AY	281	PRO
20	AY	347	GLY
20	AY	383	THR
20	AY	473	ASP
20	AY	498	ILE
20	AY	568	TYR
20	AY	600	VAL
25	BC	22	THR
25	BC	36	ALA
25	BC	43	GLU
25	BC	59	VAL
25	BC	75	VAL
25	BC	76	LEU
25	BC	96	GLY
25	BC	130	ARG
25	BC	162	ILE
25	BC	210	LEU
26	BD	36	PRO
26	BD	42	GLY
26	BD	43	ARG
26	BD	46	GLN
26	BD	78	LYS
26	BD	165	ILE
26	BD	200	ASP
26	BD	236	GLY
26	BD	239	ARG
27	BE	13	ARG
27	BE	86	PRO
27	BE	129	HIS
27	BE	187	ALA
28	BF	21	ALA

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Mol	Chain	Res	Type
28	BF	53	THR
28	BF	79	GLY
28	BF	158	THR
28	BF	194	MET
29	BG	123	ASN
29	BG	177	GLY
30	BH	45	VAL
30	BH	165	ALA
30	BH	174	GLY
32	BK	30	HIS
32	BK	63	ARG
33	BN	2	LYS
33	BN	67	LEU
33	BN	129	PRO
34	BO	5	GLN
34	BO	29	ASN
34	BO	31	LYS
34	BO	96	THR
35	BP	10	PRO
35	BP	13	ASN
35	BP	49	ARG
35	BP	50	ARG
35	BP	66	GLY
35	BP	106	LEU
35	BP	110	TYR
35	BP	149	GLU
36	BQ	4	PRO
36	BQ	6	ARG
36	BQ	30	GLY
36	BQ	92	GLY
36	BQ	134	ARG
36	BQ	139	GLU
37	BR	8	ARG
37	BR	103	ARG
38	BS	13	ARG
38	BS	14	VAL
38	BS	43	GLU
38	BS	105	ALA
39	BT	28	VAL
39	BT	59	THR
39	BT	80	SER
39	BT	83	ILE

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Mol	Chain	Res	Type
40	BU	99	ALA
40	BU	116	ALA
41	BV	50	PRO
41	BV	53	GLU
41	BV	68	LYS
41	BV	97	LYS
42	BW	25	ARG
42	BW	61	ASN
42	BW	74	ALA
42	BW	77	ASP
42	BW	80	PRO
42	BW	93	ALA
44	BY	29	GLU
44	BY	39	VAL
44	BY	41	GLY
44	BY	77	PRO
44	BY	78	ALA
45	BZ	92	SER
46	B0	13	GLY
47	B2	37	PHE
47	B2	48	HIS
49	B5	23	HIS
49	B5	25	LEU
49	B5	53	ALA
50	B6	8	LYS
50	B6	17	LYS
50	B6	27	LYS
50	B6	31	PRO
50	B6	49	HIS
51	B7	23	ARG
52	B8	18	ALA
52	B8	24	ALA
52	B8	30	ARG
52	B8	51	ALA
56	B1	22	GLY
56	B1	23	LYS
56	B1	32	LYS
56	B1	34	THR
56	B1	53	VAL
56	B1	94	LEU
57	B4	2	LYS
57	B4	4	GLY

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Mol	Chain	Res	Type
57	B4	33	VAL
58	Be	119	GLY
1	CB	34	ALA
1	CB	97	TRP
1	CB	103	THR
1	CB	164	VAL
1	CB	165	VAL
2	CC	10	PHE
2	CC	162	GLN
3	CD	5	ILE
3	CD	172	PRO
4	CE	11	ILE
4	CE	67	VAL
4	CE	77	PRO
5	CF	38	GLU
6	CG	10	ARG
6	CG	19	GLY
7	CH	43	GLY
7	CH	74	PRO
7	CH	93	VAL
7	CH	103	VAL
8	CI	109	VAL
9	CJ	81	THR
10	CK	69	ALA
10	CK	90	GLY
11	CL	58	VAL
11	CL	92	ASP
11	CL	96	VAL
11	CL	101	VAL
11	CL	104	VAL
11	CL	112	ASP
11	CL	121	GLY
11	CL	122	THR
11	CL	123	LYS
11	CL	126	LYS
12	CM	46	LYS
13	CN	15	LYS
13	CN	58	LYS
16	CQ	28	PRO
16	CQ	49	GLU
16	CQ	82	MET
18	CS	45	VAL

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Mol	Chain	Res	Type
18	CS	46	GLY
18	CS	72	GLY
19	CT	74	LYS
19	CT	79	ARG
20	CY	21	ILE
20	CY	64	THR
20	CY	102	ASP
20	CY	162	VAL
20	CY	281	PRO
20	CY	360	ALA
20	CY	384	ILE
20	CY	437	THR
20	CY	501	THR
20	CY	528	ALA
20	CY	565	VAL
20	CY	681	LYS
25	DC	3	LYS
25	DC	38	PHE
25	DC	59	VAL
25	DC	60	ARG
25	DC	61	GLY
25	DC	106	ASP
25	DC	114	VAL
25	DC	161	ARG
26	DD	43	ARG
26	DD	99	ASP
26	DD	236	GLY
26	DD	239	ARG
26	DD	249	PRO
27	DE	14	ILE
27	DE	74	PRO
27	DE	86	PRO
27	DE	130	GLY
27	DE	180	ASN
28	DF	47	GLY
28	DF	67	GLN
28	DF	158	THR
29	DG	82	LEU
29	DG	163	ALA
30	DH	41	MET
32	DK	5	VAL
32	DK	13	PRO

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Mol	Chain	Res	Type
32	DK	30	HIS
32	DK	102	GLU
32	DK	103	GLN
33	DN	24	GLY
33	DN	111	PRO
34	DO	26	LYS
34	DO	29	ASN
34	DO	96	THR
35	DP	13	ASN
35	DP	14	LYS
35	DP	17	LYS
35	DP	48	PRO
35	DP	50	ARG
35	DP	58	THR
35	DP	66	GLY
35	DP	89	ALA
35	DP	106	LEU
35	DP	107	LYS
35	DP	145	PRO
36	DQ	4	PRO
36	DQ	8	LYS
36	DQ	30	GLY
36	DQ	75	THR
38	DS	96	GLY
39	DT	2	ASN
39	DT	16	ARG
39	DT	28	VAL
39	DT	48	ILE
39	DT	50	ILE
39	DT	90	GLN
39	DT	128	GLU
40	DU	9	VAL
42	DW	25	ARG
42	DW	65	LEU
42	DW	80	PRO
43	DX	4	ALA
43	DX	62	LYS
44	DY	26	LYS
44	DY	78	ALA
44	DY	80	GLY
44	DY	97	ARG
44	DY	101	LYS

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Mol	Chain	Res	Type
44	DY	107	ASP
45	DZ	62	PRO
45	DZ	73	GLN
45	DZ	166	SER
46	D0	13	GLY
48	D3	52	HIS
49	D5	24	ALA
49	D5	53	ALA
50	D6	16	CYS
50	D6	28	ARG
50	D6	31	PRO
50	D6	49	HIS
52	D8	30	ARG
52	D8	45	GLY
52	D8	51	ALA
56	D1	32	LYS
56	D1	36	GLY
56	D1	53	VAL
57	D4	15	ILE
57	D4	33	VAL
58	De	81	ILE
1	AB	34	ALA
2	AC	75	VAL
2	AC	109	PRO
3	AD	26	CYS
3	AD	28	SER
3	AD	40	PRO
3	AD	47	ARG
3	AD	48	ALA
3	AD	142	PRO
4	AE	21	ALA
4	AE	49	PRO
6	AG	10	ARG
6	AG	129	GLU
6	AG	147	ALA
7	AH	2	LEU
7	AH	44	PHE
7	AH	54	ASP
7	AH	74	PRO
7	AH	103	VAL
7	AH	105	ARG
7	AH	107	LEU

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Mol	Chain	Res	Type
8	AI	31	GLN
8	AI	43	ALA
8	AI	104	ARG
8	AI	109	VAL
9	AJ	37	PRO
9	AJ	41	PRO
9	AJ	58	ASP
9	AJ	83	GLU
10	AK	37	GLY
10	AK	124	LYS
11	AL	22	SER
11	AL	47	LYS
11	AL	74	GLY
11	AL	89	ARG
11	AL	91	LYS
11	AL	115	LYS
11	AL	120	TYR
11	AL	125	PRO
12	AM	39	ILE
12	AM	124	PRO
13	AN	57	ARG
14	AO	23	GLY
15	AP	44	THR
15	AP	46	PRO
16	AQ	31	LEU
17	AR	28	GLU
17	AR	87	ARG
18	AS	45	VAL
18	AS	78	ARG
20	AY	53	ASP
20	AY	71	THR
20	AY	109	ASP
20	AY	170	ARG
20	AY	185	ALA
20	AY	188	TYR
20	AY	189	GLY
20	AY	191	ASP
20	AY	234	GLY
20	AY	403	GLU
20	AY	436	PRO
20	AY	535	PRO
20	AY	539	ILE

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Mol	Chain	Res	Type
20	AY	614	GLU
20	AY	638	GLY
25	BC	18	ASN
25	BC	34	ALA
25	BC	106	ASP
25	BC	112	ASP
25	BC	142	LYS
25	BC	214	TYR
25	BC	221	PRO
25	BC	224	ARG
26	BD	3	VAL
26	BD	24	ILE
26	BD	28	GLU
26	BD	86	PRO
26	BD	114	GLY
26	BD	241	PRO
26	BD	260	ARG
27	BE	53	PRO
27	BE	192	ASN
28	BF	18	ARG
28	BF	83	PHE
28	BF	171	PRO
29	BG	49	ASP
29	BG	81	LYS
29	BG	82	LEU
29	BG	142	PRO
30	BH	42	ARG
30	BH	141	VAL
30	BH	157	TYR
32	BK	7	VAL
32	BK	89	HIS
33	BN	24	GLY
33	BN	100	GLU
35	BP	31	ALA
35	BP	70	GLN
35	BP	107	LYS
36	BQ	28	ALA
36	BQ	31	ASP
36	BQ	133	ARG
36	BQ	135	ASP
37	BR	107	ASP
38	BS	94	TYR

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Mol	Chain	Res	Type
39	BT	2	ASN
39	BT	24	PRO
39	BT	35	LYS
39	BT	137	LYS
40	BU	78	THR
40	BU	90	VAL
40	BU	92	ARG
41	BV	80	GLN
41	BV	93	GLU
42	BW	14	PRO
42	BW	15	ARG
42	BW	26	GLY
44	BY	18	GLY
44	BY	28	LYS
44	BY	47	LYS
44	BY	48	ALA
44	BY	50	ARG
44	BY	56	PRO
44	BY	58	GLY
44	BY	60	PHE
44	BY	90	LEU
45	BZ	51	ALA
45	BZ	62	PRO
46	B0	33	ALA
46	B0	75	LEU
48	B3	41	PRO
49	B5	24	ALA
49	B5	49	CYS
50	B6	18	ARG
50	B6	44	ARG
50	B6	48	VAL
52	B8	3	LYS
52	B8	19	SER
52	B8	64	TYR
56	B1	15	ALA
56	B1	40	ARG
58	Be	52	ALA
1	CB	8	LYS
1	CB	105	PHE
1	CB	190	THR
2	CC	49	SER
2	CC	160	ALA

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Mol	Chain	Res	Type
2	CC	181	ASN
3	CD	28	SER
3	CD	34	GLU
3	CD	156	GLU
4	CE	129	ILE
5	CF	49	ALA
5	CF	93	SER
7	CH	105	ARG
7	CH	129	VAL
8	CI	35	GLU
8	CI	102	LEU
8	CI	104	ARG
8	CI	106	ALA
9	CJ	33	GLN
10	CK	36	ASP
10	CK	91	ARG
11	CL	17	LYS
11	CL	19	ARG
11	CL	47	LYS
11	CL	56	ALA
11	CL	102	ARG
11	CL	128	ALA
12	CM	21	TYR
12	CM	39	ILE
12	CM	62	ASN
12	CM	101	GLN
13	CN	52	GLN
14	CO	16	ALA
15	CP	28	ARG
15	CP	54	GLU
16	CQ	48	GLU
17	CR	43	PHE
17	CR	87	ARG
19	CT	78	ALA
19	CT	99	LEU
20	CY	22	ASP
20	CY	33	LEU
20	CY	66	THR
20	CY	72	CYS
20	CY	89	ASP
20	CY	99	ARG
20	CY	112	GLN

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Mol	Chain	Res	Type
20	CY	129	LYS
20	CY	175	SER
20	CY	188	TYR
20	CY	200	PRO
20	CY	253	LEU
20	CY	324	ARG
20	CY	347	GLY
20	CY	383	THR
20	CY	395	PRO
20	CY	521	SER
20	CY	539	ILE
20	CY	622	GLY
20	CY	652	MET
25	DC	18	ASN
25	DC	33	LEU
25	DC	167	ASP
25	DC	214	TYR
26	DD	147	LEU
26	DD	186	HIS
26	DD	188	GLU
26	DD	225	ALA
26	DD	232	PRO
26	DD	233	HIS
26	DD	241	PRO
26	DD	260	ARG
26	DD	272	ALA
27	DE	155	LYS
27	DE	169	ASN
27	DE	188	VAL
27	DE	204	ALA
28	DF	22	ALA
28	DF	58	ALA
28	DF	73	ALA
30	DH	123	PHE
30	DH	128	PRO
32	DK	51	ALA
32	DK	63	ARG
33	DN	56	ASN
33	DN	62	VAL
33	DN	91	LEU
33	DN	131	GLN
35	DP	35	HIS

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Mol	Chain	Res	Type
35	DP	53	GLY
35	DP	119	GLU
35	DP	123	LEU
36	DQ	6	ARG
36	DQ	62	GLY
38	DS	14	VAL
38	DS	57	LYS
39	DT	68	TYR
39	DT	78	LEU
39	DT	85	LYS
39	DT	107	ASP
40	DU	92	ARG
40	DU	99	ALA
40	DU	106	PHE
41	DV	68	LYS
41	DV	77	ALA
42	DW	22	ASP
44	DY	7	VAL
44	DY	12	THR
44	DY	48	ALA
44	DY	50	ARG
44	DY	63	LYS
44	DY	91	GLU
45	DZ	32	HIS
45	DZ	78	LYS
45	DZ	159	PRO
46	D0	11	ARG
46	D0	33	ALA
49	D5	47	PRO
50	D6	44	ARG
52	D8	3	LYS
52	D8	6	THR
52	D8	34	TRP
53	D9	5	ALA
56	D1	37	ILE
56	D1	40	ARG
56	D1	52	ARG
56	D1	92	LYS
57	D4	2	LYS
57	D4	9	LEU
1	AB	155	LEU
2	AC	53	ALA

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Mol	Chain	Res	Type
2	AC	112	SER
2	AC	162	GLN
3	AD	5	ILE
6	AG	152	ALA
9	AJ	42	THR
10	AK	35	PRO
10	AK	54	ARG
11	AL	128	ALA
12	AM	13	LYS
12	AM	101	GLN
13	AN	58	LYS
14	AO	25	THR
14	AO	87	ILE
17	AR	45	SER
18	AS	27	GLU
19	AT	46	GLU
19	AT	49	ALA
20	AY	253	LEU
20	AY	269	VAL
20	AY	296	GLY
20	AY	382	GLU
20	AY	396	ARG
20	AY	437	THR
20	AY	541	ALA
20	AY	565	VAL
20	AY	649	LEU
20	AY	652	MET
25	BC	86	GLU
25	BC	167	ASP
26	BD	30	GLU
26	BD	226	MET
26	BD	232	PRO
26	BD	259	THR
26	BD	272	ALA
27	BE	35	GLN
27	BE	72	VAL
28	BF	3	GLU
28	BF	19	GLU
28	BF	66	PRO
28	BF	105	VAL
29	BG	143	GLU
30	BH	21	PRO

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Mol	Chain	Res	Type
30	BH	81	GLU
30	BH	92	ILE
30	BH	156	ALA
32	BK	6	ALA
32	BK	73	PRO
32	BK	81	ALA
32	BK	122	ALA
33	BN	30	ILE
33	BN	119	ARG
34	BO	26	LYS
34	BO	91	LEU
35	BP	68	GLN
35	BP	103	ALA
36	BQ	29	PHE
36	BQ	78	PRO
37	BR	93	GLY
37	BR	102	GLU
38	BS	42	ASP
38	BS	100	ALA
39	BT	85	LYS
40	BU	87	GLY
41	BV	18	LEU
42	BW	73	ALA
44	BY	12	THR
44	BY	70	SER
44	BY	80	GLY
45	BZ	22	GLY
45	BZ	31	ARG
45	BZ	135	GLU
45	BZ	177	PRO
47	B2	13	ALA
48	B3	51	ALA
49	B5	47	PRO
49	B5	57	VAL
51	B7	3	ARG
52	B8	48	PHE
53	B9	27	CYS
56	B1	10	LYS
58	Be	81	ILE
1	CB	20	GLU
1	CB	157	ARG
1	CB	194	PRO

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Mol	Chain	Res	Type
1	CB	215	LEU
2	CC	51	GLY
2	CC	102	ASN
2	CC	132	ARG
2	CC	156	ARG
3	CD	89	THR
3	CD	173	TRP
4	CE	128	PRO
5	CF	51	PRO
7	CH	45	ILE
7	CH	51	VAL
7	CH	107	LEU
8	CI	39	GLY
8	CI	127	LYS
9	CJ	55	LYS
9	CJ	83	GLU
10	CK	54	ARG
10	CK	107	SER
11	CL	55	VAL
11	CL	74	GLY
11	CL	79	GLU
11	CL	93	LEU
12	CM	11	ARG
12	CM	30	ALA
12	CM	114	ARG
14	CO	23	GLY
14	CO	73	GLU
15	CP	68	ASP
16	CQ	31	LEU
17	CR	60	ALA
18	CS	63	THR
18	CS	80	TYR
20	CY	38	ARG
20	CY	50	ALA
20	CY	63	ILE
20	CY	203	GLU
20	CY	234	GLY
20	CY	397	VAL
20	CY	456	GLU
20	CY	614	GLU
20	CY	628	ARG
25	DC	51	ASP

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Mol	Chain	Res	Type
25	DC	117	THR
25	DC	130	ARG
26	DD	28	GLU
26	DD	40	THR
26	DD	164	GLN
26	DD	238	GLY
27	DE	17	ASP
27	DE	53	PRO
27	DE	70	ALA
27	DE	89	ASP
27	DE	147	PRO
28	DF	61	GLY
28	DF	68	LYS
28	DF	83	PHE
29	DG	74	LYS
30	DH	175	LYS
32	DK	89	HIS
33	DN	47	ALA
33	DN	129	PRO
35	DP	31	ALA
35	DP	68	GLN
35	DP	104	GLY
36	DQ	28	ALA
36	DQ	135	ASP
37	DR	5	LYS
37	DR	8	ARG
37	DR	11	ASN
37	DR	102	GLU
37	DR	104	ARG
38	DS	23	ARG
38	DS	94	TYR
39	DT	31	SER
39	DT	35	LYS
39	DT	39	ARG
39	DT	82	LEU
39	DT	83	ILE
39	DT	115	ARG
40	DU	30	LYS
40	DU	74	LEU
41	DV	18	LEU
41	DV	80	GLN
43	DX	85	PRO

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Mol	Chain	Res	Type
44	DY	47	LYS
45	DZ	93	ASP
51	D7	3	ARG
52	D8	48	PHE
56	D1	10	LYS
56	D1	44	PRO
57	D4	4	GLY
57	D4	10	VAL
58	De	62	VAL
58	De	108	ALA
1	AB	125	PRO
1	AB	150	SER
1	AB	194	PRO
2	AC	8	ILE
2	AC	30	ARG
2	AC	63	ASN
3	AD	132	ARG
3	AD	135	LEU
4	AE	11	ILE
5	AF	51	PRO
7	AH	43	GLY
7	AH	73	ASP
7	AH	129	VAL
8	AI	21	PRO
11	AL	40	VAL
11	AL	73	GLU
11	AL	79	GLU
12	AM	67	GLU
13	AN	27	CYS
14	AO	16	ALA
15	AP	16	HIS
15	AP	83	GLU
16	AQ	64	PRO
16	AQ	77	VAL
17	AR	43	PHE
18	AS	71	LEU
20	AY	337	SER
20	AY	345	THR
20	AY	384	ILE
20	AY	397	VAL
20	AY	598	ASP
20	AY	681	LYS

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Mol	Chain	Res	Type
25	BC	58	ASN
25	BC	97	GLY
25	BC	175	PRO
25	BC	176	VAL
25	BC	179	ALA
26	BD	40	THR
26	BD	52	ARG
26	BD	80	ALA
26	BD	140	THR
26	BD	244	ARG
27	BE	66	HIS
27	BE	141	ILE
28	BF	5	ALA
28	BF	68	LYS
29	BG	17	PRO
29	BG	74	LYS
32	BK	21	PRO
32	BK	90	LYS
32	BK	137	GLU
34	BO	49	ARG
35	BP	35	HIS
35	BP	56	SER
36	BQ	75	THR
37	BR	99	LYS
41	BV	19	LYS
42	BW	64	MET
43	BX	33	LYS
43	BX	62	LYS
44	BY	91	GLU
45	BZ	53	ILE
45	BZ	84	GLU
45	BZ	151	HIS
46	B0	3	HIS
46	B0	17	GLN
47	B2	10	LEU
49	B5	56	LYS
51	B7	13	ALA
56	B1	24	ALA
56	B1	36	GLY
56	B1	44	PRO
57	B4	7	PRO
57	B4	8	LYS

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Mol	Chain	Res	Type
1	CB	26	PRO
1	CB	153	ARG
2	CC	83	ARG
2	CC	101	LEU
4	CE	100	VAL
5	CF	40	VAL
5	CF	85	VAL
5	CF	100	ASN
8	CI	107	ARG
9	CJ	37	PRO
9	CJ	91	PRO
11	CL	115	LYS
12	CM	124	PRO
13	CN	13	THR
15	CP	24	ALA
16	CQ	73	VAL
18	CS	29	ARG
20	CY	75	LYS
20	CY	145	ASP
20	CY	296	GLY
20	CY	304	ASP
20	CY	393	ASP
20	CY	394	ALA
20	CY	535	PRO
25	DC	36	ALA
25	DC	49	GLY
25	DC	65	LEU
25	DC	107	GLY
25	DC	118	PRO
25	DC	221	PRO
25	DC	224	ARG
26	DD	24	ILE
26	DD	123	ALA
26	DD	226	MET
26	DD	244	ARG
26	DD	246	PRO
27	DE	34	VAL
27	DE	118	LYS
28	DF	5	ALA
28	DF	11	VAL
28	DF	172	TRP
28	DF	178	PRO

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Mol	Chain	Res	Type
29	DG	96	ARG
30	DH	45	VAL
30	DH	59	ARG
32	DK	14	ALA
32	DK	21	PRO
32	DK	73	PRO
32	DK	112	MET
32	DK	122	ALA
33	DN	32	THR
33	DN	104	LYS
35	DP	49	ARG
35	DP	52	GLU
35	DP	77	ARG
36	DQ	90	VAL
38	DS	24	LEU
38	DS	63	THR
40	DU	10	ARG
40	DU	86	ALA
41	DV	16	PRO
41	DV	52	VAL
42	DW	63	ASP
45	DZ	134	PRO
45	DZ	162	GLU
48	D3	13	ILE
48	D3	32	GLN
49	D5	57	VAL
50	D6	18	ARG
50	D6	33	LYS
52	D8	10	ALA
56	D1	22	GLY
57	D4	7	PRO
2	AC	12	LEU
4	AE	100	VAL
7	AH	89	PRO
7	AH	97	VAL
8	AI	119	ALA
18	AS	80	TYR
20	AY	5	VAL
20	AY	87	HIS
20	AY	129	LYS
20	AY	248	LYS
20	AY	341	VAL

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Mol	Chain	Res	Type
20	AY	554	PRO
25	BC	127	LYS
25	BC	137	LEU
26	BD	123	ALA
33	BN	127	ASP
35	BP	145	PRO
37	BR	117	VAL
39	BT	91	ARG
40	BU	79	PHE
41	BV	3	ALA
42	BW	63	ASP
43	BX	11	PRO
43	BX	52	VAL
45	BZ	136	PHE
45	BZ	166	SER
47	B2	35	LEU
51	B7	14	LYS
3	CD	39	PRO
6	CG	81	GLY
6	CG	138	LYS
7	CH	2	LEU
10	CK	121	PRO
11	CL	31	PRO
11	CL	52	LEU
11	CL	65	GLU
11	CL	99	HIS
14	CO	87	ILE
16	CQ	47	PRO
18	CS	77	THR
20	CY	258	VAL
20	CY	436	PRO
25	DC	20	VAL
25	DC	76	LEU
25	DC	139	PRO
25	DC	175	PRO
26	DD	25	THR
26	DD	242	ARG
27	DE	66	HIS
28	DF	9	ILE
28	DF	53	THR
39	DT	88	ILE
42	DW	31	GLU

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Mol	Chain	Res	Type
44	DY	70	SER
45	DZ	85	HIS
45	DZ	108	PRO
45	DZ	120	ILE
51	D7	48	LYS
52	D8	64	TYR
58	De	99	VAL
58	De	117	ALA
1	AB	233	SER
10	AK	118	GLY
11	AL	45	PRO
15	AP	53	VAL
15	AP	66	PRO
20	AY	121	VAL
20	AY	394	ALA
20	AY	532	GLY
29	BG	144	ILE
30	BH	128	PRO
35	BP	23	PRO
36	BQ	127	ILE
37	BR	92	GLY
39	BT	20	PRO
45	BZ	165	VAL
46	B0	47	PRO
56	B1	18	ILE
57	B4	10	VAL
1	CB	130	ARG
2	CC	130	VAL
7	CH	73	ASP
9	CJ	94	VAL
10	CK	113	PRO
11	CL	35	GLY
11	CL	125	PRO
12	CM	117	VAL
26	DD	100	GLY
27	DE	141	ILE
29	DG	129	GLY
30	DH	21	PRO
36	DQ	127	ILE
39	DT	20	PRO
40	DU	7	GLY
44	DY	18	GLY

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Mol	Chain	Res	Type
44	DY	98	VAL
1	AB	15	VAL
7	AH	86	ILE
12	AM	7	VAL
20	AY	258	VAL
26	BD	249	PRO
35	BP	77	ARG
36	BQ	52	VAL
38	BS	90	GLY
39	BT	88	ILE
41	BV	52	VAL
44	BY	7	VAL
45	BZ	141	VAL
47	B2	17	SER
52	B8	53	PRO
53	B9	3	VAL
9	CJ	36	GLY
20	CY	341	VAL
20	CY	402	ILE
25	DC	181	PHE
27	DE	193	GLY
30	DH	39	PRO
32	DK	7	VAL
32	DK	49	GLY
35	DP	34	GLY
35	DP	54	GLY
36	DQ	78	PRO
1	AB	127	ILE
1	AB	130	ARG
2	AC	70	VAL
2	AC	130	VAL
4	AE	22	GLY
5	AF	40	VAL
10	AK	102	GLY
11	AL	55	VAL
13	AN	14	PRO
18	AS	46	GLY
20	AY	167	PRO
20	AY	288	PRO
25	BC	20	VAL
25	BC	42	VAL
26	BD	51	VAL

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Mol	Chain	Res	Type
26	BD	100	GLY
27	BE	134	ILE
28	BF	150	GLY
35	BP	34	GLY
37	BR	83	ILE
37	BR	108	GLY
44	BY	27	VAL
44	BY	82	PRO
46	B0	63	VAL
49	B5	4	HIS
3	CD	142	PRO
4	CE	101	ILE
9	CJ	53	PRO
10	CK	39	PRO
20	CY	598	ASP
27	DE	43	GLY
35	DP	8	PRO
48	D3	2	PRO
53	D9	3	VAL
4	AE	103	GLY
7	AH	51	VAL
10	AK	108	ILE
11	AL	58	VAL
25	BC	146	VAL
28	BF	178	PRO
40	BU	82	GLY
45	BZ	161	VAL
48	B3	16	PRO
56	B1	37	ILE
5	CF	72	VAL
19	CT	101	GLY
25	DC	75	VAL
30	DH	136	ILE
33	DN	46	VAL
37	DR	93	GLY
41	DV	72	VAL
45	DZ	141	VAL
57	D4	17	GLY
58	De	83	GLY
12	AM	117	VAL
20	AY	116	PRO
29	BG	5	VAL

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Mol	Chain	Res	Type
33	BN	11	PRO
36	BQ	109	VAL
41	BV	22	VAL
41	BV	29	PRO
48	B3	13	ILE
7	CH	101	PRO
17	CR	77	GLY
58	De	118	VAL
32	DK	22	PRO
35	BP	48	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
1	AB	203/203 (100%)	164 (81%)	39 (19%)	1 7
1	CB	203/203 (100%)	177 (87%)	26 (13%)	4 22
2	AC	161/161 (100%)	125 (78%)	36 (22%)	1 4
2	CC	161/161 (100%)	122 (76%)	39 (24%)	0 4
3	AD	180/180 (100%)	143 (79%)	37 (21%)	1 6
3	CD	180/180 (100%)	142 (79%)	38 (21%)	1 5
4	AE	116/116 (100%)	96 (83%)	20 (17%)	2 11
4	CE	116/116 (100%)	95 (82%)	21 (18%)	1 9
5	AF	90/90 (100%)	76 (84%)	14 (16%)	2 16
5	CF	90/90 (100%)	74 (82%)	16 (18%)	2 10
6	AG	126/126 (100%)	111 (88%)	15 (12%)	5 25
6	CG	126/126 (100%)	112 (89%)	14 (11%)	6 28
7	AH	119/119 (100%)	94 (79%)	25 (21%)	1 5
7	CH	119/119 (100%)	91 (76%)	28 (24%)	1 4
8	AI	98/98 (100%)	82 (84%)	16 (16%)	2 13
8	CI	98/98 (100%)	77 (79%)	21 (21%)	1 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AJ	89/89 (100%)	71 (80%)	18 (20%)	1	6
9	CJ	89/89 (100%)	66 (74%)	23 (26%)	0	3
10	AK	90/90 (100%)	73 (81%)	17 (19%)	1	8
10	CK	90/90 (100%)	72 (80%)	18 (20%)	1	7
11	AL	104/104 (100%)	74 (71%)	30 (29%)	0	2
11	CL	104/104 (100%)	77 (74%)	27 (26%)	0	3
12	AM	100/100 (100%)	83 (83%)	17 (17%)	2	12
12	CM	100/100 (100%)	86 (86%)	14 (14%)	3	19
13	AN	49/49 (100%)	39 (80%)	10 (20%)	1	6
13	CN	49/49 (100%)	35 (71%)	14 (29%)	0	3
14	AO	79/79 (100%)	70 (89%)	9 (11%)	5	26
14	CO	79/79 (100%)	66 (84%)	13 (16%)	2	13
15	AP	72/72 (100%)	59 (82%)	13 (18%)	1	9
15	CP	72/72 (100%)	61 (85%)	11 (15%)	2	17
16	AQ	95/95 (100%)	82 (86%)	13 (14%)	3	20
16	CQ	95/95 (100%)	80 (84%)	15 (16%)	2	15
17	AR	61/61 (100%)	53 (87%)	8 (13%)	4	21
17	CR	61/61 (100%)	53 (87%)	8 (13%)	4	21
18	AS	69/69 (100%)	58 (84%)	11 (16%)	2	14
18	CS	69/69 (100%)	52 (75%)	17 (25%)	0	4
19	AT	76/76 (100%)	66 (87%)	10 (13%)	4	21
19	CT	76/76 (100%)	68 (90%)	8 (10%)	7	31
20	AY	579/579 (100%)	459 (79%)	120 (21%)	1	6
20	CY	579/579 (100%)	483 (83%)	96 (17%)	2	13
24	AU	2/2 (100%)	2 (100%)	0	100	100
24	CU	2/2 (100%)	2 (100%)	0	100	100
25	BC	180/180 (100%)	132 (73%)	48 (27%)	0	3
25	DC	180/180 (100%)	128 (71%)	52 (29%)	0	2
26	BD	217/217 (100%)	167 (77%)	50 (23%)	1	4
26	DD	217/217 (100%)	175 (81%)	42 (19%)	1	7
27	BE	165/165 (100%)	137 (83%)	28 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	DE	165/165 (100%)	136 (82%)	29 (18%)	2	10
28	BF	165/165 (100%)	133 (81%)	32 (19%)	1	7
28	DF	165/165 (100%)	140 (85%)	25 (15%)	3	17
29	BG	155/155 (100%)	130 (84%)	25 (16%)	2	14
29	DG	155/155 (100%)	130 (84%)	25 (16%)	2	14
30	BH	136/136 (100%)	111 (82%)	25 (18%)	1	8
30	DH	136/136 (100%)	117 (86%)	19 (14%)	3	19
32	BK	105/105 (100%)	74 (70%)	31 (30%)	0	2
32	DK	105/105 (100%)	77 (73%)	28 (27%)	0	3
33	BN	117/117 (100%)	98 (84%)	19 (16%)	2	14
33	DN	117/117 (100%)	93 (80%)	24 (20%)	1	6
34	BO	100/100 (100%)	85 (85%)	15 (15%)	3	17
34	DO	100/100 (100%)	86 (86%)	14 (14%)	3	19
35	BP	112/112 (100%)	82 (73%)	30 (27%)	0	3
35	DP	112/112 (100%)	85 (76%)	27 (24%)	0	4
36	BQ	111/111 (100%)	80 (72%)	31 (28%)	0	3
36	DQ	111/111 (100%)	84 (76%)	27 (24%)	0	4
37	BR	100/100 (100%)	79 (79%)	21 (21%)	1	5
37	DR	100/100 (100%)	78 (78%)	22 (22%)	1	5
38	BS	77/77 (100%)	60 (78%)	17 (22%)	1	5
38	DS	77/77 (100%)	59 (77%)	18 (23%)	1	4
39	BT	120/120 (100%)	94 (78%)	26 (22%)	1	5
39	DT	120/120 (100%)	93 (78%)	27 (22%)	1	4
40	BU	93/93 (100%)	75 (81%)	18 (19%)	1	7
40	DU	93/93 (100%)	70 (75%)	23 (25%)	0	4
41	BV	82/82 (100%)	60 (73%)	22 (27%)	0	3
41	DV	82/82 (100%)	62 (76%)	20 (24%)	0	4
42	BW	92/92 (100%)	69 (75%)	23 (25%)	0	4
42	DW	92/92 (100%)	76 (83%)	16 (17%)	2	11
43	BX	75/75 (100%)	56 (75%)	19 (25%)	0	3
43	DX	75/75 (100%)	58 (77%)	17 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	BY	88/88 (100%)	69 (78%)	19 (22%)	1	5
44	DY	88/88 (100%)	73 (83%)	15 (17%)	2	12
45	BZ	162/162 (100%)	128 (79%)	34 (21%)	1	5
45	DZ	162/162 (100%)	125 (77%)	37 (23%)	1	4
46	B0	66/66 (100%)	56 (85%)	10 (15%)	3	17
46	D0	66/66 (100%)	56 (85%)	10 (15%)	3	17
47	B2	66/66 (100%)	59 (89%)	7 (11%)	6	30
47	D2	66/66 (100%)	58 (88%)	8 (12%)	5	24
48	B3	52/52 (100%)	42 (81%)	10 (19%)	1	7
48	D3	52/52 (100%)	45 (86%)	7 (14%)	4	21
49	B5	51/51 (100%)	39 (76%)	12 (24%)	1	4
49	D5	51/51 (100%)	41 (80%)	10 (20%)	1	7
50	B6	49/49 (100%)	37 (76%)	12 (24%)	0	4
50	D6	49/49 (100%)	34 (69%)	15 (31%)	0	2
51	B7	42/42 (100%)	35 (83%)	7 (17%)	2	12
51	D7	42/42 (100%)	36 (86%)	6 (14%)	3	19
52	B8	54/54 (100%)	42 (78%)	12 (22%)	1	5
52	D8	54/54 (100%)	44 (82%)	10 (18%)	1	8
53	B9	34/34 (100%)	32 (94%)	2 (6%)	19	53
53	D9	34/34 (100%)	30 (88%)	4 (12%)	5	25
56	B1	78/78 (100%)	58 (74%)	20 (26%)	0	3
56	D1	78/78 (100%)	58 (74%)	20 (26%)	0	3
57	B4	31/31 (100%)	22 (71%)	9 (29%)	0	3
57	D4	31/31 (100%)	21 (68%)	10 (32%)	0	2
58	Be	54/54 (100%)	46 (85%)	8 (15%)	3	17
58	De	54/54 (100%)	46 (85%)	8 (15%)	3	17
All	All	11174/11174 (100%)	8972 (80%)	2202 (20%)	1	7

All (2202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	9	GLU
1	AB	15	VAL

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Mol	Chain	Res	Type
1	AB	16	HIS
1	AB	17	PHE
1	AB	21	ARG
1	AB	23	ARG
1	AB	33	TYR
1	AB	36	ARG
1	AB	37	ASN
1	AB	42	ILE
1	AB	56	ARG
1	AB	64	ARG
1	AB	69	LEU
1	AB	94	ASN
1	AB	96	ARG
1	AB	104	ASN
1	AB	105	PHE
1	AB	106	LYS
1	AB	121	LEU
1	AB	133	LYS
1	AB	141	GLU
1	AB	144	ARG
1	AB	146	GLN
1	AB	152	PHE
1	AB	158	LEU
1	AB	164	VAL
1	AB	168	THR
1	AB	170	GLU
1	AB	172	ILE
1	AB	185	ILE
1	AB	187	LEU
1	AB	189	ASP
1	AB	190	THR
1	AB	196	LEU
1	AB	211	ILE
1	AB	212	GLN
1	AB	221	LEU
1	AB	229	VAL
1	AB	239	VAL
2	AC	3	ASN
2	AC	12	LEU
2	AC	14	ILE
2	AC	17	ASP
2	AC	18	TRP

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Mol	Chain	Res	Type
2	AC	26	LYS
2	AC	29	TYR
2	AC	55	VAL
2	AC	62	ASP
2	AC	70	VAL
2	AC	72	LYS
2	AC	75	VAL
2	AC	84	ILE
2	AC	85	ARG
2	AC	91	LEU
2	AC	101	LEU
2	AC	103	VAL
2	AC	104	GLN
2	AC	105	GLU
2	AC	115	LEU
2	AC	124	ILE
2	AC	125	GLU
2	AC	128	PHE
2	AC	132	ARG
2	AC	134	ILE
2	AC	136	GLN
2	AC	152	ILE
2	AC	167	TRP
2	AC	173	VAL
2	AC	177	THR
2	AC	186	PHE
2	AC	188	LEU
2	AC	191	THR
2	AC	193	TYR
2	AC	195	VAL
2	AC	196	LEU
3	AD	8	VAL
3	AD	9	CYS
3	AD	10	ARG
3	AD	12	CYS
3	AD	14	ARG
3	AD	19	LEU
3	AD	26	CYS
3	AD	27	TYR
3	AD	30	LYS
3	AD	33	MET
3	AD	43	HIS

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Mol	Chain	Res	Type
3	AD	49	ARG
3	AD	52	SER
3	AD	53	ASP
3	AD	54	TYR
3	AD	57	ARG
3	AD	60	GLU
3	AD	61	LYS
3	AD	67	ILE
3	AD	72	GLU
3	AD	76	ARG
3	AD	79	PHE
3	AD	86	LYS
3	AD	89	THR
3	AD	113	SER
3	AD	116	GLN
3	AD	135	LEU
3	AD	140	VAL
3	AD	156	GLU
3	AD	159	ARG
3	AD	165	MET
3	AD	173	TRP
3	AD	176	LEU
3	AD	182	LYS
3	AD	187	ARG
3	AD	207	TYR
3	AD	208	SER
4	AE	12	LEU
4	AE	16	THR
4	AE	37	ARG
4	AE	41	VAL
4	AE	47	LYS
4	AE	60	TYR
4	AE	64	ARG
4	AE	68	GLU
4	AE	73	ASN
4	AE	78	HIS
4	AE	80	ILE
4	AE	84	PHE
4	AE	100	VAL
4	AE	111	GLU
4	AE	120	THR
4	AE	137	GLU

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Mol	Chain	Res	Type
4	AE	141	GLN
4	AE	143	ARG
4	AE	147	ASP
4	AE	150	ARG
5	AF	11	ASN
5	AF	16	GLN
5	AF	23	LYS
5	AF	27	GLN
5	AF	31	GLU
5	AF	45	LEU
5	AF	46	ARG
5	AF	47	ARG
5	AF	52	ILE
5	AF	61	LEU
5	AF	63	TYR
5	AF	69	GLU
5	AF	71	ARG
5	AF	87	ARG
6	AG	5	ARG
6	AG	16	LEU
6	AG	41	ARG
6	AG	52	GLU
6	AG	54	THR
6	AG	67	GLU
6	AG	79	ARG
6	AG	85	TYR
6	AG	97	GLN
6	AG	120	ILE
6	AG	122	HIS
6	AG	136	LYS
6	AG	139	GLU
6	AG	140	ASP
6	AG	149	ARG
7	AH	18	ARG
7	AH	26	VAL
7	AH	37	ARG
7	AH	44	PHE
7	AH	51	VAL
7	AH	61	VAL
7	AH	63	LEU
7	AH	70	GLN
7	AH	75	ARG

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Mol	Chain	Res	Type
7	AH	82	HIS
7	AH	83	ILE
7	AH	98	LYS
7	AH	99	GLU
7	AH	102	ARG
7	AH	104	ARG
7	AH	111	ILE
7	AH	112	LEU
7	AH	118	VAL
7	AH	119	LEU
7	AH	120	THR
7	AH	129	VAL
7	AH	133	LEU
7	AH	135	CYS
7	AH	136	GLU
7	AH	138	TRP
8	AI	3	GLN
8	AI	4	TYR
8	AI	7	THR
8	AI	19	LEU
8	AI	25	LYS
8	AI	36	TYR
8	AI	40	LEU
8	AI	44	VAL
8	AI	79	LEU
8	AI	88	TYR
8	AI	93	ARG
8	AI	95	LYS
8	AI	96	LEU
8	AI	107	ARG
8	AI	108	VAL
8	AI	121	ARG
9	AJ	5	ARG
9	AJ	8	LEU
9	AJ	16	LEU
9	AJ	22	LYS
9	AJ	25	GLU
9	AJ	29	ARG
9	AJ	47	PHE
9	AJ	50	ILE
9	AJ	55	LYS
9	AJ	70	ARG

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Mol	Chain	Res	Type
9	AJ	74	ILE
9	AJ	78	ASN
9	AJ	79	ARG
9	AJ	84	GLN
9	AJ	94	VAL
9	AJ	96	ILE
9	AJ	99	LYS
9	AJ	101	VAL
10	AK	18	ARG
10	AK	22	HIS
10	AK	25	TYR
10	AK	38	ASN
10	AK	40	ILE
10	AK	41	THR
10	AK	54	ARG
10	AK	57	THR
10	AK	66	LEU
10	AK	67	ASP
10	AK	71	LYS
10	AK	79	SER
10	AK	84	VAL
10	AK	103	LEU
10	AK	109	VAL
10	AK	124	LYS
10	AK	127	LYS
11	AL	17	LYS
11	AL	18	VAL
11	AL	20	LYS
11	AL	24	VAL
11	AL	33	ARG
11	AL	37	CYS
11	AL	38	THR
11	AL	43	VAL
11	AL	44	THR
11	AL	47	LYS
11	AL	49	ASN
11	AL	54	LYS
11	AL	55	VAL
11	AL	60	LEU
11	AL	66	VAL
11	AL	69	TYR
11	AL	75	HIS

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Mol	Chain	Res	Type
11	AL	76	ASN
11	AL	77	LEU
11	AL	79	GLU
11	AL	80	HIS
11	AL	84	LEU
11	AL	85	ILE
11	AL	90	VAL
11	AL	92	ASP
11	AL	93	LEU
11	AL	102	ARG
11	AL	112	ASP
11	AL	118	SER
11	AL	127	GLU
12	AM	16	ASP
12	AM	19	LEU
12	AM	25	ILE
12	AM	50	GLU
12	AM	57	ARG
12	AM	64	TRP
12	AM	69	GLU
12	AM	81	LEU
12	AM	90	LEU
12	AM	92	HIS
12	AM	99	ARG
12	AM	102	ARG
12	AM	108	ARG
12	AM	110	ARG
12	AM	111	LYS
12	AM	114	ARG
12	AM	121	LYS
13	AN	22	THR
13	AN	29	ARG
13	AN	35	ARG
13	AN	44	LEU
13	AN	49	HIS
13	AN	53	LEU
13	AN	56	VAL
13	AN	57	ARG
13	AN	58	LYS
13	AN	61	TRP
14	AO	5	LYS
14	AO	10	LYS

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Mol	Chain	Res	Type
14	AO	25	THR
14	AO	26	GLU
14	AO	38	ARG
14	AO	63	ARG
14	AO	84	LYS
14	AO	87	ILE
14	AO	88	ARG
15	AP	8	ARG
15	AP	13	HIS
15	AP	22	THR
15	AP	23	ASP
15	AP	32	TYR
15	AP	39	TYR
15	AP	45	THR
15	AP	53	VAL
15	AP	58	TYR
15	AP	59	TRP
15	AP	67	THR
15	AP	73	LEU
15	AP	76	GLN
16	AQ	19	VAL
16	AQ	20	THR
16	AQ	37	LYS
16	AQ	48	GLU
16	AQ	52	LYS
16	AQ	53	LEU
16	AQ	55	ASP
16	AQ	60	ILE
16	AQ	66	SER
16	AQ	81	ARG
16	AQ	84	LEU
16	AQ	89	LEU
16	AQ	101	ARG
17	AR	19	LYS
17	AR	32	ARG
17	AR	38	GLU
17	AR	47	THR
17	AR	62	GLU
17	AR	79	LEU
17	AR	81	PHE
17	AR	83	GLU
18	AS	6	LYS

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Mol	Chain	Res	Type
18	AS	16	LEU
18	AS	25	LYS
18	AS	29	ARG
18	AS	38	SER
18	AS	51	VAL
18	AS	58	VAL
18	AS	61	TYR
18	AS	62	ILE
18	AS	66	MET
18	AS	71	LEU
19	AT	13	LEU
19	AT	22	ARG
19	AT	26	ASN
19	AT	56	MET
19	AT	57	ARG
19	AT	70	SER
19	AT	71	THR
19	AT	74	LYS
19	AT	75	ASN
19	AT	93	GLU
20	AY	9	LEU
20	AY	20	HIS
20	AY	29	THR
20	AY	33	LEU
20	AY	35	TYR
20	AY	38	ARG
20	AY	39	ILE
20	AY	40	HIS
20	AY	59	ARG
20	AY	63	ILE
20	AY	65	ILE
20	AY	66	THR
20	AY	73	PHE
20	AY	80	ASN
20	AY	87	HIS
20	AY	88	VAL
20	AY	92	ILE
20	AY	98	MET
20	AY	99	ARG
20	AY	101	LEU
20	AY	114	VAL
20	AY	121	VAL

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Mol	Chain	Res	Type
20	AY	126	GLU
20	AY	128	TYR
20	AY	132	ARG
20	AY	133	ILE
20	AY	170	ARG
20	AY	172	ASP
20	AY	173	THR
20	AY	174	PHE
20	AY	175	SER
20	AY	178	ILE
20	AY	190	ASN
20	AY	191	ASP
20	AY	199	ILE
20	AY	203	GLU
20	AY	225	GLU
20	AY	232	LEU
20	AY	240	GLU
20	AY	248	LYS
20	AY	254	LYS
20	AY	255	ILE
20	AY	260	LEU
20	AY	270	GLN
20	AY	271	LEU
20	AY	277	VAL
20	AY	278	ASP
20	AY	282	SER
20	AY	292	THR
20	AY	304	ASP
20	AY	314	PHE
20	AY	317	MET
20	AY	325	LEU
20	AY	328	ILE
20	AY	329	ARG
20	AY	330	VAL
20	AY	334	THR
20	AY	341	VAL
20	AY	342	TYR
20	AY	344	THR
20	AY	348	ARG
20	AY	352	VAL
20	AY	356	LEU
20	AY	358	MET

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Mol	Chain	Res	Type
20	AY	381	LYS
20	AY	382	GLU
20	AY	408	VAL
20	AY	410	ASP
20	AY	420	ASP
20	AY	428	LEU
20	AY	431	LEU
20	AY	435	ASP
20	AY	439	ARG
20	AY	440	VAL
20	AY	448	GLN
20	AY	449	THR
20	AY	454	MET
20	AY	456	GLU
20	AY	457	LEU
20	AY	464	ASP
20	AY	469	GLU
20	AY	471	LYS
20	AY	472	VAL
20	AY	473	ASP
20	AY	476	VAL
20	AY	481	VAL
20	AY	487	ILE
20	AY	488	THR
20	AY	504	ARG
20	AY	507	TYR
20	AY	512	ILE
20	AY	536	LYS
20	AY	556	ILE
20	AY	563	ILE
20	AY	565	VAL
20	AY	568	TYR
20	AY	582	PHE
20	AY	583	LYS
20	AY	606	MET
20	AY	612	THR
20	AY	615	GLU
20	AY	616	TYR
20	AY	617	MET
20	AY	619	ASP
20	AY	624	LEU
20	AY	630	GLN

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Mol	Chain	Res	Type
20	AY	634	MET
20	AY	635	GLU
20	AY	641	GLN
20	AY	647	VAL
20	AY	653	PHE
20	AY	657	THR
20	AY	663	THR
20	AY	669	PHE
20	AY	671	MET
20	AY	672	PHE
20	AY	676	TYR
20	AY	677	GLN
20	AY	679	VAL
20	AY	685	GLU
25	BC	4	HIS
25	BC	13	GLU
25	BC	19	LYS
25	BC	24	ASP
25	BC	31	LYS
25	BC	38	PHE
25	BC	39	ASP
25	BC	45	HIS
25	BC	48	LEU
25	BC	53	ARG
25	BC	54	ARG
25	BC	64	SER
25	BC	67	HIS
25	BC	73	VAL
25	BC	75	VAL
25	BC	98	GLU
25	BC	110	ASP
25	BC	115	VAL
25	BC	117	THR
25	BC	119	ASP
25	BC	121	MET
25	BC	128	LEU
25	BC	130	ARG
25	BC	131	ILE
25	BC	137	LEU
25	BC	138	LEU
25	BC	145	THR
25	BC	146	VAL

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Mol	Chain	Res	Type
25	BC	148	PHE
25	BC	154	ILE
25	BC	158	LYS
25	BC	161	ARG
25	BC	166	ASN
25	BC	167	ASP
25	BC	169	THR
25	BC	172	ILE
25	BC	173	HIS
25	BC	176	VAL
25	BC	178	LYS
25	BC	181	PHE
25	BC	184	GLU
25	BC	186	LEU
25	BC	201	LYS
25	BC	203	GLU
25	BC	206	LYS
25	BC	209	PHE
25	BC	216	THR
25	BC	222	SER
26	BD	5	LYS
26	BD	10	THR
26	BD	13	ARG
26	BD	14	ARG
26	BD	15	PHE
26	BD	23	GLU
26	BD	24	ILE
26	BD	25	THR
26	BD	26	LYS
26	BD	27	THR
26	BD	31	LYS
26	BD	35	LYS
26	BD	37	LEU
26	BD	44	ASN
26	BD	60	ARG
26	BD	63	ARG
26	BD	64	ILE
26	BD	65	ILE
26	BD	78	LYS
26	BD	82	ILE
26	BD	87	ASN
26	BD	95	LEU

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Mol	Chain	Res	Type
26	BD	103	ARG
26	BD	104	TYR
26	BD	105	ILE
26	BD	109	ASP
26	BD	112	GLN
26	BD	115	GLN
26	BD	117	VAL
26	BD	122	ASP
26	BD	126	GLN
26	BD	131	LEU
26	BD	136	ILE
26	BD	140	THR
26	BD	143	HIS
26	BD	147	LEU
26	BD	150	LYS
26	BD	155	LEU
26	BD	161	THR
26	BD	171	ASP
26	BD	175	LEU
26	BD	186	HIS
26	BD	196	VAL
26	BD	198	ASN
26	BD	227	ASN
26	BD	230	ASP
26	BD	257	LEU
26	BD	259	THR
26	BD	262	ARG
26	BD	273	ARG
27	BE	4	ILE
27	BE	12	THR
27	BE	18	ASP
27	BE	26	ILE
27	BE	36	ARG
27	BE	45	THR
27	BE	52	LEU
27	BE	63	LEU
27	BE	66	HIS
27	BE	77	ILE
27	BE	78	LEU
27	BE	87	GLU
27	BE	91	VAL
27	BE	92	THR

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Mol	Chain	Res	Type
27	BE	93	VAL
27	BE	95	ILE
27	BE	113	PHE
27	BE	127	ASP
27	BE	134	ILE
27	BE	135	HIS
27	BE	141	ILE
27	BE	144	ARG
27	BE	146	THR
27	BE	163	GLU
27	BE	175	VAL
27	BE	178	GLU
27	BE	183	LEU
27	BE	197	ILE
28	BF	2	LYS
28	BF	3	GLU
28	BF	7	TYR
28	BF	12	LEU
28	BF	17	ARG
28	BF	20	LEU
28	BF	40	GLN
28	BF	45	ARG
28	BF	59	TYR
28	BF	67	GLN
28	BF	74	ARG
28	BF	78	ILE
28	BF	83	PHE
28	BF	90	PHE
28	BF	106	ARG
28	BF	110	LEU
28	BF	125	LEU
28	BF	126	VAL
28	BF	132	VAL
28	BF	136	THR
28	BF	149	ASP
28	BF	154	VAL
28	BF	156	LEU
28	BF	158	THR
28	BF	175	THR
28	BF	182	ASN
28	BF	186	ILE
28	BF	190	GLU

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Mol	Chain	Res	Type
28	BF	194	MET
28	BF	199	TRP
28	BF	200	GLU
28	BF	206	ILE
29	BG	5	VAL
29	BG	21	ARG
29	BG	31	VAL
29	BG	34	LEU
29	BG	39	ILE
29	BG	40	ASN
29	BG	43	LEU
29	BG	45	GLU
29	BG	59	GLU
29	BG	60	LEU
29	BG	82	LEU
29	BG	86	MET
29	BG	99	MET
29	BG	106	LEU
29	BG	113	ARG
29	BG	115	ARG
29	BG	121	ASN
29	BG	133	LEU
29	BG	136	ARG
29	BG	143	GLU
29	BG	146	TYR
29	BG	150	ASP
29	BG	157	ILE
29	BG	164	GLU
29	BG	172	LEU
30	BH	16	SER
30	BH	17	VAL
30	BH	23	ARG
30	BH	33	LEU
30	BH	41	MET
30	BH	42	ARG
30	BH	43	VAL
30	BH	47	GLU
30	BH	57	ASP
30	BH	61	HIS
30	BH	65	HIS
30	BH	72	ILE
30	BH	80	SER

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Mol	Chain	Res	Type
30	BH	83	TYR
30	BH	86	GLU
30	BH	99	VAL
30	BH	104	GLU
30	BH	105	LEU
30	BH	122	THR
30	BH	133	VAL
30	BH	136	ILE
30	BH	147	ASN
30	BH	152	ARG
30	BH	158	HIS
30	BH	163	TYR
32	BK	9	LYS
32	BK	10	LEU
32	BK	18	THR
32	BK	30	HIS
32	BK	37	PHE
32	BK	38	VAL
32	BK	42	ASN
32	BK	57	ILE
32	BK	59	ILE
32	BK	60	TYR
32	BK	65	PHE
32	BK	66	THR
32	BK	71	THR
32	BK	76	TYR
32	BK	78	ILE
32	BK	80	LYS
32	BK	84	LEU
32	BK	94	GLU
32	BK	95	LYS
32	BK	100	THR
32	BK	103	GLN
32	BK	105	LEU
32	BK	110	GLN
32	BK	114	ASP
32	BK	115	LEU
32	BK	117	THR
32	BK	118	THR
32	BK	125	ARG
32	BK	126	MET
32	BK	132	ARG

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Mol	Chain	Res	Type
32	BK	137	GLU
33	BN	1	MET
33	BN	5	VAL
33	BN	16	ILE
33	BN	29	LYS
33	BN	32	THR
33	BN	33	LEU
33	BN	48	MET
33	BN	61	ARG
33	BN	62	VAL
33	BN	69	GLN
33	BN	71	ILE
33	BN	76	SER
33	BN	97	ARG
33	BN	99	LEU
33	BN	119	ARG
33	BN	127	ASP
33	BN	134	ARG
33	BN	137	LYS
33	BN	138	LEU
34	BO	2	ILE
34	BO	3	GLN
34	BO	8	LEU
34	BO	14	THR
34	BO	21	CYS
34	BO	23	ARG
34	BO	29	ASN
34	BO	31	LYS
34	BO	37	ASP
34	BO	45	GLU
34	BO	82	ASN
34	BO	89	ASN
34	BO	90	GLN
34	BO	91	LEU
34	BO	117	LEU
35	BP	7	ARG
35	BP	13	ASN
35	BP	16	ARG
35	BP	17	LYS
35	BP	19	VAL
35	BP	29	LYS
35	BP	32	THR

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Mol	Chain	Res	Type
35	BP	35	HIS
35	BP	39	LYS
35	BP	46	LYS
35	BP	50	ARG
35	BP	51	PHE
35	BP	55	ARG
35	BP	59	LEU
35	BP	60	MET
35	BP	61	ARG
35	BP	62	LEU
35	BP	79	ARG
35	BP	84	ASN
35	BP	85	LEU
35	BP	90	ARG
35	BP	91	PHE
35	BP	94	GLU
35	BP	95	VAL
35	BP	96	THR
35	BP	100	LEU
35	BP	110	TYR
35	BP	130	PHE
35	BP	132	LYS
35	BP	144	GLU
36	BQ	1	MET
36	BQ	3	MET
36	BQ	6	ARG
36	BQ	7	MET
36	BQ	9	TYR
36	BQ	13	GLN
36	BQ	14	ARG
36	BQ	16	ARG
36	BQ	25	ASP
36	BQ	37	LEU
36	BQ	43	THR
36	BQ	45	GLN
36	BQ	46	GLN
36	BQ	58	PHE
36	BQ	60	ARG
36	BQ	68	ILE
36	BQ	74	TYR
36	BQ	89	ASN
36	BQ	90	VAL

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Mol	Chain	Res	Type
36	BQ	91	GLU
36	BQ	96	VAL
36	BQ	97	VAL
36	BQ	104	PHE
36	BQ	105	GLU
36	BQ	106	VAL
36	BQ	109	VAL
36	BQ	128	LYS
36	BQ	131	ILE
36	BQ	132	VAL
36	BQ	137	TYR
36	BQ	139	GLU
37	BR	3	HIS
37	BR	4	LEU
37	BR	8	ARG
37	BR	16	HIS
37	BR	29	LEU
37	BR	35	THR
37	BR	44	LEU
37	BR	45	ARG
37	BR	48	VAL
37	BR	59	ASP
37	BR	65	LEU
37	BR	67	LEU
37	BR	75	LEU
37	BR	76	VAL
37	BR	79	LEU
37	BR	81	ASP
37	BR	95	THR
37	BR	96	ARG
37	BR	98	LEU
37	BR	99	LYS
37	BR	100	LEU
38	BS	13	ARG
38	BS	15	ARG
38	BS	18	ILE
38	BS	24	LEU
38	BS	35	ILE
38	BS	42	ASP
38	BS	47	THR
38	BS	53	SER
38	BS	61	ASN

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Mol	Chain	Res	Type
38	BS	62	LYS
38	BS	63	THR
38	BS	69	VAL
38	BS	83	LYS
38	BS	84	GLN
38	BS	92	TYR
38	BS	97	ARG
38	BS	98	VAL
39	BT	1	MET
39	BT	13	ARG
39	BT	16	ARG
39	BT	21	GLU
39	BT	27	THR
39	BT	32	TYR
39	BT	38	ASN
39	BT	42	ILE
39	BT	44	ASP
39	BT	48	ILE
39	BT	49	VAL
39	BT	62	THR
39	BT	65	LYS
39	BT	70	VAL
39	BT	74	ARG
39	BT	82	LEU
39	BT	84	GLN
39	BT	105	LEU
39	BT	107	ASP
39	BT	108	ARG
39	BT	109	GLU
39	BT	114	LEU
39	BT	115	ARG
39	BT	118	ARG
39	BT	124	ASP
39	BT	128	GLU
40	BU	3	ARG
40	BU	6	THR
40	BU	8	VAL
40	BU	10	ARG
40	BU	14	HIS
40	BU	36	ARG
40	BU	44	ASN
40	BU	51	LYS

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Mol	Chain	Res	Type
40	BU	62	ILE
40	BU	64	ARG
40	BU	74	LEU
40	BU	83	LEU
40	BU	90	VAL
40	BU	98	LEU
40	BU	101	ARG
40	BU	104	GLN
40	BU	108	GLU
40	BU	117	GLN
41	BV	5	VAL
41	BV	18	LEU
41	BV	19	LYS
41	BV	21	ARG
41	BV	35	LEU
41	BV	38	LEU
41	BV	40	LEU
41	BV	45	THR
41	BV	49	THR
41	BV	53	GLU
41	BV	57	VAL
41	BV	61	VAL
41	BV	69	LYS
41	BV	71	LEU
41	BV	72	VAL
41	BV	75	PHE
41	BV	80	GLN
41	BV	87	HIS
41	BV	95	LEU
41	BV	96	ILE
41	BV	98	GLU
41	BV	99	ILE
42	BW	11	ARG
42	BW	17	VAL
42	BW	19	LEU
42	BW	22	ASP
42	BW	23	LEU
42	BW	25	ARG
42	BW	27	LYS
42	BW	37	ARG
42	BW	39	THR
42	BW	61	ASN

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Mol	Chain	Res	Type
42	BW	64	MET
42	BW	66	GLU
42	BW	70	TYR
42	BW	77	ASP
42	BW	88	ARG
42	BW	94	ASP
42	BW	95	ILE
42	BW	96	ILE
42	BW	97	LYS
42	BW	99	ARG
42	BW	100	THR
42	BW	103	ILE
42	BW	107	LEU
43	BX	3	THR
43	BX	23	GLU
43	BX	27	THR
43	BX	31	HIS
43	BX	35	THR
43	BX	54	VAL
43	BX	57	LEU
43	BX	58	HIS
43	BX	62	LYS
43	BX	63	LYS
43	BX	65	ARG
43	BX	66	LEU
43	BX	68	ARG
43	BX	69	TYR
43	BX	72	LYS
43	BX	76	ARG
43	BX	80	ILE
43	BX	87	GLN
43	BX	92	LEU
44	BY	2	ARG
44	BY	3	VAL
44	BY	4	LYS
44	BY	5	MET
44	BY	6	HIS
44	BY	7	VAL
44	BY	9	LYS
44	BY	13	VAL
44	BY	19	LYS
44	BY	35	TYR

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Mol	Chain	Res	Type
44	BY	39	VAL
44	BY	44	ILE
44	BY	45	VAL
44	BY	47	LYS
44	BY	50	ARG
44	BY	88	LYS
44	BY	90	LEU
44	BY	97	ARG
44	BY	107	ASP
45	BZ	3	TYR
45	BZ	9	TYR
45	BZ	14	LYS
45	BZ	28	MET
45	BZ	29	TYR
45	BZ	32	HIS
45	BZ	34	ASN
45	BZ	36	LYS
45	BZ	39	VAL
45	BZ	57	ILE
45	BZ	59	LEU
45	BZ	70	LEU
45	BZ	72	ARG
45	BZ	81	ARG
45	BZ	82	ARG
45	BZ	86	VAL
45	BZ	87	ASP
45	BZ	94	GLU
45	BZ	98	MET
45	BZ	124	ILE
45	BZ	127	LYS
45	BZ	133	ILE
45	BZ	136	PHE
45	BZ	139	VAL
45	BZ	151	HIS
45	BZ	154	ASP
45	BZ	156	LYS
45	BZ	162	GLU
45	BZ	163	LEU
45	BZ	165	VAL
45	BZ	179	ASP
45	BZ	181	GLU
45	BZ	185	GLU

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Mol	Chain	Res	Type
45	BZ	186	GLU
46	B0	11	ARG
46	B0	27	GLU
46	B0	30	VAL
46	B0	35	ASN
46	B0	41	ARG
46	B0	55	ARG
46	B0	63	VAL
46	B0	64	ASP
46	B0	71	ASP
46	B0	75	LEU
47	B2	37	PHE
47	B2	44	LEU
47	B2	47	ASN
47	B2	50	ILE
47	B2	53	LEU
47	B2	55	ARG
47	B2	59	ARG
48	B3	4	LEU
48	B3	20	LYS
48	B3	29	ARG
48	B3	31	LEU
48	B3	33	GLN
48	B3	36	VAL
48	B3	46	ASN
48	B3	53	LEU
48	B3	55	ARG
48	B3	59	VAL
49	B5	3	LYS
49	B5	13	LYS
49	B5	25	LEU
49	B5	31	VAL
49	B5	33	CYS
49	B5	36	CYS
49	B5	44	THR
49	B5	45	VAL
49	B5	48	GLU
49	B5	51	TYR
49	B5	55	ARG
49	B5	58	LEU
50	B6	6	ARG
50	B6	9	LEU

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Mol	Chain	Res	Type
50	B6	10	LEU
50	B6	11	LEU
50	B6	18	ARG
50	B6	19	ARG
50	B6	23	THR
50	B6	25	LYS
50	B6	28	ARG
50	B6	43	CYS
50	B6	45	LYS
50	B6	48	VAL
51	B7	3	ARG
51	B7	6	GLN
51	B7	19	ARG
51	B7	24	THR
51	B7	30	VAL
51	B7	40	TRP
51	B7	42	LEU
52	B8	6	THR
52	B8	30	ARG
52	B8	32	LEU
52	B8	34	TRP
52	B8	36	LYS
52	B8	40	GLU
52	B8	49	VAL
52	B8	52	LYS
52	B8	53	PRO
52	B8	59	LYS
52	B8	60	LEU
52	B8	64	TYR
53	B9	4	ARG
53	B9	7	VAL
56	B1	13	ILE
56	B1	23	LYS
56	B1	26	ARG
56	B1	32	LYS
56	B1	34	THR
56	B1	40	ARG
56	B1	41	ARG
56	B1	43	TYR
56	B1	46	LEU
56	B1	50	ARG
56	B1	57	GLU

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Mol	Chain	Res	Type
56	B1	58	ILE
56	B1	59	THR
56	B1	60	PHE
56	B1	61	ARG
56	B1	67	ILE
56	B1	73	LEU
56	B1	82	LEU
56	B1	88	LYS
56	B1	90	ILE
57	B4	1	MET
57	B4	6	HIS
57	B4	8	LYS
57	B4	9	LEU
57	B4	10	VAL
57	B4	14	ILE
57	B4	27	THR
57	B4	30	GLU
57	B4	32	TYR
58	Be	61	ASP
58	Be	73	GLU
58	Be	78	LEU
58	Be	94	GLU
58	Be	100	LYS
58	Be	101	GLU
58	Be	106	GLN
58	Be	111	ILE
1	CB	15	VAL
1	CB	16	HIS
1	CB	17	PHE
1	CB	36	ARG
1	CB	39	ILE
1	CB	42	ILE
1	CB	56	ARG
1	CB	59	GLU
1	CB	63	MET
1	CB	69	LEU
1	CB	94	ASN
1	CB	96	ARG
1	CB	103	THR
1	CB	144	ARG
1	CB	152	PHE
1	CB	164	VAL

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Mol	Chain	Res	Type
1	CB	168	THR
1	CB	170	GLU
1	CB	184	VAL
1	CB	195	ASP
1	CB	200	ILE
1	CB	211	ILE
1	CB	213	LEU
1	CB	221	LEU
1	CB	238	LEU
1	CB	239	VAL
2	CC	15	THR
2	CC	16	ARG
2	CC	17	ASP
2	CC	18	TRP
2	CC	26	LYS
2	CC	28	GLN
2	CC	29	TYR
2	CC	34	LEU
2	CC	36	ASP
2	CC	38	ARG
2	CC	43	LEU
2	CC	55	VAL
2	CC	56	ASP
2	CC	62	ASP
2	CC	70	VAL
2	CC	72	LYS
2	CC	76	VAL
2	CC	83	ARG
2	CC	91	LEU
2	CC	101	LEU
2	CC	104	GLN
2	CC	105	GLU
2	CC	115	LEU
2	CC	124	ILE
2	CC	125	GLU
2	CC	128	PHE
2	CC	132	ARG
2	CC	134	ILE
2	CC	136	GLN
2	CC	152	ILE
2	CC	153	VAL
2	CC	162	GLN

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Mol	Chain	Res	Type
2	CC	166	GLU
2	CC	173	VAL
2	CC	175	LEU
2	CC	186	PHE
2	CC	188	LEU
2	CC	196	LEU
2	CC	206	GLU
3	CD	9	CYS
3	CD	10	ARG
3	CD	12	CYS
3	CD	13	ARG
3	CD	26	CYS
3	CD	27	TYR
3	CD	33	MET
3	CD	42	GLN
3	CD	49	ARG
3	CD	50	ARG
3	CD	54	TYR
3	CD	57	ARG
3	CD	60	GLU
3	CD	61	LYS
3	CD	67	ILE
3	CD	70	ILE
3	CD	76	ARG
3	CD	77	ASN
3	CD	86	LYS
3	CD	89	THR
3	CD	97	LEU
3	CD	98	GLU
3	CD	103	ASN
3	CD	107	ARG
3	CD	110	PHE
3	CD	113	SER
3	CD	135	LEU
3	CD	140	VAL
3	CD	141	ARG
3	CD	148	VAL
3	CD	156	GLU
3	CD	159	ARG
3	CD	173	TRP
3	CD	176	LEU
3	CD	178	VAL

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Mol	Chain	Res	Type
3	CD	187	ARG
3	CD	193	ASP
3	CD	207	TYR
4	CE	5	ASP
4	CE	12	LEU
4	CE	16	THR
4	CE	37	ARG
4	CE	41	VAL
4	CE	45	PHE
4	CE	60	TYR
4	CE	64	ARG
4	CE	68	GLU
4	CE	73	ASN
4	CE	76	ILE
4	CE	78	HIS
4	CE	80	ILE
4	CE	87	SER
4	CE	91	LEU
4	CE	112	LEU
4	CE	119	LEU
4	CE	120	THR
4	CE	126	ARG
4	CE	137	GLU
4	CE	143	ARG
5	CF	11	ASN
5	CF	13	ASN
5	CF	16	GLN
5	CF	23	LYS
5	CF	36	ARG
5	CF	45	LEU
5	CF	46	ARG
5	CF	57	GLN
5	CF	61	LEU
5	CF	69	GLU
5	CF	70	ASP
5	CF	74	ASP
5	CF	78	GLU
5	CF	82	ARG
5	CF	87	ARG
5	CF	89	MET
6	CG	13	GLN
6	CG	17	VAL

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Mol	Chain	Res	Type
6	CG	18	TYR
6	CG	56	GLN
6	CG	78	ARG
6	CG	79	ARG
6	CG	80	VAL
6	CG	106	GLN
6	CG	113	GLU
6	CG	114	ARG
6	CG	122	HIS
6	CG	126	ASP
6	CG	136	LYS
6	CG	140	ASP
7	CH	8	ASP
7	CH	29	SER
7	CH	37	ARG
7	CH	44	PHE
7	CH	49	GLU
7	CH	51	VAL
7	CH	58	TYR
7	CH	59	LEU
7	CH	61	VAL
7	CH	63	LEU
7	CH	70	GLN
7	CH	73	ASP
7	CH	77	GLU
7	CH	83	ILE
7	CH	99	GLU
7	CH	102	ARG
7	CH	104	ARG
7	CH	107	LEU
7	CH	109	ILE
7	CH	111	ILE
7	CH	112	LEU
7	CH	119	LEU
7	CH	120	THR
7	CH	129	VAL
7	CH	133	LEU
7	CH	135	CYS
7	CH	136	GLU
7	CH	138	TRP
8	CI	19	LEU
8	CI	25	LYS

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Mol	Chain	Res	Type
8	CI	27	THR
8	CI	53	VAL
8	CI	70	LYS
8	CI	71	SER
8	CI	79	LEU
8	CI	88	TYR
8	CI	91	ASP
8	CI	93	ARG
8	CI	95	LYS
8	CI	96	LEU
8	CI	102	LEU
8	CI	107	ARG
8	CI	108	VAL
8	CI	113	LYS
8	CI	114	TYR
8	CI	117	HIS
8	CI	118	LYS
8	CI	121	ARG
8	CI	124	GLN
9	CJ	5	ARG
9	CJ	8	LEU
9	CJ	11	PHE
9	CJ	16	LEU
9	CJ	22	LYS
9	CJ	25	GLU
9	CJ	28	ARG
9	CJ	30	SER
9	CJ	47	PHE
9	CJ	48	THR
9	CJ	50	ILE
9	CJ	55	LYS
9	CJ	66	ARG
9	CJ	67	THR
9	CJ	70	ARG
9	CJ	74	ILE
9	CJ	78	ASN
9	CJ	79	ARG
9	CJ	81	THR
9	CJ	83	GLU
9	CJ	84	GLN
9	CJ	95	GLU
9	CJ	96	ILE

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Mol	Chain	Res	Type
10	CK	18	ARG
10	CK	25	TYR
10	CK	29	ILE
10	CK	33	THR
10	CK	34	ASP
10	CK	36	ASP
10	CK	40	ILE
10	CK	41	THR
10	CK	48	ILE
10	CK	54	ARG
10	CK	57	THR
10	CK	75	TYR
10	CK	84	VAL
10	CK	101	SER
10	CK	103	LEU
10	CK	107	SER
10	CK	124	LYS
10	CK	127	LYS
11	CL	6	THR
11	CL	18	VAL
11	CL	20	LYS
11	CL	24	VAL
11	CL	33	ARG
11	CL	37	CYS
11	CL	38	THR
11	CL	43	VAL
11	CL	47	LYS
11	CL	52	LEU
11	CL	54	LYS
11	CL	55	VAL
11	CL	60	LEU
11	CL	67	THR
11	CL	69	TYR
11	CL	75	HIS
11	CL	76	ASN
11	CL	77	LEU
11	CL	80	HIS
11	CL	85	ILE
11	CL	92	ASP
11	CL	93	LEU
11	CL	96	VAL
11	CL	101	VAL

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Mol	Chain	Res	Type
11	CL	112	ASP
11	CL	123	LYS
11	CL	127	GLU
12	CM	17	VAL
12	CM	31	LYS
12	CM	36	LYS
12	CM	43	THR
12	CM	46	LYS
12	CM	50	GLU
12	CM	57	ARG
12	CM	64	TRP
12	CM	81	LEU
12	CM	92	HIS
12	CM	99	ARG
12	CM	108	ARG
12	CM	110	ARG
12	CM	121	LYS
13	CN	9	LYS
13	CN	16	PHE
13	CN	22	THR
13	CN	29	ARG
13	CN	35	ARG
13	CN	36	PHE
13	CN	40	CYS
13	CN	44	LEU
13	CN	47	LEU
13	CN	53	LEU
13	CN	56	VAL
13	CN	57	ARG
13	CN	58	LYS
13	CN	61	TRP
14	CO	17	ARG
14	CO	21	ASP
14	CO	25	THR
14	CO	26	GLU
14	CO	38	ARG
14	CO	39	LEU
14	CO	43	LEU
14	CO	47	LYS
14	CO	54	ARG
14	CO	63	ARG
14	CO	79	ARG

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Mol	Chain	Res	Type
14	CO	87	ILE
14	CO	88	ARG
15	CP	1	MET
15	CP	3	LYS
15	CP	12	LYS
15	CP	13	HIS
15	CP	22	THR
15	CP	32	TYR
15	CP	49	LEU
15	CP	58	TYR
15	CP	59	TRP
15	CP	69	THR
15	CP	73	LEU
16	CQ	10	VAL
16	CQ	19	VAL
16	CQ	36	ILE
16	CQ	37	LYS
16	CQ	48	GLU
16	CQ	52	LYS
16	CQ	53	LEU
16	CQ	55	ASP
16	CQ	63	ARG
16	CQ	66	SER
16	CQ	81	ARG
16	CQ	83	ASP
16	CQ	85	VAL
16	CQ	87	LYS
16	CQ	92	ARG
17	CR	19	LYS
17	CR	23	LYS
17	CR	34	TYR
17	CR	38	GLU
17	CR	47	THR
17	CR	53	ARG
17	CR	62	GLU
17	CR	81	PHE
18	CS	5	LEU
18	CS	6	LYS
18	CS	9	VAL
18	CS	13	ASP
18	CS	25	LYS
18	CS	27	GLU

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Mol	Chain	Res	Type
18	CS	29	ARG
18	CS	33	THR
18	CS	34	TRP
18	CS	37	ARG
18	CS	47	HIS
18	CS	61	TYR
18	CS	62	ILE
18	CS	63	THR
18	CS	66	MET
18	CS	67	VAL
18	CS	71	LEU
19	CT	11	SER
19	CT	13	LEU
19	CT	15	ARG
19	CT	43	LEU
19	CT	71	THR
19	CT	74	LYS
19	CT	92	LEU
19	CT	93	GLU
20	CY	8	ASP
20	CY	9	LEU
20	CY	14	ASN
20	CY	20	HIS
20	CY	26	THR
20	CY	33	LEU
20	CY	35	TYR
20	CY	39	ILE
20	CY	61	ARG
20	CY	66	THR
20	CY	84	THR
20	CY	92	ILE
20	CY	94	VAL
20	CY	98	MET
20	CY	99	ARG
20	CY	105	ILE
20	CY	114	VAL
20	CY	126	GLU
20	CY	128	TYR
20	CY	132	ARG
20	CY	133	ILE
20	CY	135	PHE
20	CY	152	THR

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Mol	Chain	Res	Type
20	CY	153	MET
20	CY	170	ARG
20	CY	171	GLU
20	CY	173	THR
20	CY	174	PHE
20	CY	178	ILE
20	CY	179	ASP
20	CY	190	ASN
20	CY	199	ILE
20	CY	203	GLU
20	CY	204	GLU
20	CY	224	ASP
20	CY	225	GLU
20	CY	232	LEU
20	CY	260	LEU
20	CY	266	ASN
20	CY	271	LEU
20	CY	277	VAL
20	CY	290	LYS
20	CY	292	THR
20	CY	300	GLU
20	CY	304	ASP
20	CY	312	LEU
20	CY	328	ILE
20	CY	342	TYR
20	CY	344	THR
20	CY	382	GLU
20	CY	398	ILE
20	CY	406	GLU
20	CY	408	VAL
20	CY	410	ASP
20	CY	422	GLU
20	CY	424	LEU
20	CY	428	LEU
20	CY	437	THR
20	CY	438	PHE
20	CY	448	GLN
20	CY	451	ILE
20	CY	454	MET
20	CY	456	GLU
20	CY	457	LEU
20	CY	468	ARG

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Mol	Chain	Res	Type
20	CY	472	VAL
20	CY	476	VAL
20	CY	487	ILE
20	CY	488	THR
20	CY	493	VAL
20	CY	497	PHE
20	CY	504	ARG
20	CY	507	TYR
20	CY	510	VAL
20	CY	512	ILE
20	CY	525	PHE
20	CY	526	VAL
20	CY	542	VAL
20	CY	556	ILE
20	CY	568	TYR
20	CY	572	TYR
20	CY	574	GLU
20	CY	579	GLU
20	CY	601	ILE
20	CY	606	MET
20	CY	608	VAL
20	CY	614	GLU
20	CY	617	MET
20	CY	623	ASP
20	CY	630	GLN
20	CY	663	THR
20	CY	669	PHE
20	CY	671	MET
20	CY	676	TYR
20	CY	677	GLN
20	CY	679	VAL
25	DC	7	ARG
25	DC	9	ARG
25	DC	12	LEU
25	DC	14	LYS
25	DC	19	LYS
25	DC	28	ARG
25	DC	31	LYS
25	DC	41	THR
25	DC	42	VAL
25	DC	45	HIS
25	DC	48	LEU

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Mol	Chain	Res	Type
25	DC	51	ASP
25	DC	53	ARG
25	DC	54	ARG
25	DC	57	GLN
25	DC	73	VAL
25	DC	75	VAL
25	DC	83	LYS
25	DC	85	LYS
25	DC	86	GLU
25	DC	93	ASP
25	DC	95	VAL
25	DC	98	GLU
25	DC	100	ILE
25	DC	105	LEU
25	DC	109	MET
25	DC	115	VAL
25	DC	117	THR
25	DC	119	ASP
25	DC	121	MET
25	DC	130	ARG
25	DC	131	ILE
25	DC	132	LEU
25	DC	138	LEU
25	DC	148	PHE
25	DC	149	ASN
25	DC	155	ARG
25	DC	158	LYS
25	DC	161	ARG
25	DC	164	PHE
25	DC	168	LYS
25	DC	169	THR
25	DC	172	ILE
25	DC	173	HIS
25	DC	176	VAL
25	DC	201	LYS
25	DC	203	GLU
25	DC	206	LYS
25	DC	209	PHE
25	DC	211	ARG
25	DC	213	VAL
25	DC	216	THR
26	DD	4	LYS

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Mol	Chain	Res	Type
26	DD	5	LYS
26	DD	9	TYR
26	DD	10	THR
26	DD	14	ARG
26	DD	15	PHE
26	DD	23	GLU
26	DD	24	ILE
26	DD	25	THR
26	DD	26	LYS
26	DD	30	GLU
26	DD	31	LYS
26	DD	35	LYS
26	DD	37	LEU
26	DD	62	TYR
26	DD	64	ILE
26	DD	65	ILE
26	DD	69	ARG
26	DD	78	LYS
26	DD	82	ILE
26	DD	83	GLU
26	DD	92	ILE
26	DD	95	LEU
26	DD	103	ARG
26	DD	104	TYR
26	DD	105	ILE
26	DD	115	GLN
26	DD	134	ARG
26	DD	136	ILE
26	DD	140	THR
26	DD	143	HIS
26	DD	155	LEU
26	DD	161	THR
26	DD	175	LEU
26	DD	196	VAL
26	DD	229	VAL
26	DD	230	ASP
26	DD	237	GLU
26	DD	242	ARG
26	DD	248	SER
26	DD	264	LYS
26	DD	267	SER
27	DE	4	ILE

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Mol	Chain	Res	Type
27	DE	9	VAL
27	DE	11	MET
27	DE	18	ASP
27	DE	26	ILE
27	DE	35	GLN
27	DE	52	LEU
27	DE	54	GLN
27	DE	57	LYS
27	DE	61	ARG
27	DE	77	ILE
27	DE	78	LEU
27	DE	79	ARG
27	DE	87	GLU
27	DE	89	ASP
27	DE	93	VAL
27	DE	94	GLU
27	DE	95	ILE
27	DE	132	HIS
27	DE	134	ILE
27	DE	135	HIS
27	DE	141	ILE
27	DE	146	THR
27	DE	159	HIS
27	DE	160	TYR
27	DE	163	GLU
27	DE	180	ASN
27	DE	192	ASN
27	DE	199	ARG
28	DF	3	GLU
28	DF	6	VAL
28	DF	7	TYR
28	DF	12	LEU
28	DF	17	ARG
28	DF	38	ARG
28	DF	40	GLN
28	DF	53	THR
28	DF	56	GLU
28	DF	72	ARG
28	DF	74	ARG
28	DF	106	ARG
28	DF	125	LEU
28	DF	126	VAL

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Mol	Chain	Res	Type
28	DF	132	VAL
28	DF	136	THR
28	DF	149	ASP
28	DF	154	VAL
28	DF	175	THR
28	DF	185	ASP
28	DF	191	ARG
28	DF	196	LEU
28	DF	199	TRP
28	DF	200	GLU
28	DF	206	ILE
29	DG	5	VAL
29	DG	9	ARG
29	DG	21	ARG
29	DG	34	LEU
29	DG	39	ILE
29	DG	40	ASN
29	DG	43	LEU
29	DG	45	GLU
29	DG	58	GLN
29	DG	60	LEU
29	DG	66	GLN
29	DG	82	LEU
29	DG	83	ARG
29	DG	84	LYS
29	DG	86	MET
29	DG	99	MET
29	DG	113	ARG
29	DG	115	ARG
29	DG	126	ASP
29	DG	133	LEU
29	DG	135	LEU
29	DG	138	GLN
29	DG	146	TYR
29	DG	147	ASP
29	DG	172	LEU
30	DH	17	VAL
30	DH	23	ARG
30	DH	33	LEU
30	DH	41	MET
30	DH	43	VAL
30	DH	67	LEU

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Mol	Chain	Res	Type
30	DH	70	THR
30	DH	72	ILE
30	DH	79	VAL
30	DH	83	TYR
30	DH	86	GLU
30	DH	88	LEU
30	DH	107	VAL
30	DH	114	VAL
30	DH	116	GLU
30	DH	122	THR
30	DH	133	VAL
30	DH	136	ILE
30	DH	159	GLU
32	DK	9	LYS
32	DK	10	LEU
32	DK	27	LEU
32	DK	37	PHE
32	DK	45	THR
32	DK	57	ILE
32	DK	58	THR
32	DK	60	TYR
32	DK	63	ARG
32	DK	64	SER
32	DK	65	PHE
32	DK	69	THR
32	DK	78	ILE
32	DK	84	LEU
32	DK	95	LYS
32	DK	96	VAL
32	DK	98	ARG
32	DK	102	GLU
32	DK	105	LEU
32	DK	106	GLU
32	DK	110	GLN
32	DK	111	LYS
32	DK	114	ASP
32	DK	115	LEU
32	DK	118	THR
32	DK	125	ARG
32	DK	132	ARG
32	DK	133	SER
33	DN	22	THR

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Mol	Chain	Res	Type
33	DN	25	ARG
33	DN	28	THR
33	DN	29	LYS
33	DN	32	THR
33	DN	33	LEU
33	DN	41	ASP
33	DN	48	MET
33	DN	65	LYS
33	DN	76	SER
33	DN	84	LYS
33	DN	87	LEU
33	DN	93	THR
33	DN	98	VAL
33	DN	106	MET
33	DN	112	LEU
33	DN	114	ARG
33	DN	119	ARG
33	DN	120	LEU
33	DN	127	ASP
33	DN	131	GLN
33	DN	134	ARG
33	DN	137	LYS
33	DN	138	LEU
34	DO	2	ILE
34	DO	8	LEU
34	DO	37	ASP
34	DO	42	SER
34	DO	45	GLU
34	DO	70	LYS
34	DO	78	ARG
34	DO	80	ASP
34	DO	82	ASN
34	DO	89	ASN
34	DO	91	LEU
34	DO	92	GLU
34	DO	94	ARG
34	DO	117	LEU
35	DP	7	ARG
35	DP	16	ARG
35	DP	19	VAL
35	DP	27	HIS
35	DP	29	LYS

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Mol	Chain	Res	Type
35	DP	32	THR
35	DP	35	HIS
35	DP	39	LYS
35	DP	46	LYS
35	DP	50	ARG
35	DP	51	PHE
35	DP	55	ARG
35	DP	60	MET
35	DP	61	ARG
35	DP	62	LEU
35	DP	65	ARG
35	DP	68	GLN
35	DP	71	VAL
35	DP	77	ARG
35	DP	79	ARG
35	DP	84	ASN
35	DP	91	PHE
35	DP	100	LEU
35	DP	101	VAL
35	DP	110	TYR
35	DP	123	LEU
35	DP	130	PHE
36	DQ	1	MET
36	DQ	3	MET
36	DQ	7	MET
36	DQ	14	ARG
36	DQ	16	ARG
36	DQ	17	LEU
36	DQ	25	ASP
36	DQ	35	VAL
36	DQ	37	LEU
36	DQ	43	THR
36	DQ	45	GLN
36	DQ	46	GLN
36	DQ	56	ARG
36	DQ	57	HIS
36	DQ	58	PHE
36	DQ	59	ARG
36	DQ	60	ARG
36	DQ	68	ILE
36	DQ	91	GLU
36	DQ	104	PHE

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Mol	Chain	Res	Type
36	DQ	105	GLU
36	DQ	106	VAL
36	DQ	112	GLU
36	DQ	128	LYS
36	DQ	131	ILE
36	DQ	132	VAL
36	DQ	137	TYR
37	DR	3	HIS
37	DR	4	LEU
37	DR	11	ASN
37	DR	13	HIS
37	DR	16	HIS
37	DR	29	LEU
37	DR	37	THR
37	DR	43	GLU
37	DR	44	LEU
37	DR	45	ARG
37	DR	49	ASP
37	DR	59	ASP
37	DR	65	LEU
37	DR	71	GLN
37	DR	72	ASP
37	DR	76	VAL
37	DR	79	LEU
37	DR	82	GLU
37	DR	97	VAL
37	DR	99	LYS
37	DR	100	LEU
37	DR	107	ASP
38	DS	13	ARG
38	DS	15	ARG
38	DS	16	ASN
38	DS	23	ARG
38	DS	24	LEU
38	DS	47	THR
38	DS	50	SER
38	DS	62	LYS
38	DS	67	ARG
38	DS	69	VAL
38	DS	78	LEU
38	DS	84	GLN
38	DS	87	PHE

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Mol	Chain	Res	Type
38	DS	92	TYR
38	DS	95	HIS
38	DS	97	ARG
38	DS	98	VAL
38	DS	99	LYS
39	DT	1	MET
39	DT	13	ARG
39	DT	16	ARG
39	DT	27	THR
39	DT	30	VAL
39	DT	33	LYS
39	DT	38	ASN
39	DT	42	ILE
39	DT	44	ASP
39	DT	46	GLU
39	DT	48	ILE
39	DT	57	PHE
39	DT	64	ARG
39	DT	70	VAL
39	DT	74	ARG
39	DT	80	SER
39	DT	82	LEU
39	DT	96	ARG
39	DT	105	LEU
39	DT	107	ASP
39	DT	108	ARG
39	DT	109	GLU
39	DT	111	ARG
39	DT	114	LEU
39	DT	115	ARG
39	DT	118	ARG
39	DT	124	ASP
40	DU	6	THR
40	DU	14	HIS
40	DU	18	LEU
40	DU	34	LYS
40	DU	38	THR
40	DU	39	LEU
40	DU	44	ASN
40	DU	51	LYS
40	DU	54	LYS
40	DU	58	ARG

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Mol	Chain	Res	Type
40	DU	59	ARG
40	DU	64	ARG
40	DU	74	LEU
40	DU	83	LEU
40	DU	90	VAL
40	DU	97	ASP
40	DU	98	LEU
40	DU	101	ARG
40	DU	104	GLN
40	DU	105	VAL
40	DU	108	GLU
40	DU	114	LYS
40	DU	117	GLN
41	DV	14	VAL
41	DV	18	LEU
41	DV	19	LYS
41	DV	21	ARG
41	DV	37	VAL
41	DV	38	LEU
41	DV	40	LEU
41	DV	47	VAL
41	DV	57	VAL
41	DV	60	GLU
41	DV	69	LYS
41	DV	71	LEU
41	DV	73	SER
41	DV	75	PHE
41	DV	80	GLN
41	DV	82	ARG
41	DV	85	LYS
41	DV	87	HIS
41	DV	98	GLU
41	DV	99	ILE
42	DW	11	ARG
42	DW	12	ILE
42	DW	17	VAL
42	DW	19	LEU
42	DW	27	LYS
42	DW	37	ARG
42	DW	39	THR
42	DW	61	ASN
42	DW	64	MET

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Mol	Chain	Res	Type
42	DW	66	GLU
42	DW	70	TYR
42	DW	88	ARG
42	DW	95	ILE
42	DW	96	ILE
42	DW	99	ARG
42	DW	107	LEU
43	DX	3	THR
43	DX	6	ASP
43	DX	15	GLU
43	DX	27	THR
43	DX	53	LYS
43	DX	54	VAL
43	DX	56	THR
43	DX	57	LEU
43	DX	58	HIS
43	DX	66	LEU
43	DX	68	ARG
43	DX	69	TYR
43	DX	72	LYS
43	DX	75	ASP
43	DX	76	ARG
43	DX	87	GLN
43	DX	92	LEU
44	DY	2	ARG
44	DY	4	LYS
44	DY	5	MET
44	DY	6	HIS
44	DY	7	VAL
44	DY	9	LYS
44	DY	13	VAL
44	DY	19	LYS
44	DY	35	TYR
44	DY	39	VAL
44	DY	44	ILE
44	DY	47	LYS
44	DY	50	ARG
44	DY	62	GLU
44	DY	76	CYS
45	DZ	3	TYR
45	DZ	24	LEU
45	DZ	31	ARG

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Mol	Chain	Res	Type
45	DZ	34	ASN
45	DZ	36	LYS
45	DZ	37	VAL
45	DZ	39	VAL
45	DZ	46	LYS
45	DZ	52	SER
45	DZ	57	ILE
45	DZ	59	LEU
45	DZ	70	LEU
45	DZ	72	ARG
45	DZ	81	ARG
45	DZ	82	ARG
45	DZ	86	VAL
45	DZ	87	ASP
45	DZ	98	MET
45	DZ	102	LEU
45	DZ	124	ILE
45	DZ	126	VAL
45	DZ	127	LYS
45	DZ	133	ILE
45	DZ	136	PHE
45	DZ	140	ASP
45	DZ	145	GLU
45	DZ	148	ASP
45	DZ	151	HIS
45	DZ	153	SER
45	DZ	154	ASP
45	DZ	155	LEU
45	DZ	156	LYS
45	DZ	165	VAL
45	DZ	179	ASP
45	DZ	181	GLU
45	DZ	185	GLU
45	DZ	186	GLU
46	D0	11	ARG
46	D0	21	LEU
46	D0	27	GLU
46	D0	30	VAL
46	D0	35	ASN
46	D0	36	ILE
46	D0	41	ARG
46	D0	43	THR

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Mol	Chain	Res	Type
46	D0	57	PHE
46	D0	82	ARG
47	D2	9	GLN
47	D2	17	SER
47	D2	21	LEU
47	D2	35	LEU
47	D2	40	SER
47	D2	47	ASN
47	D2	55	ARG
47	D2	71	ASN
48	D3	8	LEU
48	D3	17	LYS
48	D3	19	GLN
48	D3	29	ARG
48	D3	36	VAL
48	D3	48	GLU
48	D3	60	GLU
49	D5	3	LYS
49	D5	20	ARG
49	D5	25	LEU
49	D5	26	THR
49	D5	31	VAL
49	D5	44	THR
49	D5	48	GLU
49	D5	51	TYR
49	D5	52	TYR
49	D5	58	LEU
50	D6	6	ARG
50	D6	9	LEU
50	D6	10	LEU
50	D6	11	LEU
50	D6	18	ARG
50	D6	19	ARG
50	D6	23	THR
50	D6	25	LYS
50	D6	28	ARG
50	D6	34	LEU
50	D6	43	CYS
50	D6	46	HIS
50	D6	47	THR
50	D6	53	LYS
50	D6	54	ILE

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Mol	Chain	Res	Type
51	D7	6	GLN
51	D7	19	ARG
51	D7	24	THR
51	D7	39	ARG
51	D7	40	TRP
51	D7	47	ARG
52	D8	33	ASN
52	D8	34	TRP
52	D8	36	LYS
52	D8	40	GLU
52	D8	44	LYS
52	D8	49	VAL
52	D8	53	PRO
52	D8	59	LYS
52	D8	61	LEU
52	D8	64	TYR
53	D9	11	CYS
53	D9	17	ILE
53	D9	27	CYS
53	D9	35	ARG
56	D1	5	CYS
56	D1	14	VAL
56	D1	20	ARG
56	D1	25	LYS
56	D1	27	GLU
56	D1	32	LYS
56	D1	40	ARG
56	D1	41	ARG
56	D1	43	TYR
56	D1	45	ASN
56	D1	46	LEU
56	D1	47	GLN
56	D1	50	ARG
56	D1	57	GLU
56	D1	58	ILE
56	D1	61	ARG
56	D1	67	ILE
56	D1	88	LYS
56	D1	90	ILE
56	D1	94	LEU
57	D4	1	MET
57	D4	6	HIS

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Mol	Chain	Res	Type
57	D4	8	LYS
57	D4	9	LEU
57	D4	10	VAL
57	D4	15	ILE
57	D4	23	GLU
57	D4	26	SER
57	D4	32	TYR
57	D4	34	GLU
58	De	61	ASP
58	De	70	LYS
58	De	73	GLU
58	De	78	LEU
58	De	90	LYS
58	De	94	GLU
58	De	95	LYS
58	De	101	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	16	HIS
1	AB	104	ASN
2	AC	107	GLN
3	AD	161	ASN
6	AG	96	GLN
7	AH	78	GLN
10	AK	117	ASN
11	AL	99	HIS
14	AO	71	GLN
15	AP	65	GLN
20	AY	77	HIS
20	AY	137	ASN
20	AY	165	GLN
20	AY	595	GLN
20	AY	682	GLN
25	BC	18	ASN
25	BC	189	ASN
26	BD	164	GLN
27	BE	35	GLN
27	BE	159	HIS
28	BF	40	GLN
28	BF	169	ASN

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Mol	Chain	Res	Type
29	BG	138	GLN
32	BK	30	HIS
34	BO	90	GLN
35	BP	68	GLN
36	BQ	12	GLN
39	BT	123	GLN
45	BZ	75	ASN
49	B5	23	HIS
50	B6	32	ASN
3	CD	161	ASN
4	CE	78	HIS
5	CF	32	ASN
6	CG	148	ASN
10	CK	27	ASN
10	CK	116	HIS
12	CM	92	HIS
16	CQ	96	GLN
19	CT	18	GLN
20	CY	40	HIS
20	CY	80	ASN
20	CY	137	ASN
26	DD	87	ASN
26	DD	126	GLN
26	DD	231	HIS
27	DE	180	ASN
28	DF	40	GLN
28	DF	169	ASN
29	DG	27	ASN
32	DK	30	HIS
33	DN	131	GLN
35	DP	9	ASN
35	DP	68	GLN
36	DQ	12	GLN
36	DQ	89	ASN
36	DQ	123	HIS
37	DR	23	ASN
38	DS	34	HIS
38	DS	38	GLN
39	DT	84	GLN
41	DV	87	HIS
41	DV	89	GLN
43	DX	58	HIS

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Mol	Chain	Res	Type
43	DX	87	GLN
45	DZ	118	GLN
46	D0	80	HIS
50	D6	26	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1511/1511 (100%)	326 (21%)	19 (1%)
21	CA	1511/1511 (100%)	310 (20%)	16 (1%)
22	AW	76/77 (98%)	22 (28%)	1 (1%)
22	CW	76/77 (98%)	19 (25%)	1 (1%)
23	AV	22/23 (95%)	11 (50%)	2 (9%)
23	CV	22/23 (95%)	9 (40%)	3 (13%)
59	BA	2878/2879 (99%)	666 (23%)	21 (0%)
59	DA	2878/2879 (99%)	629 (21%)	17 (0%)
60	BB	118/119 (99%)	20 (16%)	4 (3%)
60	DB	118/119 (99%)	19 (16%)	3 (2%)
All	All	9210/9218 (99%)	2031 (22%)	87 (0%)

All (2031) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	G
21	AA	8	A
21	AA	9	G
21	AA	13	U
21	AA	22	G
21	AA	31	G
21	AA	32	A
21	AA	39	G
21	AA	47	C
21	AA	48	C
21	AA	50	A
21	AA	51	A
21	AA	54	C
21	AA	65	U
21	AA	66	G
21	AA	68	G
21	AA	68(H)	G

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Mol	Chain	Res	Type
21	AA	68(L)	U
21	AA	68(P)	C
21	AA	68(R)	C
21	AA	68(S)	C
21	AA	109	A
21	AA	116	A
21	AA	121	C
21	AA	129(A)	G
21	AA	131	C
21	AA	134	A
21	AA	135	C
21	AA	136	C
21	AA	144	G
21	AA	148	G
21	AA	163	C
21	AA	170	U
21	AA	174	C
21	AA	186(H)	U
21	AA	191	G
21	AA	195	A
21	AA	197	A
21	AA	201	C
21	AA	201(A)	U
21	AA	201(C)	U
21	AA	216	G
21	AA	222	U
21	AA	233	C
21	AA	247	G
21	AA	251	G
21	AA	264	U
21	AA	267	C
21	AA	281	G
21	AA	283	C
21	AA	289	G
21	AA	290	C
21	AA	294	U
21	AA	306	G
21	AA	313	A
21	AA	315	A
21	AA	316	G
21	AA	321	A
21	AA	328	C

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Mol	Chain	Res	Type
21	AA	329	A
21	AA	332	G
21	AA	340	U
21	AA	345	C
21	AA	346	G
21	AA	347	G
21	AA	348	G
21	AA	352	C
21	AA	353	A
21	AA	354	G
21	AA	367	U
21	AA	372	C
21	AA	388	G
21	AA	389	A
21	AA	390	C
21	AA	392	G
21	AA	397	A
21	AA	398	C
21	AA	406	G
21	AA	410	G
21	AA	412	A
21	AA	413	G
21	AA	414	A
21	AA	422	C
21	AA	424	G
21	AA	429	U
21	AA	430	A
21	AA	432	A
21	AA	440	A
21	AA	444	C
21	AA	452	A
21	AA	453	A
21	AA	457	C
21	AA	458(B)	A
21	AA	475	G
21	AA	481	G
21	AA	482	A
21	AA	484	G
21	AA	485	G
21	AA	486	U
21	AA	497	A
21	AA	498	U

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Mol	Chain	Res	Type
21	AA	505	G
21	AA	509	A
21	AA	511	C
21	AA	518	C
21	AA	520	A
21	AA	521	G
21	AA	524	G
21	AA	527	G
21	AA	531	U
21	AA	532	A
21	AA	533	A
21	AA	535	A
21	AA	536	C
21	AA	547	A
21	AA	559	A
21	AA	561	U
21	AA	562	C
21	AA	564	C
21	AA	565	U
21	AA	568	G
21	AA	572	A
21	AA	573	A
21	AA	574	A
21	AA	576	G
21	AA	577	G
21	AA	596	C
21	AA	618	C
21	AA	653	A
21	AA	659	U
21	AA	665	A
21	AA	666	G
21	AA	678	U
21	AA	688	G
21	AA	693	G
21	AA	702	A
21	AA	703	G
21	AA	706	A
21	AA	717	C
21	AA	720	C
21	AA	721	G
21	AA	724	G
21	AA	733	A

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Mol	Chain	Res	Type
21	AA	734	G
21	AA	737	A
21	AA	749	C
21	AA	755	G
21	AA	777	A
21	AA	793	U
21	AA	794	A
21	AA	796	C
21	AA	816	A
21	AA	817	C
21	AA	818	G
21	AA	819	A
21	AA	828	A
21	AA	838(A)	U
21	AA	838(B)	C
21	AA	838(C)	U
21	AA	848	C
21	AA	852	G
21	AA	853	G
21	AA	855	G
21	AA	859	A
21	AA	889	A
21	AA	907	A
21	AA	916	G
21	AA	918	A
21	AA	923	A
21	AA	926	G
21	AA	927	G
21	AA	934	C
21	AA	935	A
21	AA	939	G
21	AA	960	U
21	AA	961	U
21	AA	968	A
21	AA	969	A
21	AA	971	G
21	AA	974	A
21	AA	976	G
21	AA	977	A
21	AA	978	A
21	AA	980	C
21	AA	983	A

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Mol	Chain	Res	Type
21	AA	992	U
21	AA	993	G
21	AA	1004	A
21	AA	1005	A
21	AA	1006	C
21	AA	1008	C
21	AA	1020	U
21	AA	1025	U
21	AA	1028(B)	C
21	AA	1028(C)	G
21	AA	1036	G
21	AA	1037	C
21	AA	1045	C
21	AA	1054	C
21	AA	1055	A
21	AA	1060	C
21	AA	1065	U
21	AA	1066	C
21	AA	1068	G
21	AA	1081	G
21	AA	1084	G
21	AA	1089	G
21	AA	1094	G
21	AA	1095	U
21	AA	1101	A
21	AA	1102	A
21	AA	1108	G
21	AA	1115	C
21	AA	1117	G
21	AA	1118	C
21	AA	1120	G
21	AA	1125	U
21	AA	1126	U
21	AA	1127	G
21	AA	1128	C
21	AA	1129	C
21	AA	1130	A
21	AA	1131	G
21	AA	1136	U
21	AA	1137	C
21	AA	1138	G
21	AA	1139	G

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Mol	Chain	Res	Type
21	AA	1146	A
21	AA	1150	U
21	AA	1152	A
21	AA	1158	C
21	AA	1159	U
21	AA	1160	G
21	AA	1171	G
21	AA	1181	G
21	AA	1182	G
21	AA	1190	G
21	AA	1191	A
21	AA	1193	G
21	AA	1196	U
21	AA	1197	G
21	AA	1210	C
21	AA	1211	U
21	AA	1212	U
21	AA	1213	A
21	AA	1220	G
21	AA	1222	G
21	AA	1225	A
21	AA	1226	C
21	AA	1228	C
21	AA	1236	A
21	AA	1238	A
21	AA	1239	A
21	AA	1240	U
21	AA	1249	C
21	AA	1256	A
21	AA	1257	U
21	AA	1260	C
21	AA	1270	C
21	AA	1280	A
21	AA	1281	U
21	AA	1287	A
21	AA	1300	G
21	AA	1301	U
21	AA	1302	U
21	AA	1303	C
21	AA	1305	G
21	AA	1311	G
21	AA	1317	C

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Mol	Chain	Res	Type
21	AA	1320	C
21	AA	1322	C
21	AA	1331	G
21	AA	1335	C
21	AA	1338	G
21	AA	1345	U
21	AA	1347	G
21	AA	1357	A
21	AA	1358	U
21	AA	1359	C
21	AA	1362(A)	C
21	AA	1363	A
21	AA	1364	U
21	AA	1365	G
21	AA	1370	G
21	AA	1377	A
21	AA	1378	C
21	AA	1379	G
21	AA	1381	U
21	AA	1394	A
21	AA	1397	C
21	AA	1413	A
21	AA	1419	G
21	AA	1440(B)	G
21	AA	1440(C)	G
21	AA	1440(D)	A
21	AA	1440(I)	A
21	AA	1440(J)	C
21	AA	1440(K)	G
21	AA	1440(L)	G
21	AA	1475	G
21	AA	1484	C
21	AA	1487	G
21	AA	1489	G
21	AA	1491	G
21	AA	1492	A
21	AA	1493	A
21	AA	1494	G
21	AA	1497	G
21	AA	1502	A
21	AA	1503	A
21	AA	1504	G

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Mol	Chain	Res	Type
21	AA	1505	G
21	AA	1506	U
21	AA	1507	A
21	AA	1517	G
21	AA	1520	G
21	AA	1525	G
21	AA	1529	G
21	AA	1530	G
21	AA	1532	U
21	AA	1533	C
21	AA	1534	A
21	AA	1535	C
21	AA	1536	C
21	AA	1538	C
22	AW	6	C
22	AW	8	U
22	AW	9	A
22	AW	16	U
22	AW	17	U
22	AW	18	G
22	AW	19	G
22	AW	20	U
22	AW	20(A)	U
22	AW	21	A
22	AW	22	G
22	AW	25	C
22	AW	29	U
22	AW	46	G
22	AW	47	U
22	AW	48	C
22	AW	50	C
22	AW	58	A
22	AW	60	U
22	AW	61	C
22	AW	66	C
22	AW	76	A
23	AV	5	A
23	AV	9	G
23	AV	10	G
23	AV	11	U
23	AV	12	A
23	AV	15	A

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Mol	Chain	Res	Type
23	AV	16	A
23	AV	18	G
23	AV	19	G
23	AV	22	A
23	AV	23	A
59	BA	9	U
59	BA	12	U
59	BA	13	A
59	BA	27	G
59	BA	34	C
59	BA	46	C
59	BA	47	C
59	BA	49	A
59	BA	50	U
59	BA	51	G
59	BA	61	G
59	BA	68	G
59	BA	70	G
59	BA	72	U
59	BA	73	A
59	BA	74	A
59	BA	75	G
59	BA	84	A
59	BA	90	U
59	BA	93	C
59	BA	94	G
59	BA	98	G
59	BA	101	G
59	BA	102	G
59	BA	104	U
59	BA	113	G
59	BA	116	C
59	BA	118	A
59	BA	119	A
59	BA	120	U
59	BA	121	G
59	BA	134	C
59	BA	138	G
59	BA	149	A
59	BA	163	U
59	BA	164	U
59	BA	181	A

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Mol	Chain	Res	Type
59	BA	196	A
59	BA	197	A
59	BA	199	A
59	BA	204	A
59	BA	205	G
59	BA	215	G
59	BA	216	A
59	BA	221	A
59	BA	222	A
59	BA	227	A
59	BA	228	A
59	BA	229	A
59	BA	230	U
59	BA	232	G
59	BA	233	A
59	BA	248	G
59	BA	252	G
59	BA	264	C
59	BA	265	A
59	BA	266	G
59	BA	270(L)	C
59	BA	270(M)	U
59	BA	270(N)	U
59	BA	270(O)	G
59	BA	270(Q)	C
59	BA	270(R)	C
59	BA	271(D)	U
59	BA	271	G
59	BA	274	G
59	BA	278	A
59	BA	279	C
59	BA	294	A
59	BA	295	G
59	BA	300	A
59	BA	302	C
59	BA	310	A
59	BA	322	A
59	BA	323	G
59	BA	325	G
59	BA	329	G
59	BA	330	A
59	BA	331	A

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Mol	Chain	Res	Type
59	BA	352	G
59	BA	354	G
59	BA	363(A)	G
59	BA	363(B)	A
59	BA	363(G)	A
59	BA	364	C
59	BA	372	G
59	BA	386	G
59	BA	387	U
59	BA	388	G
59	BA	389	G
59	BA	396	G
59	BA	405	U
59	BA	408	G
59	BA	411	G
59	BA	412	A
59	BA	425	G
59	BA	444	C
59	BA	447	A
59	BA	448	U
59	BA	449	A
59	BA	451	C
59	BA	454	A
59	BA	455	C
59	BA	456	C
59	BA	457	A
59	BA	458	G
59	BA	459	U
59	BA	464	U
59	BA	470	A
59	BA	473	G
59	BA	474	G
59	BA	475	U
59	BA	480	A
59	BA	481	G
59	BA	489	G
59	BA	492	A
59	BA	505	A
59	BA	508	G
59	BA	509	C
59	BA	513	A
59	BA	527	C

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Mol	Chain	Res	Type
59	BA	528	A
59	BA	530	G
59	BA	531	C
59	BA	532	A
59	BA	544	C
59	BA	546	C
59	BA	548	A
59	BA	556	G
59	BA	560	C
59	BA	563	G
59	BA	568	U
59	BA	569	U
59	BA	572	A
59	BA	573	G
59	BA	575	A
59	BA	586	A
59	BA	587	C
59	BA	599	G
59	BA	603	A
59	BA	604	G
59	BA	615	G
59	BA	616	A
59	BA	617	G
59	BA	620	G
59	BA	621	A
59	BA	627	A
59	BA	634	C
59	BA	637	A
59	BA	645	C
59	BA	646	A
59	BA	653	C
59	BA	654	U
59	BA	655	A
59	BA	671	C
59	BA	675	A
59	BA	682	G
59	BA	683	C
59	BA	685	A
59	BA	686	G
59	BA	717	G
59	BA	723	G
59	BA	730	C

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Mol	Chain	Res	Type
59	BA	738	G
59	BA	747	U
59	BA	748	G
59	BA	752	A
59	BA	753	C
59	BA	764	A
59	BA	776	G
59	BA	778	G
59	BA	779	U
59	BA	782	A
59	BA	784	A
59	BA	785	G
59	BA	788	A
59	BA	789	A
59	BA	792	G
59	BA	793	A
59	BA	800	A
59	BA	805	G
59	BA	812	C
59	BA	819	A
59	BA	821	A
59	BA	822	U
59	BA	824	A
59	BA	827	U
59	BA	831	G
59	BA	832	G
59	BA	846	C
59	BA	847	U
59	BA	852	G
59	BA	859	G
59	BA	860	U
59	BA	861	A
59	BA	866	A
59	BA	869	G
59	BA	870	A
59	BA	877	U
59	BA	879	G
59	BA	881	G
59	BA	882	G
59	BA	887	A
59	BA	890	A
59	BA	895	U

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Mol	Chain	Res	Type
59	BA	896	A
59	BA	897	C
59	BA	910	A
59	BA	914	C
59	BA	917	A
59	BA	929	G
59	BA	932	G
59	BA	933	A
59	BA	941	A
59	BA	943	U
59	BA	946	G
59	BA	951	C
59	BA	953	A
59	BA	959	A
59	BA	961	C
59	BA	970	C
59	BA	974(A)	G
59	BA	974(B)	C
59	BA	980	A
59	BA	983	A
59	BA	991	C
59	BA	996	A
59	BA	997	G
59	BA	999	U
59	BA	1008	C
59	BA	1009	A
59	BA	1011	G
59	BA	1012	U
59	BA	1013	C
59	BA	1017	G
59	BA	1021	A
59	BA	1022	G
59	BA	1023	U
59	BA	1024	G
59	BA	1025	G
59	BA	1026	U
59	BA	1027	A
59	BA	1030	G
59	BA	1033	U
59	BA	1034	G
59	BA	1047	G
59	BA	1048	A

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Mol	Chain	Res	Type
59	BA	1060	U
59	BA	1061	U
59	BA	1062	G
59	BA	1063	G
59	BA	1070	A
59	BA	1072	C
59	BA	1077	A
59	BA	1078	U
59	BA	1079	C
59	BA	1086	A
59	BA	1088	A
59	BA	1090	U
59	BA	1096	A
59	BA	1097	U
59	BA	1105	U
59	BA	1106	G
59	BA	1110	G
59	BA	1112	G
59	BA	1123	C
59	BA	1128	A
59	BA	1130	U
59	BA	1136	G
59	BA	1139	G
59	BA	1141	U
59	BA	114(B)	A
59	BA	1144	G
59	BA	1154	G
59	BA	1155	A
59	BA	1175	U
59	BA	1176	G
59	BA	1179	C
59	BA	1186	G
59	BA	1199	U
59	BA	1204	A
59	BA	1205	U
59	BA	1210	A
59	BA	1211	U
59	BA	1212	G
59	BA	1220	A
59	BA	1221	C
59	BA	1241	A
59	BA	1247	A

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Mol	Chain	Res	Type
59	BA	1248	G
59	BA	1249	U
59	BA	1253	A
59	BA	1256	G
59	BA	1265	A
59	BA	1271	G
59	BA	1272	A
59	BA	1286	A
59	BA	1294	U
59	BA	1300	U
59	BA	1301	A
59	BA	1302	A
59	BA	1309	G
59	BA	1311	G
59	BA	1312	U
59	BA	1313	U
59	BA	1314	C
59	BA	1321	A
59	BA	1322	A
59	BA	1325	G
59	BA	1329	U
59	BA	1330	C
59	BA	1331	A
59	BA	1332	G
59	BA	1333	C
59	BA	1341	U
59	BA	1343	G
59	BA	1348	G
59	BA	1349	A
59	BA	1352	U
59	BA	1359	A
59	BA	1360	A
59	BA	1365	A
59	BA	1378	A
59	BA	1379	A
59	BA	1384	A
59	BA	1385	G
59	BA	1395	A
59	BA	1396	U
59	BA	1398	C
59	BA	1416	G
59	BA	1417	C

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Mol	Chain	Res	Type
59	BA	1418	G
59	BA	1420	U
59	BA	1421	G
59	BA	1428	C
59	BA	1430	C
59	BA	144(B)	A
59	BA	149(B)	A
59	BA	1449	G
59	BA	1453	A
59	BA	1454	U
59	BA	1455	G
59	BA	1458	C
59	BA	1460	A
59	BA	1467	C
59	BA	1478	G
59	BA	1483	G
59	BA	1490	A
59	BA	1491	G
59	BA	1493	C
59	BA	1494	A
59	BA	1495	A
59	BA	1497	U
59	BA	1498	C
59	BA	1509	A
59	BA	1510	A
59	BA	1523	U
59	BA	1528	A
59	BA	1535	U
59	BA	1536	A
59	BA	1538	G
59	BA	1539	G
59	BA	1540	G
59	BA	1541	U
59	BA	1542	G
59	BA	1543	A
59	BA	1544	C
59	BA	1545	A
59	BA	154(B)	C
59	BA	1547	C
59	BA	1558	A
59	BA	1559	G
59	BA	1566	A

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Mol	Chain	Res	Type
59	BA	1569	A
59	BA	1580	A
59	BA	1581	G
59	BA	1583	A
59	BA	1585	C
59	BA	1602	U
59	BA	1603	A
59	BA	1608	A
59	BA	1609	A
59	BA	1616	A
59	BA	1617	C
59	BA	1618	A
59	BA	1635	G
59	BA	1639	U
59	BA	1640	C
59	BA	1644	C
59	BA	1646	C
59	BA	1648	C
59	BA	1654	A
59	BA	1656	C
59	BA	1672	C
59	BA	1674	G
59	BA	1691	C
59	BA	1694	C
59	BA	1729	A
59	BA	1732	A
59	BA	1735	U
59	BA	1755	A
59	BA	1757	U
59	BA	1762	A
59	BA	1763	G
59	BA	1764	G
59	BA	1769	G
59	BA	1773	A
59	BA	1781	C
59	BA	1783	A
59	BA	1784	A
59	BA	1787	A
59	BA	1791	A
59	BA	1800	C
59	BA	1801	G
59	BA	1809	A

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Mol	Chain	Res	Type
59	BA	1816	G
59	BA	1820	U
59	BA	1821	A
59	BA	1829	A
59	BA	1836	C
59	BA	1837	C
59	BA	1847	A
59	BA	1859	A
59	BA	1888	G
59	BA	1889	A
59	BA	1900	A
59	BA	1903	G
59	BA	1906	G
59	BA	1908	C
59	BA	1909	C
59	BA	1911	U
59	BA	1912	A
59	BA	1913	A
59	BA	1914	C
59	BA	1929	G
59	BA	1930	G
59	BA	1931	U
59	BA	1935	G
59	BA	1936	A
59	BA	1937	A
59	BA	1938	A
59	BA	1939	U
59	BA	1940	U
59	BA	1944	U
59	BA	1955	U
59	BA	1963	U
59	BA	1964	G
59	BA	1967	C
59	BA	1970	A
59	BA	1971	A
59	BA	1972	A
59	BA	1980	G
59	BA	1981	A
59	BA	1982	C
59	BA	1992	G
59	BA	1993	U
59	BA	1996	C

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Mol	Chain	Res	Type
59	BA	2013	A
59	BA	2020	A
59	BA	2023	G
59	BA	2024	G
59	BA	2027	G
59	BA	2028	U
59	BA	2030	A
59	BA	2031	A
59	BA	2032	G
59	BA	2033	A
59	BA	2034	U
59	BA	2036	C
59	BA	2043	C
59	BA	2044	C
59	BA	2051	A
59	BA	2052	G
59	BA	2055	C
59	BA	2056	G
59	BA	2060	A
59	BA	2061	G
59	BA	2062	A
59	BA	2069	G
59	BA	2093	G
59	BA	2111	C
59	BA	2113	U
59	BA	2117	A
59	BA	2118	U
59	BA	2120	G
59	BA	2126	A
59	BA	2131	G
59	BA	2133	G
59	BA	2134	A
59	BA	2144	U
59	BA	2154	G
59	BA	2159	G
59	BA	2161	C
59	BA	2166	G
59	BA	2168	G
59	BA	2171	A
59	BA	2173	A
59	BA	2174	C
59	BA	2184	G

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Mol	Chain	Res	Type
59	BA	2198	A
59	BA	2199	A
59	BA	2210	G
59	BA	2211	G
59	BA	2212	A
59	BA	2213	U
59	BA	2225	A
59	BA	2238	G
59	BA	2239	G
59	BA	2246	G
59	BA	2249	U
59	BA	2252	G
59	BA	2269	A
59	BA	2274	A
59	BA	2275	C
59	BA	2279	G
59	BA	2281	C
59	BA	2283	C
59	BA	2287	A
59	BA	2288	A
59	BA	2289	G
59	BA	2305	A
59	BA	2308	G
59	BA	2311	A
59	BA	2320	A
59	BA	2321	G
59	BA	2322	A
59	BA	2325	G
59	BA	2326	C
59	BA	2327	A
59	BA	2334	G
59	BA	2336	A
59	BA	2345	G
59	BA	2346	A
59	BA	2347	C
59	BA	2348	U
59	BA	2362	G
59	BA	2365	G
59	BA	2377	A
59	BA	2379	G
59	BA	2383	G
59	BA	2385	C

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Mol	Chain	Res	Type
59	BA	2391	G
59	BA	2392	A
59	BA	2402	C
59	BA	2406	U
59	BA	2423	U
59	BA	2425	A
59	BA	2426	A
59	BA	2427	C
59	BA	2429	G
59	BA	2430	A
59	BA	2431	U
59	BA	2435	A
59	BA	2437	U
59	BA	2439	A
59	BA	2441	C
59	BA	2448	A
59	BA	2469	A
59	BA	2470	G
59	BA	2476	A
59	BA	2477	C
59	BA	2480	C
59	BA	2481	G
59	BA	2482	G
59	BA	2491	U
59	BA	2497	A
59	BA	2500	U
59	BA	2502	G
59	BA	2503	A
59	BA	2504	U
59	BA	2505	G
59	BA	2514	U
59	BA	2518	A
59	BA	2520	C
59	BA	2525	G
59	BA	2529	G
59	BA	2530	A
59	BA	2532	G
59	BA	2535	G
59	BA	2539	C
59	BA	2542	A
59	BA	2543	G
59	BA	2552	U

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Mol	Chain	Res	Type
59	BA	2554	U
59	BA	2562	U
59	BA	2563	U
59	BA	2564	A
59	BA	2566	A
59	BA	2567	G
59	BA	2572	A
59	BA	2573	C
59	BA	2585	U
59	BA	2586	C
59	BA	2593	U
59	BA	2602	A
59	BA	2603	G
59	BA	2609	U
59	BA	2612	C
59	BA	2613	U
59	BA	2614	A
59	BA	2615	U
59	BA	2623	G
59	BA	2624	G
59	BA	2630	G
59	BA	2642	G
59	BA	2645	G
59	BA	2646	C
59	BA	2657	A
59	BA	2663	G
59	BA	2665	A
59	BA	2667	C
59	BA	2682	U
59	BA	2689	U
59	BA	2691	C
59	BA	2702	U
59	BA	2703	C
59	BA	2706	G
59	BA	2707	G
59	BA	2712	U
59	BA	712(B)	A
59	BA	2713	A
59	BA	2714	G
59	BA	2718	G
59	BA	2720	U
59	BA	2726	U

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Mol	Chain	Res	Type
59	BA	2732	G
59	BA	2733	A
59	BA	2748	A
59	BA	2758	A
59	BA	2760	C
59	BA	2764	A
59	BA	2765	A
59	BA	2766	G
59	BA	2770	G
59	BA	2778	A
59	BA	2779	U
59	BA	2780	G
59	BA	2781	A
59	BA	2782	G
59	BA	2786	U
59	BA	2790	A
59	BA	2791	C
59	BA	2792	G
59	BA	2797	U
59	BA	2798	C
59	BA	2811	G
59	BA	2818	G
59	BA	2820	A
59	BA	2821	A
59	BA	2823	A
59	BA	2833	G
59	BA	2834	G
59	BA	2835	A
59	BA	2849	U
59	BA	2851	A
59	BA	2853	C
59	BA	2866	U
59	BA	2871	C
59	BA	2872	G
59	BA	2876	G
59	BA	2879	C
59	BA	2880	C
59	BA	2886	G
59	BA	2892	A
59	BA	2894	G
59	BA	2895	U
60	BB	12	C

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Mol	Chain	Res	Type
60	BB	13	A
60	BB	15	A
60	BB	16	G
60	BB	25	A
60	BB	26	A
60	BB	35	U
60	BB	41	U
60	BB	42	C
60	BB	45	A
60	BB	50	G
60	BB	53	A
60	BB	58	A
60	BB	67	G
60	BB	73	A
60	BB	74	U
60	BB	85	G
60	BB	102	G
60	BB	109	G
60	BB	118	G
21	CA	6	G
21	CA	8	A
21	CA	9	G
21	CA	10	A
21	CA	13	U
21	CA	22	G
21	CA	31	G
21	CA	32	A
21	CA	39	G
21	CA	47	C
21	CA	48	C
21	CA	51	A
21	CA	54	C
21	CA	65	U
21	CA	66	G
21	CA	68(H)	G
21	CA	68(L)	U
21	CA	68(N)	U
21	CA	68(P)	C
21	CA	68(R)	C
21	CA	68(S)	C
21	CA	109	A
21	CA	116	A

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Mol	Chain	Res	Type
21	CA	121	C
21	CA	122	G
21	CA	129(A)	G
21	CA	131	C
21	CA	134	A
21	CA	135	C
21	CA	136	C
21	CA	153	C
21	CA	163	C
21	CA	169	C
21	CA	172	A
21	CA	174	C
21	CA	186(I)	U
21	CA	186(K)	G
21	CA	192	U
21	CA	195	A
21	CA	197	A
21	CA	201	C
21	CA	201(C)	U
21	CA	216	G
21	CA	221	C
21	CA	243	A
21	CA	247	G
21	CA	251	G
21	CA	267	C
21	CA	279	A
21	CA	281	G
21	CA	285	G
21	CA	289	G
21	CA	296	U
21	CA	301	G
21	CA	315	A
21	CA	316	G
21	CA	321	A
21	CA	328	C
21	CA	329	A
21	CA	332	G
21	CA	345	C
21	CA	346	G
21	CA	347	G
21	CA	348	G
21	CA	352	C

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Mol	Chain	Res	Type
21	CA	353	A
21	CA	354	G
21	CA	366	C
21	CA	367	U
21	CA	368	U
21	CA	372	C
21	CA	373	A
21	CA	388	G
21	CA	389	A
21	CA	390	C
21	CA	392	G
21	CA	397	A
21	CA	398	C
21	CA	406	G
21	CA	410	G
21	CA	412	A
21	CA	414	A
21	CA	421	U
21	CA	422	C
21	CA	423	G
21	CA	424	G
21	CA	429	U
21	CA	430	A
21	CA	440	A
21	CA	452	A
21	CA	453	A
21	CA	457	C
21	CA	458(B)	A
21	CA	475	G
21	CA	481	G
21	CA	484	G
21	CA	485	G
21	CA	497	A
21	CA	498	U
21	CA	501	C
21	CA	505	G
21	CA	509	A
21	CA	511	C
21	CA	512	U
21	CA	518	C
21	CA	521	G
21	CA	524	G

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Mol	Chain	Res	Type
21	CA	525	C
21	CA	527	G
21	CA	531	U
21	CA	532	A
21	CA	533	A
21	CA	535	A
21	CA	547	A
21	CA	552	U
21	CA	559	A
21	CA	562	C
21	CA	567	G
21	CA	568	G
21	CA	572	A
21	CA	573	A
21	CA	574	A
21	CA	575	G
21	CA	576	G
21	CA	577	G
21	CA	603	U
21	CA	653	A
21	CA	659	U
21	CA	665	A
21	CA	666	G
21	CA	688	G
21	CA	693	G
21	CA	695	A
21	CA	702	A
21	CA	703	G
21	CA	706	A
21	CA	711	G
21	CA	717	C
21	CA	721	G
21	CA	737	A
21	CA	741	G
21	CA	749	C
21	CA	753	A
21	CA	755	G
21	CA	777	A
21	CA	781	A
21	CA	793	U
21	CA	794	A
21	CA	809	G

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Mol	Chain	Res	Type
21	CA	815	A
21	CA	816	A
21	CA	817	C
21	CA	818	G
21	CA	819	A
21	CA	821	G
21	CA	828	A
21	CA	838(A)	U
21	CA	838(B)	C
21	CA	838(C)	U
21	CA	848	C
21	CA	849	C
21	CA	859	A
21	CA	867	G
21	CA	872	A
21	CA	885	G
21	CA	889	A
21	CA	890	G
21	CA	916	G
21	CA	926	G
21	CA	927	G
21	CA	934	C
21	CA	935	A
21	CA	946	A
21	CA	960	U
21	CA	961	U
21	CA	966	G
21	CA	969	A
21	CA	971	G
21	CA	972	C
21	CA	974	A
21	CA	976	G
21	CA	977	A
21	CA	978	A
21	CA	979	C
21	CA	980	C
21	CA	992	U
21	CA	993	G
21	CA	1004	A
21	CA	1005	A
21	CA	1025	U
21	CA	1028	C

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Mol	Chain	Res	Type
21	CA	1028(B)	C
21	CA	1028(C)	G
21	CA	1037	C
21	CA	1045	C
21	CA	1054	C
21	CA	1055	A
21	CA	1060	C
21	CA	1065	U
21	CA	1094	G
21	CA	1095	U
21	CA	1101	A
21	CA	1102	A
21	CA	1104	G
21	CA	1108	G
21	CA	1125	U
21	CA	1126	U
21	CA	1128	C
21	CA	1129	C
21	CA	1130	A
21	CA	1131	G
21	CA	1137	C
21	CA	1138	G
21	CA	1139	G
21	CA	1149	C
21	CA	1152	A
21	CA	1159	U
21	CA	1171	G
21	CA	1178	G
21	CA	1181	G
21	CA	1190	G
21	CA	1191	A
21	CA	1196	U
21	CA	1197	G
21	CA	1198	G
21	CA	1204	A
21	CA	1212	U
21	CA	1213	A
21	CA	1215	G
21	CA	1220	G
21	CA	1225	A
21	CA	1227	A
21	CA	1228	C

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Mol	Chain	Res	Type
21	CA	1236	A
21	CA	1238	A
21	CA	1239	A
21	CA	1256	A
21	CA	1257	U
21	CA	1260	C
21	CA	1270	C
21	CA	1272	G
21	CA	1280	A
21	CA	1281	U
21	CA	1282	C
21	CA	1287	A
21	CA	1290	G
21	CA	1293	G
21	CA	1300	G
21	CA	1301	U
21	CA	1302	U
21	CA	1305	G
21	CA	1309	G
21	CA	1314	C
21	CA	1317	C
21	CA	1320	C
21	CA	1322	C
21	CA	1323	G
21	CA	1325	C
21	CA	1331	G
21	CA	1335	C
21	CA	1345	U
21	CA	1346	A
21	CA	1347	G
21	CA	1359	C
21	CA	1362(A)	C
21	CA	1364	U
21	CA	1370	G
21	CA	1373	G
21	CA	1377	A
21	CA	1378	C
21	CA	1379	G
21	CA	1381	U
21	CA	1382	C
21	CA	1394	A
21	CA	1397	C

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Mol	Chain	Res	Type
21	CA	1399	C
21	CA	1413	A
21	CA	1419	G
21	CA	1435	G
21	CA	1440(B)	G
21	CA	1440(C)	G
21	CA	1440(D)	A
21	CA	1440(J)	C
21	CA	1440(K)	G
21	CA	1440(L)	G
21	CA	1491	G
21	CA	1492	A
21	CA	1493	A
21	CA	1494	G
21	CA	1497	G
21	CA	1499	A
21	CA	1502	A
21	CA	1503	A
21	CA	1504	G
21	CA	1505	G
21	CA	1506	U
21	CA	1507	A
21	CA	1517	G
21	CA	1518	A
21	CA	1519	A
21	CA	1520	G
21	CA	1529	G
21	CA	1530	G
21	CA	1532	U
21	CA	1533	C
21	CA	1534	A
21	CA	1535	C
21	CA	1536	C
21	CA	1537	U
21	CA	1538	C
22	CW	8	U
22	CW	16	U
22	CW	17	U
22	CW	18	G
22	CW	20	U
22	CW	20(A)	U
22	CW	21	A

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Mol	Chain	Res	Type
22	CW	22	G
22	CW	23	A
22	CW	29	U
22	CW	42	U
22	CW	46	G
22	CW	47	U
22	CW	48	C
22	CW	58	A
22	CW	60	U
22	CW	61	C
22	CW	74	C
22	CW	76	A
23	CV	5	A
23	CV	9	G
23	CV	11	U
23	CV	12	A
23	CV	15	A
23	CV	16	A
23	CV	18	G
23	CV	19	G
23	CV	23	A
59	DA	10	G
59	DA	12	U
59	DA	13	A
59	DA	15	G
59	DA	23	G
59	DA	25	U
59	DA	27	G
59	DA	28	A
59	DA	34	C
59	DA	35	G
59	DA	46	C
59	DA	50	U
59	DA	51	G
59	DA	52	A
59	DA	64	A
59	DA	70	G
59	DA	73	A
59	DA	74	A
59	DA	75	G
59	DA	84	A
59	DA	90	U

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Mol	Chain	Res	Type
59	DA	98	G
59	DA	101	G
59	DA	102	G
59	DA	113	G
59	DA	118	A
59	DA	119	A
59	DA	120	U
59	DA	121	G
59	DA	138	G
59	DA	140	A
59	DA	141(A)	A
59	DA	163	U
59	DA	178	G
59	DA	181	A
59	DA	196	A
59	DA	197	A
59	DA	199	A
59	DA	204	A
59	DA	205	G
59	DA	216	A
59	DA	221	A
59	DA	222	A
59	DA	225	A
59	DA	227	A
59	DA	228	A
59	DA	229	A
59	DA	230	U
59	DA	232	G
59	DA	233	A
59	DA	241	A
59	DA	248	G
59	DA	250	G
59	DA	251	A
59	DA	252	G
59	DA	265	A
59	DA	270(C)	A
59	DA	270(L)	C
59	DA	270(M)	U
59	DA	270(N)	U
59	DA	270(O)	G
59	DA	270(P)	U
59	DA	270(Q)	C

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Mol	Chain	Res	Type
59	DA	270(R)	C
59	DA	271(D)	U
59	DA	271	G
59	DA	274	G
59	DA	275	G
59	DA	277	C
59	DA	279	C
59	DA	294	A
59	DA	301	G
59	DA	302	C
59	DA	310	A
59	DA	322	A
59	DA	324	A
59	DA	329	G
59	DA	330	A
59	DA	352	G
59	DA	360	G
59	DA	363(A)	G
59	DA	363(B)	A
59	DA	363(D)	G
59	DA	363(G)	A
59	DA	384	U
59	DA	386	G
59	DA	387	U
59	DA	389	G
59	DA	396	G
59	DA	405	U
59	DA	407	G
59	DA	411	G
59	DA	422	A
59	DA	438	G
59	DA	444	C
59	DA	446	G
59	DA	447	A
59	DA	448	U
59	DA	449	A
59	DA	451	C
59	DA	455	C
59	DA	456	C
59	DA	457	A
59	DA	458	G
59	DA	459	U

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Mol	Chain	Res	Type
59	DA	464	U
59	DA	470	A
59	DA	473	G
59	DA	474	G
59	DA	475	U
59	DA	480	A
59	DA	481	G
59	DA	489	G
59	DA	491	G
59	DA	505	A
59	DA	506	G
59	DA	507	A
59	DA	508	G
59	DA	509	C
59	DA	513	A
59	DA	527	C
59	DA	528	A
59	DA	530	G
59	DA	531	C
59	DA	532	A
59	DA	542	C
59	DA	546	C
59	DA	548	A
59	DA	556	G
59	DA	563	G
59	DA	572	A
59	DA	573	G
59	DA	575	A
59	DA	586	A
59	DA	587	C
59	DA	603	A
59	DA	614	U
59	DA	615	G
59	DA	616	A
59	DA	617	G
59	DA	620	G
59	DA	621	A
59	DA	627	A
59	DA	637	A
59	DA	643	A
59	DA	645	C
59	DA	646	A

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Mol	Chain	Res	Type
59	DA	653	C
59	DA	654	U
59	DA	671	C
59	DA	686	G
59	DA	695	G
59	DA	701	G
59	DA	707	G
59	DA	730	C
59	DA	738	G
59	DA	747	U
59	DA	749	C
59	DA	764	A
59	DA	771	G
59	DA	776	G
59	DA	778	G
59	DA	779	U
59	DA	781	A
59	DA	782	A
59	DA	783	A
59	DA	784	A
59	DA	785	G
59	DA	786	C
59	DA	788	A
59	DA	789	A
59	DA	790	C
59	DA	792	G
59	DA	794	G
59	DA	799	G
59	DA	800	A
59	DA	805	G
59	DA	812	C
59	DA	819	A
59	DA	822	U
59	DA	827	U
59	DA	829	A
59	DA	838	C
59	DA	846	C
59	DA	847	U
59	DA	852	G
59	DA	859	G
59	DA	866	A
59	DA	869	G

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Mol	Chain	Res	Type
59	DA	877	U
59	DA	878	A
59	DA	879	G
59	DA	881	G
59	DA	882	G
59	DA	886	C
59	DA	887	A
59	DA	890	A
59	DA	896	A
59	DA	897	C
59	DA	906	G
59	DA	907	U
59	DA	910	A
59	DA	917	A
59	DA	932	G
59	DA	933	A
59	DA	941	A
59	DA	943	U
59	DA	945	A
59	DA	946	G
59	DA	959	A
59	DA	961	C
59	DA	970	C
59	DA	972	G
59	DA	974(A)	G
59	DA	974(B)	C
59	DA	980	A
59	DA	983	A
59	DA	990	A
59	DA	991	C
59	DA	996	A
59	DA	1007	C
59	DA	1008	C
59	DA	1009	A
59	DA	1010	A
59	DA	1011	G
59	DA	1012	U
59	DA	1013	C
59	DA	1017	G
59	DA	1022	G
59	DA	1023	U
59	DA	1024	G

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Mol	Chain	Res	Type
59	DA	1025	G
59	DA	1026	U
59	DA	1033	U
59	DA	1045	A
59	DA	1046	A
59	DA	1047	G
59	DA	1048	A
59	DA	1056	G
59	DA	1057	A
59	DA	1060	U
59	DA	1065	U
59	DA	1070	A
59	DA	1072	C
59	DA	1078	U
59	DA	1079	C
59	DA	1086	A
59	DA	1087	G
59	DA	1088	A
59	DA	1090	U
59	DA	1105	U
59	DA	1106	G
59	DA	1107	G
59	DA	1110	G
59	DA	1112	G
59	DA	1123	C
59	DA	1126	A
59	DA	1132	A
59	DA	1136	G
59	DA	1139	G
59	DA	1141	U
59	DA	114(B)	A
59	DA	1144	G
59	DA	1155	A
59	DA	1156	A
59	DA	1157	G
59	DA	1173	G
59	DA	1175	U
59	DA	1176	G
59	DA	1179	C
59	DA	1186	G
59	DA	1204	A
59	DA	1205	U

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Mol	Chain	Res	Type
59	DA	1206	G
59	DA	1210	A
59	DA	1211	U
59	DA	1212	G
59	DA	1221	C
59	DA	1241	A
59	DA	1248	G
59	DA	1249	U
59	DA	1253	A
59	DA	1256	G
59	DA	1265	A
59	DA	1271	G
59	DA	1272	A
59	DA	1286	A
59	DA	1300	U
59	DA	1301	A
59	DA	1302	A
59	DA	1312	U
59	DA	1314	C
59	DA	1321	A
59	DA	1322	A
59	DA	1325	G
59	DA	1329	U
59	DA	1330	C
59	DA	1332	G
59	DA	1333	C
59	DA	1349	A
59	DA	1359	A
59	DA	1365	A
59	DA	1368	G
59	DA	1378	A
59	DA	1379	A
59	DA	1380	G
59	DA	1384	A
59	DA	1385	G
59	DA	1395	A
59	DA	1396	U
59	DA	1398	C
59	DA	1416	G
59	DA	1417	C
59	DA	1418	G
59	DA	1420	U

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Mol	Chain	Res	Type
59	DA	1421	G
59	DA	1428	C
59	DA	144(B)	A
59	DA	149(B)	A
59	DA	1449	G
59	DA	1453	A
59	DA	1454	U
59	DA	1455	G
59	DA	1458	C
59	DA	1460	A
59	DA	1467	C
59	DA	1478	G
59	DA	1483	G
59	DA	1491	G
59	DA	1493	C
59	DA	1495	A
59	DA	1497	U
59	DA	1498	C
59	DA	1510	A
59	DA	1523	U
59	DA	1531	C
59	DA	1535	U
59	DA	1536	A
59	DA	1538	G
59	DA	1539	G
59	DA	1540	G
59	DA	1541	U
59	DA	1542	G
59	DA	1543	A
59	DA	1545	A
59	DA	1547	C
59	DA	1558	A
59	DA	1559	G
59	DA	1566	A
59	DA	1569	A
59	DA	1578	U
59	DA	1583	A
59	DA	1585	C
59	DA	1593	G
59	DA	1602	U
59	DA	1603	A
59	DA	1608	A

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Mol	Chain	Res	Type
59	DA	1609	A
59	DA	1615	C
59	DA	1616	A
59	DA	1617	C
59	DA	1618	A
59	DA	1619	G
59	DA	1631	A
59	DA	1640	C
59	DA	1641	A
59	DA	1644	C
59	DA	1646	C
59	DA	1648	C
59	DA	1665	A
59	DA	1674	G
59	DA	1677	A
59	DA	1678	G
59	DA	1694	C
59	DA	1695	G
59	DA	1696	G
59	DA	1729	A
59	DA	1732	A
59	DA	1755	A
59	DA	1757	U
59	DA	1762	A
59	DA	1763	G
59	DA	1764	G
59	DA	1773	A
59	DA	1781	C
59	DA	1782	C
59	DA	1784	A
59	DA	1785	A
59	DA	1786	A
59	DA	1787	A
59	DA	1800	C
59	DA	1802	A
59	DA	1815	A
59	DA	1816	G
59	DA	1820	U
59	DA	1821	A
59	DA	1829	A
59	DA	1833	U
59	DA	1837	C

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Mol	Chain	Res	Type
59	DA	1847	A
59	DA	1858	G
59	DA	1870	C
59	DA	1872	A
59	DA	1888	G
59	DA	1889	A
59	DA	1900	A
59	DA	1902	C
59	DA	1903	G
59	DA	1906	G
59	DA	1909	C
59	DA	1912	A
59	DA	1913	A
59	DA	1914	C
59	DA	1929	G
59	DA	1936	A
59	DA	1937	A
59	DA	1939	U
59	DA	1940	U
59	DA	1944	U
59	DA	1955	U
59	DA	1963	U
59	DA	1964	G
59	DA	1967	C
59	DA	1970	A
59	DA	1971	A
59	DA	1972	A
59	DA	1981	A
59	DA	1982	C
59	DA	1991	U
59	DA	1992	G
59	DA	1993	U
59	DA	2005	A
59	DA	2013	A
59	DA	2023	G
59	DA	2030	A
59	DA	2031	A
59	DA	2032	G
59	DA	2033	A
59	DA	2034	U
59	DA	2036	C
59	DA	2043	C

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Mol	Chain	Res	Type
59	DA	2051	A
59	DA	2052	G
59	DA	2055	C
59	DA	2056	G
59	DA	2060	A
59	DA	2061	G
59	DA	2062	A
59	DA	2065	C
59	DA	2069	G
59	DA	2078	C
59	DA	2093	G
59	DA	2108	C
59	DA	2110	G
59	DA	2112	G
59	DA	2113	U
59	DA	2116	G
59	DA	2117	A
59	DA	2118	U
59	DA	2126	A
59	DA	2131	G
59	DA	2133	G
59	DA	2134	A
59	DA	2144	U
59	DA	2159	G
59	DA	2165	G
59	DA	2167	U
59	DA	2168	G
59	DA	2171	A
59	DA	2173	A
59	DA	2184	G
59	DA	2190	G
59	DA	2199	A
59	DA	2210	G
59	DA	2211	G
59	DA	2212	A
59	DA	2213	U
59	DA	2225	A
59	DA	2239	G
59	DA	2246	G
59	DA	2266	A
59	DA	2267	A
59	DA	2268	A

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Mol	Chain	Res	Type
59	DA	2274	A
59	DA	2275	C
59	DA	2280	G
59	DA	2283	C
59	DA	2287	A
59	DA	2289	G
59	DA	2305	A
59	DA	2308	G
59	DA	2310	A
59	DA	2311	A
59	DA	2320	A
59	DA	2322	A
59	DA	2325	G
59	DA	2327	A
59	DA	2334	G
59	DA	2336	A
59	DA	2345	G
59	DA	2346	A
59	DA	2347	C
59	DA	2350	C
59	DA	2366	A
59	DA	2377	A
59	DA	2383	G
59	DA	2385	C
59	DA	2389	G
59	DA	2401	U
59	DA	2402	C
59	DA	2405	G
59	DA	2406	U
59	DA	2422	A
59	DA	2423	U
59	DA	2425	A
59	DA	2426	A
59	DA	2427	C
59	DA	2428	G
59	DA	2429	G
59	DA	2430	A
59	DA	2435	A
59	DA	2439	A
59	DA	2441	C
59	DA	2448	A
59	DA	2450	A

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Mol	Chain	Res	Type
59	DA	2469	A
59	DA	2470	G
59	DA	2474	C
59	DA	2476	A
59	DA	2477	C
59	DA	2478	A
59	DA	2480	C
59	DA	2482	G
59	DA	2497	A
59	DA	2502	G
59	DA	2503	A
59	DA	2505	G
59	DA	2513	G
59	DA	2514	U
59	DA	2518	A
59	DA	2520	C
59	DA	2526	G
59	DA	2529	G
59	DA	2530	A
59	DA	2532	G
59	DA	2533	A
59	DA	2542	A
59	DA	2543	G
59	DA	2546	U
59	DA	2554	U
59	DA	2563	U
59	DA	2564	A
59	DA	2566	A
59	DA	2567	G
59	DA	2572	A
59	DA	2573	C
59	DA	2578	G
59	DA	2586	C
59	DA	2593	U
59	DA	2602	A
59	DA	2603	G
59	DA	2609	U
59	DA	2610	C
59	DA	2612	C
59	DA	2615	U
59	DA	2623	G
59	DA	2630	G

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Mol	Chain	Res	Type
59	DA	2633	G
59	DA	2638	G
59	DA	2641	G
59	DA	2645	G
59	DA	2646	C
59	DA	2657	A
59	DA	2663	G
59	DA	2665	A
59	DA	2667	C
59	DA	2681	C
59	DA	2682	U
59	DA	2689	U
59	DA	2691	C
59	DA	2702	U
59	DA	2703	C
59	DA	2706	G
59	DA	2711	A
59	DA	2712	U
59	DA	712(B)	A
59	DA	2713	A
59	DA	2714	G
59	DA	2718	G
59	DA	2720	U
59	DA	2721	A
59	DA	2726	U
59	DA	2733	A
59	DA	2748	A
59	DA	2760	C
59	DA	2764	A
59	DA	2765	A
59	DA	2766	G
59	DA	2770	G
59	DA	2778	A
59	DA	2779	U
59	DA	2780	G
59	DA	2781	A
59	DA	2782	G
59	DA	2786	U
59	DA	2790	A
59	DA	2791	C
59	DA	2797	U
59	DA	2798	C

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Mol	Chain	Res	Type
59	DA	2811	G
59	DA	2820	A
59	DA	2821	A
59	DA	2823	A
59	DA	2825	U
59	DA	2832	U
59	DA	2833	G
59	DA	2834	G
59	DA	2835	A
59	DA	2849	U
59	DA	2866	U
59	DA	2871	C
59	DA	2872	G
59	DA	2876	G
59	DA	2879	C
59	DA	2880	C
59	DA	2892	A
59	DA	2893	G
59	DA	2894	G
59	DA	2895	U
60	DB	7	G
60	DB	13	A
60	DB	15	A
60	DB	16	G
60	DB	25	A
60	DB	35	U
60	DB	41	U
60	DB	42	C
60	DB	45	A
60	DB	47	C
60	DB	50	G
60	DB	53	A
60	DB	55	U
60	DB	65	C
60	DB	67	G
60	DB	73	A
60	DB	87	G
60	DB	109	G
60	DB	115	G

All (87) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	115	G
21	AA	266	G
21	AA	282	A
21	AA	328	C
21	AA	409	G
21	AA	429	U
21	AA	687	A
21	AA	748	C
21	AA	992	U
21	AA	1064	G
21	AA	1067	A
21	AA	1101	A
21	AA	1136	U
21	AA	1145	C
21	AA	1493	A
21	AA	1496	C
21	AA	1504	G
21	AA	1537	U
22	AW	20(A)	U
23	AV	8	A
23	AV	18	G
59	BA	214	G
59	BA	221	A
59	BA	271(C)	G
59	BA	363(G)	A
59	BA	474	G
59	BA	479	A
59	BA	586	A
59	BA	614	U
59	BA	615	G
59	BA	1022	G
59	BA	1210	A
59	BA	1240	U
59	BA	1248	G
59	BA	1377	G
59	BA	1558	A
59	BA	1786	A
59	BA	1858	G
59	BA	2092	U
59	BA	2422	A
59	BA	2447	G
59	BA	2780	G

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Mol	Chain	Res	Type
60	BB	41	U
60	BB	56	G
60	BB	66	A
60	BB	108	C
21	CA	5	U
21	CA	115	G
21	CA	266	G
21	CA	328	C
21	CA	409	G
21	CA	429	U
21	CA	687	A
21	CA	705	U
21	CA	748	C
21	CA	992	U
21	CA	1064	G
21	CA	1101	A
21	CA	1324	A
21	CA	1493	A
21	CA	1504	G
21	CA	1537	U
22	CW	20(A)	U
23	CV	8	A
23	CV	16	A
23	CV	18	G
59	DA	221	A
59	DA	271(C)	G
59	DA	474	G
59	DA	479	A
59	DA	586	A
59	DA	1012	U
59	DA	1022	G
59	DA	1210	A
59	DA	1240	U
59	DA	1377	G
59	DA	1558	A
59	DA	1786	A
59	DA	1899	G
59	DA	2092	U
59	DA	2422	A
59	DA	2447	G
59	DA	2780	G
60	DB	41	U

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Mol	Chain	Res	Type
60	DB	66	A
60	DB	108	C

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

8 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	$\#\|Z\| > 2$
24	UAL	CU	5	24	7,8,9	2.41	3 (42%)	5,9,11	1.45	1 (20%)
24	KBE	AU	1	24	8,8,9	0.65	0	7,8,10	1.44	1 (14%)
24	5OH	CU	6	24	8,12,13	0.76	0	3,16,18	1.07	0
24	5OH	AU	6	24	8,12,13	0.75	0	3,16,18	1.07	0
24	KBE	CU	1	24	8,8,9	0.64	0	7,8,10	1.45	1 (14%)
24	DPP	AU	2	24	3,5,6	0.33	0	1,5,7	0.99	0
24	DPP	CU	2	24	3,5,6	0.33	0	1,5,7	0.99	0
24	UAL	AU	5	24	7,8,9	2.41	3 (42%)	5,9,11	1.44	1 (20%)

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
24	UAL	CU	5	24	-	0/3/7/9	-
24	KBE	AU	1	24	-	1/7/7/8	-
24	5OH	CU	6	24	-	0/2/18/20	0/1/1/1
24	5OH	AU	6	24	-	0/2/18/20	0/1/1/1
24	KBE	CU	1	24	-	1/7/7/8	-
24	DPP	AU	2	24	-	0/2/4/6	-
24	DPP	CU	2	24	-	0/2/4/6	-
24	UAL	AU	5	24	-	0/3/7/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CU	5	UAL	C-CA	4.72	1.52	1.45
24	AU	5	UAL	C-CA	4.71	1.52	1.45
24	AU	5	UAL	C1-N1	-3.32	1.35	1.40
24	CU	5	UAL	C1-N1	-3.30	1.35	1.40
24	AU	5	UAL	CB-N1	-2.14	1.30	1.35
24	CU	5	UAL	CB-N1	-2.14	1.30	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	CU	1	KBE	CB-CA-C	3.33	117.15	112.25
24	AU	1	KBE	CB-CA-C	3.30	117.11	112.25
24	AU	5	UAL	O-C-CA	-2.47	122.25	125.39
24	CU	5	UAL	O-C-CA	-2.47	122.25	125.39

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AU	1	KBE	CG-CD-CE-NZ
24	CU	1	KBE	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
61	GNP	CY	701	62	29,34,34	1.55	4 (13%)	33,54,54	2.68	13 (39%)
61	GNP	AY	701	62	29,34,34	1.55	4 (13%)	33,54,54	2.68	13 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	GNP	CY	701	62	-	7/14/38/38	0/3/3/3
61	GNP	AY	701	62	-	7/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	GNP	PG-O1G	4.78	1.53	1.46
61	CY	701	GNP	PG-O1G	4.75	1.53	1.46
61	CY	701	GNP	C6-N1	3.61	1.39	1.33
61	AY	701	GNP	C6-N1	3.60	1.39	1.33
61	AY	701	GNP	PB-O3A	-2.39	1.56	1.59
61	CY	701	GNP	PB-O3A	-2.37	1.56	1.59
61	AY	701	GNP	PA-O2A	-2.14	1.45	1.55
61	CY	701	GNP	PA-O2A	-2.14	1.45	1.55

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	AY	701	GNP	C5-C6-N1	-8.59	111.69	123.43
61	CY	701	GNP	C5-C6-N1	-8.56	111.72	123.43
61	AY	701	GNP	C2-N1-C6	5.79	125.14	115.93
61	CY	701	GNP	C2-N1-C6	5.77	125.10	115.93
61	AY	701	GNP	C2-N3-C4	-4.79	109.88	115.36
61	CY	701	GNP	C2-N3-C4	-4.79	109.89	115.36
61	CY	701	GNP	PB-O3A-PA	-4.72	115.98	132.62
61	AY	701	GNP	PB-O3A-PA	-4.72	116.00	132.62
61	CY	701	GNP	O2B-PB-O1B	3.49	117.23	109.92
61	AY	701	GNP	O2B-PB-O1B	3.48	117.22	109.92
61	AY	701	GNP	O2G-PG-O3G	3.31	116.46	107.64
61	CY	701	GNP	O2G-PG-O3G	3.30	116.43	107.64
61	CY	701	GNP	C4-C5-N7	3.10	112.63	109.40
61	AY	701	GNP	C4-C5-N7	3.06	112.59	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AY	701	GNP	O3G-PG-O1G	-2.97	105.99	113.45
61	CY	701	GNP	O3G-PG-O1G	-2.97	106.00	113.45
61	CY	701	GNP	O1B-PB-N3B	2.81	115.91	111.77
61	AY	701	GNP	O1B-PB-N3B	2.81	115.91	111.77
61	CY	701	GNP	C4-C5-C6	-2.63	118.29	120.80
61	AY	701	GNP	C4-C5-C6	-2.59	118.32	120.80
61	AY	701	GNP	N3-C2-N1	-2.27	124.19	127.22
61	CY	701	GNP	N3-C2-N1	-2.26	124.21	127.22
61	AY	701	GNP	C5'-C4'-C3'	-2.23	106.81	115.18
61	CY	701	GNP	C5'-C4'-C3'	-2.22	106.84	115.18
61	AY	701	GNP	O1G-PG-N3B	-2.21	108.51	111.77
61	CY	701	GNP	O1G-PG-N3B	-2.20	108.54	111.77

There are no chirality outliers.

All (14) torsion outliers are listed below:

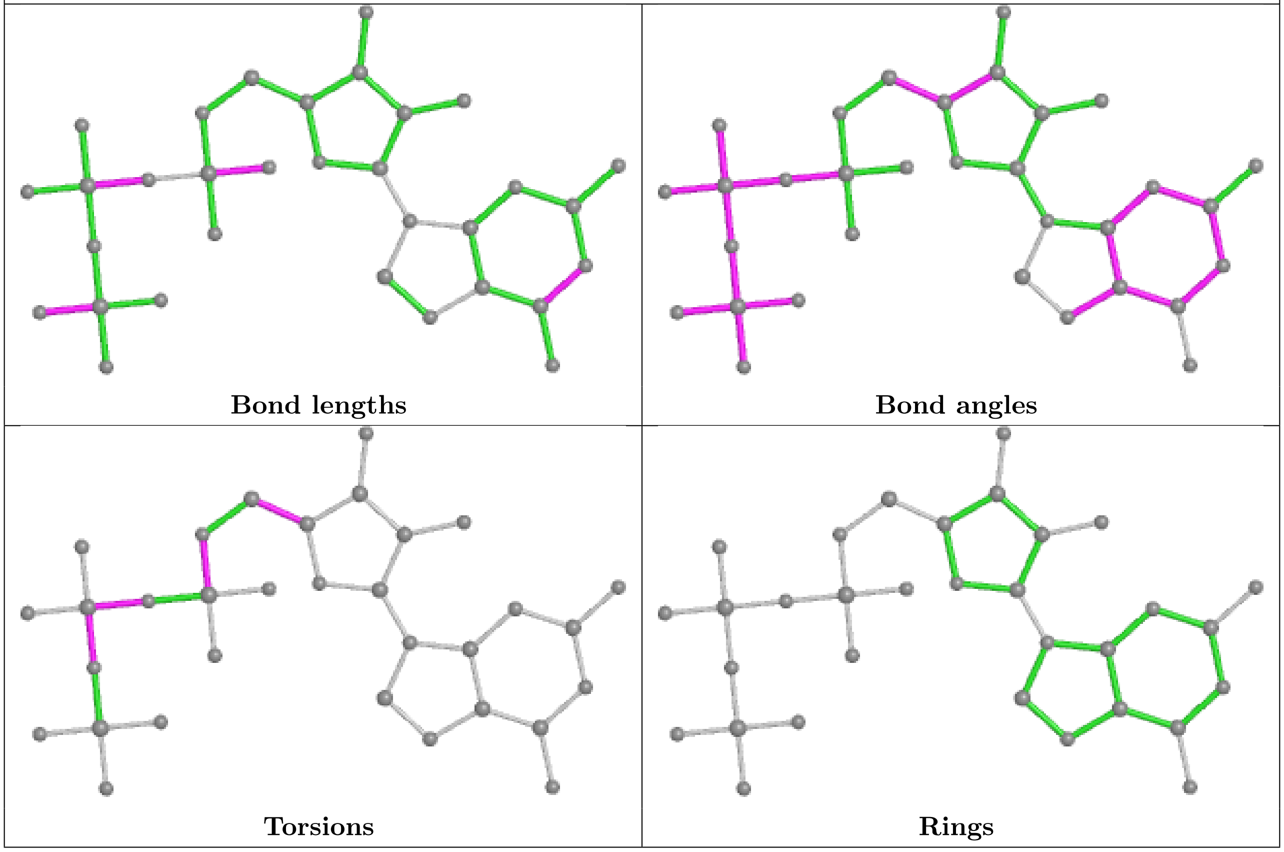
Mol	Chain	Res	Type	Atoms
61	AY	701	GNP	PG-N3B-PB-O1B
61	AY	701	GNP	PG-N3B-PB-O3A
61	AY	701	GNP	PA-O3A-PB-O1B
61	AY	701	GNP	PA-O3A-PB-O2B
61	AY	701	GNP	C5'-O5'-PA-O3A
61	AY	701	GNP	C5'-O5'-PA-O1A
61	CY	701	GNP	PG-N3B-PB-O1B
61	CY	701	GNP	PG-N3B-PB-O3A
61	CY	701	GNP	PA-O3A-PB-O1B
61	CY	701	GNP	PA-O3A-PB-O2B
61	CY	701	GNP	C5'-O5'-PA-O3A
61	CY	701	GNP	C5'-O5'-PA-O1A
61	AY	701	GNP	C3'-C4'-C5'-O5'
61	CY	701	GNP	C3'-C4'-C5'-O5'

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 GNP CY 701



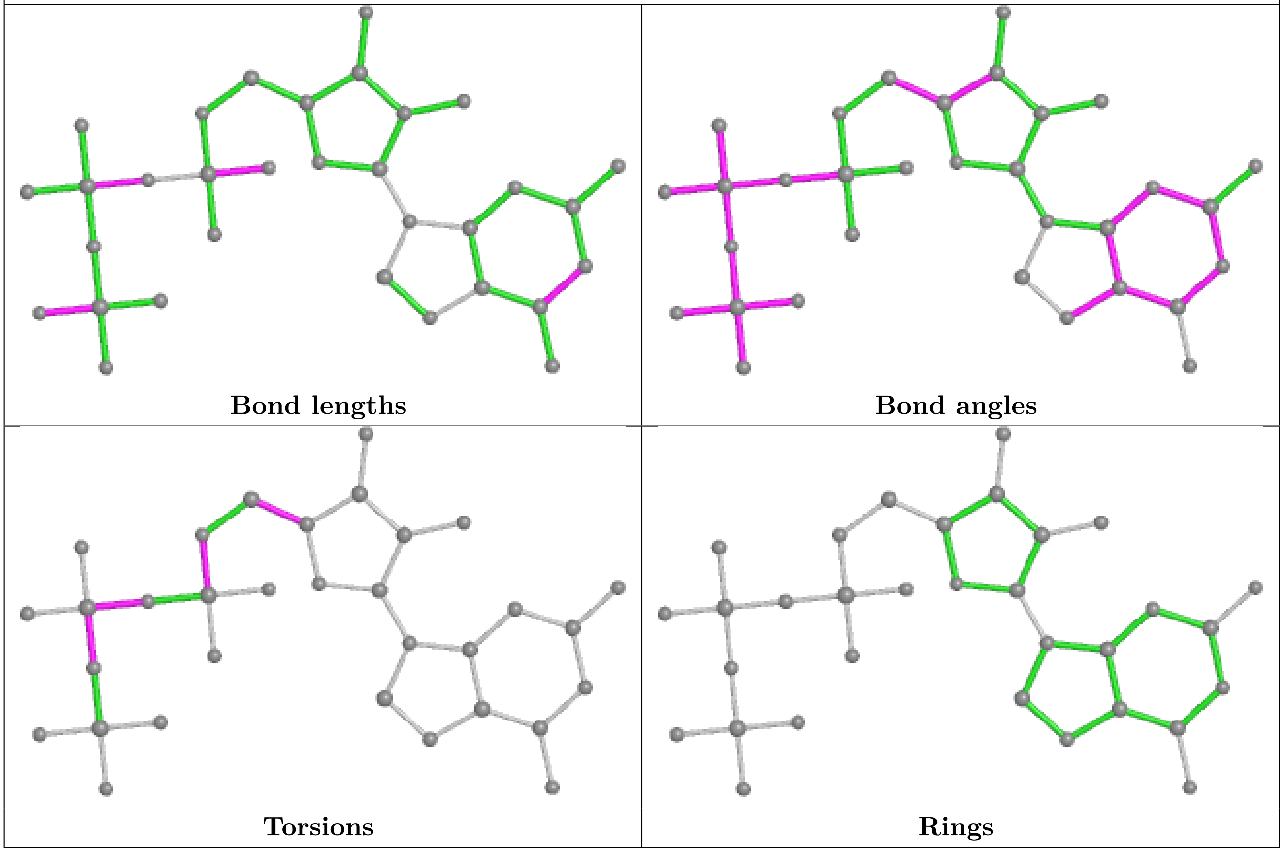
Bond lengths

Bond angles

Torsions

Rings

Ligand GNP AY 701



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
58	De	1
58	Be	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	De	30:UNK	C	51:ALA	N	36.11
1	Be	30:UNK	C	51:ALA	N	35.10

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	AB	235/235 (100%)	-0.08	6 (2%)	56	49	30, 75, 127, 171	0
1	CB	235/235 (100%)	0.41	16 (6%)	17	16	34, 86, 153, 201	0
2	AC	207/207 (100%)	0.28	14 (6%)	17	16	27, 59, 115, 156	0
2	CC	207/207 (100%)	1.01	41 (19%)	1	1	23, 74, 130, 190	0
3	AD	208/208 (100%)	-0.57	0	100	100	24, 72, 124, 159	0
3	CD	208/208 (100%)	-0.29	3 (1%)	75	69	23, 85, 142, 184	0
4	AE	151/151 (100%)	-0.41	0	100	100	17, 48, 101, 156	0
4	CE	151/151 (100%)	-0.02	7 (4%)	32	28	14, 58, 106, 151	0
5	AF	101/101 (100%)	-0.47	1 (0%)	82	77	15, 50, 100, 133	0
5	CF	101/101 (100%)	-0.62	1 (0%)	82	77	29, 61, 123, 148	0
6	AG	155/155 (100%)	-0.68	1 (0%)	89	86	30, 80, 139, 199	0
6	CG	155/155 (100%)	-0.80	0	100	100	38, 82, 137, 180	0
7	AH	138/138 (100%)	-0.16	4 (2%)	51	45	28, 59, 103, 142	0
7	CH	138/138 (100%)	0.15	5 (3%)	42	38	25, 75, 121, 155	0
8	AI	127/127 (100%)	-0.76	0	100	100	0, 71, 117, 134	0
8	CI	127/127 (100%)	-0.56	0	100	100	0, 84, 149, 220	0
9	AJ	99/99 (100%)	0.15	6 (6%)	21	19	25, 62, 116, 159	0
9	CJ	99/99 (100%)	0.90	13 (13%)	3	4	31, 75, 127, 166	0
10	AK	119/119 (100%)	-0.34	1 (0%)	86	81	31, 69, 116, 157	0
10	CK	119/119 (100%)	-0.57	1 (0%)	86	81	38, 72, 133, 151	0
11	AL	125/125 (100%)	-0.12	3 (2%)	59	53	10, 66, 120, 181	0
11	CL	125/125 (100%)	0.25	13 (10%)	6	7	29, 69, 136, 170	0
12	AM	125/125 (100%)	0.06	11 (8%)	10	10	49, 86, 144, 212	0
12	CM	125/125 (100%)	0.25	14 (11%)	5	6	53, 100, 158, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AN	60/60 (100%)	0.40	7 (11%) 4 5	28, 52, 87, 120	0
13	CN	60/60 (100%)	0.93	11 (18%) 1 1	39, 69, 117, 135	0
14	AO	88/88 (100%)	-0.31	0 100 100	22, 60, 114, 139	0
14	CO	88/88 (100%)	-0.32	0 100 100	25, 68, 119, 170	0
15	AP	84/84 (100%)	0.05	4 (4%) 30 27	26, 66, 109, 117	0
15	CP	84/84 (100%)	0.05	2 (2%) 59 53	52, 81, 127, 153	0
16	AQ	100/100 (100%)	0.25	6 (6%) 21 19	0, 67, 117, 139	0
16	CQ	100/100 (100%)	0.41	8 (8%) 12 12	0, 68, 126, 150	0
17	AR	70/70 (100%)	-0.21	3 (4%) 35 31	14, 54, 120, 154	0
17	CR	70/70 (100%)	-0.29	1 (1%) 75 69	38, 63, 113, 155	0
18	AS	79/79 (100%)	0.90	14 (17%) 1 1	47, 92, 136, 169	0
18	CS	79/79 (100%)	0.62	10 (12%) 3 4	44, 99, 145, 189	0
19	AT	99/99 (100%)	-0.50	0 100 100	0, 77, 128, 159	0
19	CT	99/99 (100%)	-0.28	2 (2%) 65 60	0, 79, 131, 166	0
20	AY	687/687 (100%)	0.00	50 (7%) 15 15	23, 84, 139, 174	0
20	CY	687/687 (100%)	0.02	49 (7%) 16 15	40, 92, 149, 204	0
21	AA	1511/1511 (100%)	-0.60	3 (0%) 95 93	15, 67, 145, 258	0
21	CA	1511/1511 (100%)	-0.61	1 (0%) 95 95	18, 70, 157, 272	0
22	AW	77/77 (100%)	-0.73	0 100 100	32, 90, 174, 205	0
22	CW	77/77 (100%)	-0.74	0 100 100	39, 101, 193, 240	0
23	AV	23/23 (100%)	-0.70	0 100 100	41, 100, 156, 172	0
23	CV	23/23 (100%)	-0.27	1 (4%) 35 31	41, 118, 186, 216	0
24	AU	2/6 (33%)	-0.75	0 100 100	114, 114, 114, 114	0
24	CU	2/6 (33%)	-0.94	0 100 100	119, 119, 119, 119	0
25	BC	228/228 (100%)	1.42	73 (32%) 0 0	81, 124, 178, 222	0
25	DC	228/228 (100%)	1.57	74 (32%) 0 0	102, 162, 214, 247	0
26	BD	275/275 (100%)	-0.49	2 (0%) 87 83	11, 47, 102, 126	0
26	DD	275/275 (100%)	-0.45	4 (1%) 73 68	23, 54, 107, 147	0
27	BE	205/205 (100%)	-0.37	3 (1%) 73 68	19, 55, 101, 193	0
27	DE	205/205 (100%)	-0.20	4 (1%) 65 60	12, 60, 120, 175	0
28	BF	208/208 (100%)	-0.02	14 (6%) 17 16	16, 69, 131, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	DF	208/208 (100%)	-0.05	11 (5%)	26	24	34, 83, 176, 205	0
29	BG	181/181 (100%)	0.90	38 (20%)	1	1	41, 90, 132, 195	0
29	DG	181/181 (100%)	1.39	53 (29%)	0	0	44, 104, 159, 196	0
30	BH	167/167 (100%)	-0.46	1 (0%)	89	86	21, 68, 123, 159	0
30	DH	167/167 (100%)	-0.42	2 (1%)	79	73	36, 72, 140, 192	0
31	BJ	0/170	-	-			-	-
31	DJ	0/170	-	-			-	-
32	BK	140/140 (100%)	-0.06	9 (6%)	19	18	60, 114, 165, 206	0
32	DK	140/140 (100%)	0.43	24 (17%)	1	1	72, 142, 197, 229	0
33	BN	138/138 (100%)	0.36	12 (8%)	10	11	59, 83, 108, 111	0
33	DN	138/138 (100%)	0.25	7 (5%)	28	25	61, 89, 110, 118	0
34	BO	122/122 (100%)	-0.06	5 (4%)	37	33	23, 44, 90, 158	0
34	DO	122/122 (100%)	0.06	4 (3%)	46	41	26, 47, 96, 121	0
35	BP	146/146 (100%)	-0.45	2 (1%)	75	69	23, 71, 132, 167	0
35	DP	146/146 (100%)	-0.32	5 (3%)	45	40	19, 88, 140, 212	0
36	BQ	141/141 (100%)	-0.56	1 (0%)	87	83	32, 53, 103, 155	0
36	DQ	141/141 (100%)	-0.64	1 (0%)	87	83	34, 58, 126, 178	0
37	BR	117/117 (100%)	-0.14	2 (1%)	70	64	22, 57, 106, 123	0
37	DR	117/117 (100%)	-0.18	0	100	100	34, 67, 108, 138	0
38	BS	99/99 (100%)	1.23	29 (29%)	0	0	41, 104, 177, 190	0
38	DS	99/99 (100%)	1.66	36 (36%)	0	0	44, 114, 168, 203	0
39	BT	138/138 (100%)	-0.27	3 (2%)	62	56	23, 68, 126, 162	0
39	DT	138/138 (100%)	-0.28	4 (2%)	51	45	25, 71, 133, 177	0
40	BU	117/117 (100%)	-0.11	1 (0%)	84	79	20, 45, 102, 140	0
40	DU	117/117 (100%)	0.09	4 (3%)	45	40	29, 54, 89, 222	0
41	BV	101/101 (100%)	0.29	8 (7%)	12	13	22, 58, 105, 172	0
41	DV	101/101 (100%)	0.10	8 (7%)	12	13	28, 60, 114, 177	0
42	BW	113/113 (100%)	-0.19	3 (2%)	54	48	14, 43, 101, 135	0
42	DW	113/113 (100%)	0.02	2 (1%)	68	62	11, 60, 133, 215	0
43	BX	93/93 (100%)	-0.50	0	100	100	16, 55, 107, 137	0
43	DX	93/93 (100%)	-0.69	0	100	100	16, 66, 134, 180	0
44	BY	107/107 (100%)	-0.12	4 (3%)	41	37	38, 88, 141, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	DY	107/107 (100%)	0.19	10 (9%) 8 9	45, 96, 167, 200	0
45	BZ	185/185 (100%)	-0.57	1 (0%) 91 88	36, 70, 124, 167	0
45	DZ	185/185 (100%)	-0.58	4 (2%) 62 56	48, 82, 136, 193	0
46	B0	84/84 (100%)	-0.36	1 (1%) 79 73	24, 65, 112, 142	0
46	D0	84/84 (100%)	0.28	6 (7%) 16 15	47, 77, 140, 162	0
47	B2	71/71 (100%)	-0.30	1 (1%) 75 69	34, 64, 118, 140	0
47	D2	71/71 (100%)	-0.20	2 (2%) 53 47	33, 85, 127, 141	0
48	B3	60/60 (100%)	-0.03	2 (3%) 46 41	28, 61, 116, 135	0
48	D3	60/60 (100%)	0.07	3 (5%) 28 25	32, 73, 137, 160	0
49	B5	59/59 (100%)	-0.28	1 (1%) 70 64	22, 55, 125, 138	0
49	D5	59/59 (100%)	-0.08	2 (3%) 45 40	29, 75, 130, 161	0
50	B6	50/50 (100%)	-0.57	0 100 100	36, 74, 120, 139	0
50	D6	50/50 (100%)	0.15	4 (8%) 12 12	49, 81, 143, 164	0
51	B7	49/49 (100%)	-0.36	1 (2%) 65 60	43, 53, 102, 126	0
51	D7	49/49 (100%)	-0.30	4 (8%) 11 12	34, 61, 112, 165	0
52	B8	64/64 (100%)	-0.42	1 (1%) 72 66	22, 66, 108, 137	0
52	D8	64/64 (100%)	-0.14	3 (4%) 31 28	33, 70, 118, 139	0
53	B9	37/37 (100%)	-0.02	2 (5%) 25 23	39, 60, 122, 134	0
53	D9	37/37 (100%)	-0.42	1 (2%) 54 48	46, 60, 134, 159	0
54	Bf	0/31	-	-	-	-
54	Bg	0/31	-	-	-	-
54	Df	0/31	-	-	-	-
54	Dg	0/31	-	-	-	-
55	Bh	0/30	-	-	-	-
55	Dh	0/30	-	-	-	-
56	B1	93/93 (100%)	-0.16	5 (5%) 25 23	22, 78, 160, 236	0
56	D1	93/93 (100%)	0.18	10 (10%) 5 6	41, 89, 159, 194	0
57	B4	35/35 (100%)	1.25	8 (22%) 0 0	67, 116, 167, 189	0
57	D4	35/35 (100%)	1.54	10 (28%) 0 0	73, 136, 168, 196	0
58	Be	72/102 (70%)	1.53	23 (31%) 0 0	77, 113, 160, 174	0
58	De	72/102 (70%)	2.84	40 (55%) 0 0	87, 141, 192, 236	0
59	BA	2879/2879 (100%)	-0.59	11 (0%) 92 90	9, 59, 146, 260	0
59	DA	2879/2879 (100%)	-0.58	9 (0%) 94 91	5, 63, 160, 308	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
60	BB	119/119 (100%)	-0.57	1 (0%)	86	81	36, 102, 157, 192	0
60	DB	119/119 (100%)	-0.44	1 (0%)	86	81	33, 108, 159, 193	0
All	All	22726/23318 (97%)	-0.23	953 (4%)	36	32	0, 72, 150, 308	0

All (953) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
58	De	59	GLU	13.9
32	DK	62	ASP	13.5
59	DA	2799	A	12.6
58	De	55	GLU	12.1
25	DC	2	PRO	11.2
32	BK	62	ASP	11.2
58	De	58	THR	10.1
25	BC	33	LEU	9.7
20	CY	4	LYS	9.5
12	AM	125	ARG	9.3
25	DC	69	LEU	9.2
44	DY	108	THR	8.8
25	DC	227	PRO	8.8
25	DC	221	PRO	8.5
40	DU	118	GLY	8.4
38	BS	52	SER	8.3
38	BS	53	SER	8.2
58	De	122	VAL	8.0
32	DK	61	ALA	7.8
38	BS	54	LEU	7.8
32	BK	61	ALA	7.7
25	DC	36	ALA	7.6
42	DW	113	LYS	7.3
58	Be	107	GLU	7.2
58	De	107	GLU	7.2
58	De	57	LYS	7.2
32	DK	2	LYS	7.1
25	BC	2	PRO	7.1
29	DG	132	ASN	6.9
44	DY	107	ASP	6.9
57	B4	1	MET	6.8
1	CB	128	GLU	6.8
25	DC	113	ALA	6.8
25	DC	162	ILE	6.8

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Mol	Chain	Res	Type	RSRZ
56	D1	15	ALA	6.8
1	AB	170	GLU	6.6
38	DS	109	GLY	6.6
25	BC	221	PRO	6.5
58	De	56	GLU	6.5
58	De	116	GLU	6.4
29	DG	90	LEU	6.4
25	BC	32	GLU	6.3
20	AY	46	HIS	6.3
3	CD	198	VAL	6.3
38	BS	82	ILE	6.1
57	B4	14	ILE	6.0
38	DS	57	LYS	5.9
20	AY	64	THR	5.9
58	De	88	GLU	5.9
57	D4	24	THR	5.9
25	DC	170	GLY	5.8
25	DC	48	LEU	5.8
2	CC	206	GLU	5.8
25	DC	228	HIS	5.7
20	AY	231	TYR	5.7
29	DG	97	ASP	5.7
20	CY	571	SER	5.7
20	AY	232	LEU	5.7
29	DG	41	GLN	5.6
25	DC	50	ILE	5.6
29	DG	6	ALA	5.6
25	DC	70	GLY	5.6
25	DC	17	PRO	5.6
32	DK	64	SER	5.6
18	AS	8	GLY	5.5
18	CS	33	THR	5.5
27	DE	58	ARG	5.5
25	DC	114	VAL	5.5
57	D4	1	MET	5.5
9	CJ	64	GLU	5.5
32	DK	63	ARG	5.4
25	DC	49	GLY	5.4
59	BA	2799	A	5.4
58	De	105	LYS	5.3
25	DC	34	ALA	5.3
25	DC	206	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
58	De	106	GLN	5.2
25	DC	149	ASN	5.2
25	BC	15	VAL	5.1
38	DS	56	LEU	5.1
38	DS	32	LEU	5.1
58	De	60	PHE	5.1
29	BG	39	ILE	5.1
12	CM	102	ARG	5.0
38	DS	82	ILE	5.0
18	AS	47	HIS	5.0
15	AP	64	ALA	5.0
38	BS	28	VAL	5.0
25	BC	128	LEU	4.9
29	DG	44	GLY	4.9
20	AY	200	PRO	4.9
2	CC	26	LYS	4.9
58	Be	63	ILE	4.9
20	CY	43	GLY	4.9
9	AJ	8	LEU	4.9
29	DG	39	ILE	4.9
20	CY	54	PHE	4.8
25	DC	193	PHE	4.8
29	BG	90	LEU	4.8
38	DS	101	LEU	4.8
38	BS	27	SER	4.8
25	DC	153	ILE	4.8
29	DG	88	ILE	4.8
58	De	52	ALA	4.8
20	AY	63	ILE	4.8
38	DS	33	LYS	4.8
58	De	66	GLU	4.8
12	AM	124	PRO	4.8
38	DS	88	ASP	4.7
11	CL	20	LYS	4.7
38	DS	26	LEU	4.7
2	AC	149	ALA	4.7
29	BG	102	PHE	4.7
25	DC	134	PRO	4.6
58	De	100	LYS	4.6
56	D1	16	ASN	4.6
16	CQ	38	ARG	4.6
38	DS	27	SER	4.6

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Mol	Chain	Res	Type	RSRZ
58	De	61	ASP	4.6
9	CJ	25	GLU	4.6
25	DC	127	LYS	4.6
29	DG	42	GLY	4.6
38	DS	55	ALA	4.6
58	De	53	PRO	4.6
9	AJ	98	ILE	4.5
38	BS	34	HIS	4.5
12	CM	124	PRO	4.5
58	Be	64	LEU	4.5
29	DG	49	ASP	4.5
58	Be	66	GLU	4.5
20	AY	51	THR	4.5
38	DS	39	ILE	4.5
16	AQ	24	GLU	4.5
33	DN	1	MET	4.5
20	AY	257	PRO	4.5
25	DC	139	PRO	4.5
13	CN	57	ARG	4.5
12	CM	125	ARG	4.4
2	CC	207	VAL	4.4
1	CB	170	GLU	4.4
59	BA	2794	C	4.4
5	CF	101	ALA	4.4
11	CL	21	LYS	4.4
38	BS	101	LEU	4.4
20	CY	234	GLY	4.4
25	BC	50	ILE	4.4
25	BC	190	ILE	4.4
9	CJ	8	LEU	4.4
28	BF	11	VAL	4.4
38	DS	65	VAL	4.4
2	CC	99	VAL	4.3
28	BF	176	LEU	4.3
58	Be	56	GLU	4.3
25	BC	16	ASP	4.3
29	DG	177	GLY	4.3
29	BG	38	VAL	4.3
20	AY	321	TYR	4.3
32	DK	19	PRO	4.3
32	DK	66	THR	4.3
12	CM	123	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
20	CY	181	LEU	4.3
29	BG	60	LEU	4.3
57	B4	23	GLU	4.3
25	DC	40	GLU	4.2
27	BE	73	GLU	4.2
18	AS	33	THR	4.2
38	BS	14	VAL	4.2
57	B4	13	ARG	4.2
13	CN	58	LYS	4.2
16	AQ	58	GLU	4.2
58	Be	58	THR	4.2
57	D4	25	TYR	4.2
17	AR	26	LEU	4.2
56	D1	38	SER	4.2
49	B5	2	ALA	4.1
2	CC	59	ARG	4.1
12	AM	85	GLY	4.1
25	BC	101	ILE	4.1
29	DG	98	ARG	4.1
29	BG	135	LEU	4.1
57	D4	4	GLY	4.1
32	DK	67	PHE	4.1
29	DG	150	ASP	4.1
25	BC	3	LYS	4.0
37	BR	2	ARG	4.0
41	BV	81	TYR	4.0
23	CV	26	A	4.0
28	DF	8	GLN	4.0
7	CH	24	THR	4.0
29	DG	179	PRO	4.0
45	DZ	66	SER	4.0
25	BC	79	ALA	4.0
58	Be	109	GLU	4.0
57	B4	4	GLY	4.0
25	DC	128	LEU	4.0
58	De	73	GLU	4.0
58	De	119	GLY	4.0
32	DK	55	VAL	4.0
1	CB	222	ILE	3.9
20	AY	104	ALA	3.9
59	BA	2894	G	3.9
59	BA	2132	U	3.9

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Mol	Chain	Res	Type	RSRZ
38	DS	87	PHE	3.9
18	AS	48	THR	3.9
26	BD	34	VAL	3.9
12	AM	123	ALA	3.9
39	DT	1	MET	3.9
1	CB	188	ALA	3.9
2	CC	69	HIS	3.9
58	Be	90	LYS	3.9
2	CC	20	SER	3.9
29	DG	131	TYR	3.9
38	BS	58	LEU	3.9
58	De	62	VAL	3.9
58	De	121	VAL	3.9
32	DK	9	LYS	3.9
25	DC	157	ILE	3.9
12	AM	122	LYS	3.9
2	CC	108	ASN	3.9
25	DC	180	SER	3.8
48	D3	28	LEU	3.8
25	BC	97	GLY	3.8
20	CY	200	PRO	3.8
58	De	117	ALA	3.8
33	BN	43	THR	3.8
25	BC	150	ILE	3.8
33	BN	42	TRP	3.8
32	BK	64	SER	3.8
58	Be	88	GLU	3.8
58	De	104	SER	3.8
25	DC	189	ASN	3.8
25	BC	125	GLY	3.7
25	BC	35	THR	3.7
12	AM	97	PRO	3.7
25	BC	30	VAL	3.7
29	BG	134	GLY	3.7
32	DK	20	ALA	3.7
20	AY	177	ILE	3.7
12	CM	85	GLY	3.7
38	BS	65	VAL	3.7
39	DT	76	PHE	3.7
25	DC	220	GLY	3.7
18	CS	35	SER	3.7
56	D1	42	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
57	D4	14	ILE	3.7
20	AY	50	ALA	3.7
29	DG	87	PRO	3.7
59	DA	2798	C	3.6
29	DG	157	ILE	3.6
56	D1	18	ILE	3.6
58	De	63	ILE	3.6
25	BC	34	ALA	3.6
38	DS	108	GLY	3.6
28	DF	125	LEU	3.6
13	CN	46	GLU	3.6
12	CM	101	GLN	3.6
35	BP	53	GLY	3.6
29	BG	144	ILE	3.6
38	DS	106	ARG	3.6
25	BC	127	LYS	3.6
49	D5	2	ALA	3.6
18	CS	36	ARG	3.6
57	D4	23	GLU	3.6
28	DF	176	LEU	3.6
38	DS	54	LEU	3.6
58	Be	112	LYS	3.5
25	DC	205	ALA	3.5
38	BS	39	ILE	3.5
25	BC	69	LEU	3.5
28	DF	10	PRO	3.5
11	AL	35	GLY	3.5
25	DC	152	GLU	3.5
25	DC	3	LYS	3.5
38	BS	108	GLY	3.5
25	DC	161	ARG	3.5
25	BC	18	ASN	3.5
25	BC	111	PHE	3.5
25	DC	37	LYS	3.5
2	CC	11	ARG	3.5
9	CJ	44	VAL	3.5
38	BS	57	LYS	3.5
40	DU	12	ARG	3.5
58	Be	59	GLU	3.5
29	BG	106	LEU	3.5
56	B1	38	SER	3.5
20	CY	378	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
2	CC	17	ASP	3.5
25	BC	126	SER	3.5
25	BC	17	PRO	3.4
32	BK	60	TYR	3.4
25	BC	42	VAL	3.4
38	BS	38	GLN	3.4
16	AQ	39	SER	3.4
11	CL	83	VAL	3.4
29	BG	35	GLU	3.4
25	DC	173	HIS	3.4
2	CC	25	GLY	3.4
20	CY	291	GLY	3.4
58	De	77	GLU	3.4
58	De	108	ALA	3.4
29	DG	48	GLU	3.4
7	AH	113	SER	3.4
12	AM	102	ARG	3.4
41	BV	75	PHE	3.4
38	DS	37	ALA	3.4
48	B3	28	LEU	3.4
1	CB	107	THR	3.4
25	DC	169	THR	3.4
29	BG	41	GLN	3.4
57	D4	7	PRO	3.4
38	DS	20	ARG	3.4
10	CK	41	THR	3.4
11	CL	30	ALA	3.4
20	CY	47	GLU	3.4
20	CY	5	VAL	3.4
15	CP	73	LEU	3.3
18	CS	15	LEU	3.3
25	BC	116	ALA	3.3
18	CS	44	MET	3.3
2	AC	97	LYS	3.3
20	AY	5	VAL	3.3
36	DQ	140	ALA	3.3
38	BS	55	ALA	3.3
41	BV	74	LYS	3.3
29	DG	53	LEU	3.3
25	DC	135	ARG	3.3
18	AS	9	VAL	3.3
38	DS	38	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
29	BG	25	TYR	3.3
2	AC	47	LEU	3.3
25	BC	100	ILE	3.3
25	DC	197	LEU	3.3
11	CL	28	LYS	3.3
25	DC	190	ILE	3.3
29	BG	5	VAL	3.3
2	CC	197	GLY	3.2
29	BG	37	VAL	3.2
29	BG	109	VAL	3.2
38	DS	52	SER	3.2
28	DF	181	LEU	3.2
58	Be	121	VAL	3.2
25	DC	32	GLU	3.2
2	CC	189	ALA	3.2
30	DH	57	ASP	3.2
2	CC	200	ALA	3.2
29	DG	158	ALA	3.2
2	CC	75	VAL	3.2
20	CY	60	GLU	3.2
52	B8	63	PRO	3.2
25	DC	112	ASP	3.2
29	DG	176	LEU	3.2
38	DS	53	SER	3.2
9	CJ	62	HIS	3.2
18	CS	57	HIS	3.2
59	DA	2793	G	3.2
58	Be	117	ALA	3.2
58	De	54	ALA	3.2
25	DC	172	ILE	3.2
58	De	111	ILE	3.2
25	BC	87	ALA	3.2
9	CJ	68	HIS	3.2
57	B4	24	THR	3.2
38	DS	83	LYS	3.2
38	BS	49	VAL	3.2
18	AS	50	ALA	3.1
57	D4	31	ILE	3.1
9	AJ	44	VAL	3.1
29	BG	64	THR	3.1
11	CL	89	ARG	3.1
38	DS	36	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
25	DC	160	GLY	3.1
20	CY	84	THR	3.1
25	BC	223	VAL	3.1
19	CT	72	LEU	3.1
2	CC	24	ALA	3.1
9	CJ	86	MET	3.1
20	AY	259	PHE	3.1
20	CY	59	ARG	3.1
2	CC	196	LEU	3.1
13	AN	53	LEU	3.1
25	BC	76	LEU	3.1
25	BC	197	LEU	3.1
29	BG	49	ASP	3.1
20	AY	199	ILE	3.1
44	DY	16	ALA	3.1
20	AY	570	GLY	3.1
25	DC	175	PRO	3.1
20	CY	587	SER	3.1
2	CC	67	THR	3.1
45	BZ	7	ALA	3.1
56	D1	14	VAL	3.1
20	CY	83	ASP	3.1
25	BC	213	VAL	3.1
1	CB	30	ARG	3.0
17	AR	23	LYS	3.0
29	DG	66	GLN	3.0
56	D1	33	LYS	3.0
58	De	82	THR	3.0
44	DY	106	LEU	3.0
20	CY	435	ASP	3.0
25	BC	8	TYR	3.0
29	DG	46	ALA	3.0
12	CM	104	ARG	3.0
39	DT	75	ILE	3.0
41	DV	61	VAL	3.0
29	DG	57	ALA	3.0
20	AY	666	ARG	3.0
1	CB	27	LYS	3.0
56	B1	25	LYS	3.0
29	DG	151	ALA	3.0
9	CJ	65	LEU	3.0
7	CH	116	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
20	CY	233	GLU	3.0
28	DF	18	ARG	3.0
58	Be	89	ALA	3.0
2	CC	204	LEU	3.0
20	CY	49	ALA	3.0
25	DC	174	ALA	3.0
18	AS	49	ILE	3.0
20	AY	358	MET	3.0
20	CY	227	ILE	3.0
25	DC	186	LEU	3.0
2	AC	154	SER	2.9
38	BS	41	ASP	2.9
2	CC	74	GLY	2.9
11	CL	56	ALA	2.9
25	BC	12	LEU	2.9
29	DG	155	MET	2.9
25	BC	169	THR	2.9
20	AY	105	ILE	2.9
13	CN	54	PRO	2.9
38	BS	50	SER	2.9
12	CM	70	LEU	2.9
29	BG	53	LEU	2.9
20	CY	311	ALA	2.9
56	D1	17	SER	2.9
25	DC	35	THR	2.9
29	BG	65	GLY	2.9
16	CQ	26	GLN	2.9
20	CY	16	GLY	2.9
16	CQ	69	LYS	2.9
29	DG	159	VAL	2.9
58	De	112	LYS	2.9
27	DE	205	ALA	2.9
29	DG	40	ASN	2.9
3	CD	96	LEU	2.9
25	BC	46	ALA	2.9
28	BF	181	LEU	2.9
20	CY	310	ALA	2.9
25	BC	113	ALA	2.9
26	DD	240	ALA	2.9
28	DF	155	LEU	2.9
38	DS	34	HIS	2.9
58	De	102	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
29	DG	45	GLU	2.9
38	DS	50	SER	2.9
25	DC	31	LYS	2.8
33	BN	38	HIS	2.8
34	DO	77	ILE	2.8
58	De	87	LYS	2.8
59	BA	2795	G	2.8
51	D7	49	ARG	2.8
20	CY	349	LYS	2.8
38	DS	40	ILE	2.8
29	BG	34	LEU	2.8
29	DG	32	PRO	2.8
9	CJ	10	GLY	2.8
25	BC	124	VAL	2.8
25	DC	26	ALA	2.8
38	DS	66	ALA	2.8
15	AP	16	HIS	2.8
18	AS	32	LYS	2.8
44	DY	102	CYS	2.8
13	CN	53	LEU	2.8
18	AS	31	ILE	2.8
25	DC	219	MET	2.8
29	DG	178	PHE	2.8
32	BK	65	PHE	2.8
16	AQ	41	LYS	2.8
7	CH	80	ILE	2.8
27	BE	15	PHE	2.8
12	AM	87	TYR	2.8
25	BC	75	VAL	2.8
20	CY	66	THR	2.8
25	DC	208	THR	2.8
25	DC	150	ILE	2.8
58	De	109	GLU	2.8
15	AP	51	VAL	2.8
18	AS	61	TYR	2.8
20	AY	531	GLY	2.8
21	CA	68(L)	U	2.8
15	CP	74	LEU	2.8
25	BC	44	VAL	2.8
59	BA	888	C	2.8
33	BN	82	LEU	2.8
2	CC	184	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
4	CE	135	THR	2.8
2	CC	110	ASN	2.8
12	AM	91	ARG	2.7
25	DC	75	VAL	2.7
38	DS	107	GLU	2.7
35	DP	5	ASP	2.7
29	DG	106	LEU	2.7
29	BG	136	ARG	2.7
1	CB	102	LEU	2.7
2	CC	149	ALA	2.7
13	CN	59	ALA	2.7
10	AK	70	LYS	2.7
20	CY	65	ILE	2.7
25	DC	185	LYS	2.7
53	B9	1	MET	2.7
12	AM	65	LYS	2.7
46	B0	15	ASP	2.7
20	AY	133	ILE	2.7
35	BP	144	GLU	2.7
59	BA	2116	G	2.7
25	BC	6	LYS	2.7
20	CY	237	PRO	2.7
29	DG	37	VAL	2.7
58	De	99	VAL	2.7
11	CL	19	ARG	2.7
13	CN	55	GLY	2.7
28	BF	158	THR	2.7
32	DK	27	LEU	2.7
29	DG	92	VAL	2.7
33	BN	19	GLU	2.7
29	DG	96	ARG	2.7
44	DY	54	LYS	2.7
46	D0	37	LEU	2.7
2	CC	82	GLU	2.7
25	BC	140	ASN	2.7
29	BG	158	ALA	2.7
1	CB	111	ARG	2.7
20	AY	6	GLU	2.7
29	DG	33	ARG	2.7
12	CM	68	GLY	2.7
32	DK	15	GLY	2.7
2	CC	18	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
13	CN	34	TYR	2.7
59	BA	2152	G	2.7
13	AN	55	GLY	2.7
38	DS	100	ALA	2.7
12	CM	81	LEU	2.7
25	DC	210	LEU	2.7
25	DC	225	ILE	2.7
1	AB	148	TYR	2.6
28	BF	127	GLU	2.6
25	BC	229	SER	2.6
11	CL	32	PHE	2.6
25	DC	68	GLY	2.6
42	DW	93	ALA	2.6
9	AJ	4	ILE	2.6
29	BG	107	LEU	2.6
38	DS	102	ALA	2.6
33	BN	133	GLN	2.6
3	CD	15	GLU	2.6
20	CY	85	PRO	2.6
20	AY	261	GLY	2.6
29	BG	132	ASN	2.6
38	DS	58	LEU	2.6
16	AQ	5	VAL	2.6
25	DC	229	SER	2.6
53	D9	1	MET	2.6
44	BY	90	LEU	2.6
25	BC	174	ALA	2.6
38	DS	28	VAL	2.6
20	AY	456	GLU	2.6
39	BT	114	LEU	2.6
46	D0	6	GLY	2.6
20	CY	255	ILE	2.6
1	CB	16	HIS	2.6
32	DK	10	LEU	2.6
11	CL	17	LYS	2.6
28	BF	114	VAL	2.6
1	CB	80	ILE	2.6
2	CC	201	TYR	2.6
9	CJ	59	SER	2.6
20	AY	4	LYS	2.6
25	DC	15	VAL	2.6
34	BO	76	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
25	BC	198	GLU	2.6
33	DN	116	LEU	2.6
28	BF	185	ASP	2.6
29	BG	159	VAL	2.6
40	BU	118	GLY	2.6
2	CC	16	ARG	2.6
59	BA	890	A	2.6
29	BG	103	LEU	2.6
2	AC	170	GLN	2.6
33	BN	1	MET	2.6
58	Be	87	LYS	2.6
20	CY	321	TYR	2.5
21	AA	823	G	2.5
38	BS	56	LEU	2.5
52	D8	15	LYS	2.5
33	DN	133	GLN	2.5
35	DP	7	ARG	2.5
1	AB	238	LEU	2.5
32	DK	99	ILE	2.5
11	CL	18	VAL	2.5
29	BG	146	TYR	2.5
9	AJ	46	ARG	2.5
29	BG	32	PRO	2.5
6	AG	62	PHE	2.5
7	CH	32	LYS	2.5
38	BS	88	ASP	2.5
57	B4	31	ILE	2.5
20	CY	182	ARG	2.5
18	CS	32	LYS	2.5
29	BG	57	ALA	2.5
29	DG	75	LYS	2.5
20	AY	229	LEU	2.5
38	BS	40	ILE	2.5
16	CQ	58	GLU	2.5
25	BC	115	VAL	2.5
25	DC	156	GLU	2.5
26	DD	12	SER	2.5
20	CY	232	LEU	2.5
33	BN	44	PRO	2.5
25	BC	72	GLN	2.5
2	CC	72	LYS	2.5
60	BB	53	A	2.5

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Mol	Chain	Res	Type	RSRZ
36	BQ	34	LEU	2.5
25	DC	30	VAL	2.5
25	DC	163	GLU	2.5
25	BC	147	GLY	2.5
38	BS	109	GLY	2.5
38	DS	35	ILE	2.5
25	BC	193	PHE	2.5
38	BS	48	LEU	2.5
18	AS	40	ILE	2.5
2	CC	56	ASP	2.5
2	CC	185	GLY	2.5
25	BC	186	LEU	2.5
28	BF	166	ALA	2.5
2	AC	200	ALA	2.5
33	BN	39	ARG	2.5
59	DA	311	A	2.5
4	CE	47	LYS	2.5
20	AY	233	GLU	2.5
29	DG	107	LEU	2.5
44	BY	31	LEU	2.5
2	CC	182	ILE	2.5
1	CB	152	PHE	2.5
40	DU	32	PHE	2.5
28	BF	155	LEU	2.4
32	DK	115	LEU	2.4
20	AY	532	GLY	2.4
57	B4	5	ILE	2.4
1	CB	84	GLU	2.4
20	CY	56	GLU	2.4
42	BW	87	PRO	2.4
39	BT	88	ILE	2.4
58	Be	108	ALA	2.4
32	DK	116	ASN	2.4
28	BF	129	PHE	2.4
20	CY	322	VAL	2.4
29	BG	115	ARG	2.4
30	BH	43	VAL	2.4
47	B2	14	ARG	2.4
9	CJ	4	ILE	2.4
29	DG	110	ALA	2.4
41	DV	101	GLY	2.4
25	DC	168	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
41	BV	5	VAL	2.4
58	De	79	ARG	2.4
29	BG	63	ILE	2.4
1	CB	166	ASP	2.4
2	CC	154	SER	2.4
25	BC	214	TYR	2.4
7	AH	66	GLY	2.4
25	BC	227	PRO	2.4
26	DD	191	ALA	2.4
25	DC	33	LEU	2.4
18	AS	65	ASN	2.4
38	BS	44	LYS	2.4
27	BE	72	VAL	2.4
37	BR	69	ASP	2.4
9	CJ	89	ASP	2.4
32	DK	60	TYR	2.4
20	CY	199	ILE	2.4
16	CQ	101	ARG	2.4
25	BC	40	GLU	2.4
28	BF	78	ILE	2.4
41	DV	60	GLU	2.4
7	CH	78	GLN	2.4
20	CY	258	VAL	2.4
25	BC	210	LEU	2.4
20	CY	426	GLN	2.4
44	BY	83	THR	2.4
58	De	91	ASP	2.4
59	DA	889	C	2.4
20	AY	237	PRO	2.4
52	D8	34	TRP	2.4
20	AY	215	LYS	2.4
25	BC	14	LYS	2.4
29	DG	103	LEU	2.4
29	DG	181	ARG	2.4
39	BT	106	SER	2.4
16	CQ	10	VAL	2.4
32	BK	23	VAL	2.4
41	BV	7	THR	2.4
58	De	64	LEU	2.4
2	CC	202	ILE	2.4
20	AY	185	ALA	2.4
20	CY	399	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
29	DG	69	ALA	2.4
20	CY	82	ILE	2.4
2	AC	155	GLY	2.4
57	D4	13	ARG	2.4
2	CC	66	VAL	2.4
48	B3	31	LEU	2.4
29	BG	75	LYS	2.4
44	BY	88	LYS	2.4
48	D3	8	LEU	2.3
52	D8	25	MET	2.3
20	AY	255	ILE	2.3
20	AY	202	PRO	2.3
28	DF	182	ASN	2.3
38	BS	29	PHE	2.3
2	CC	85	ARG	2.3
20	AY	53	ASP	2.3
46	D0	79	VAL	2.3
16	CQ	37	LYS	2.3
29	DG	36	LYS	2.3
58	De	120	ALA	2.3
15	AP	32	TYR	2.3
20	CY	212	TYR	2.3
2	CC	166	GLU	2.3
2	CC	150	LYS	2.3
25	BC	170	GLY	2.3
35	DP	68	GLN	2.3
16	AQ	59	ILE	2.3
20	AY	106	VAL	2.3
20	AY	182	ARG	2.3
33	BN	63	THR	2.3
51	D7	41	ARG	2.3
20	CY	46	HIS	2.3
25	DC	47	LYS	2.3
41	BV	44	LYS	2.3
48	D3	10	LYS	2.3
25	DC	209	PHE	2.3
39	DT	138	ALA	2.3
42	BW	74	ALA	2.3
2	AC	15	THR	2.3
46	D0	31	VAL	2.3
57	D4	21	VAL	2.3
19	CT	76	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
38	BS	106	ARG	2.3
41	DV	94	LEU	2.3
25	BC	22	THR	2.3
25	BC	182	PRO	2.3
47	D2	25	VAL	2.3
20	AY	18	ALA	2.3
20	CY	221	ALA	2.3
59	DA	2894	G	2.3
12	CM	122	LYS	2.3
1	CB	183	PRO	2.3
2	AC	11	ARG	2.3
2	CC	164	ARG	2.3
12	AM	88	ARG	2.3
20	CY	104	ALA	2.3
25	BC	188	ASP	2.3
28	BF	167	ALA	2.3
34	DO	34	THR	2.3
38	BS	59	LYS	2.3
45	DZ	115	GLY	2.3
13	AN	6	LEU	2.3
29	DG	77	ILE	2.3
29	BG	92	VAL	2.3
32	DK	65	PHE	2.3
29	BG	6	ALA	2.3
29	BG	69	ALA	2.3
38	DS	59	LYS	2.3
32	DK	4	VAL	2.3
34	BO	98	VAL	2.3
20	AY	47	GLU	2.2
44	DY	84	ARG	2.2
50	D6	37	ARG	2.2
7	AH	32	LYS	2.2
29	DG	34	LEU	2.2
12	CM	108	ARG	2.2
58	Be	82	THR	2.2
59	DA	887	A	2.2
25	BC	180	SER	2.2
29	BG	56	ALA	2.2
11	CL	98	TYR	2.2
29	DG	101	ILE	2.2
20	AY	156	ARG	2.2
9	AJ	6	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
17	CR	22	VAL	2.2
33	BN	48	MET	2.2
34	DO	1	MET	2.2
35	DP	67	MET	2.2
20	CY	570	GLY	2.2
25	DC	151	GLY	2.2
25	BC	4	HIS	2.2
2	AC	72	LYS	2.2
25	BC	162	ILE	2.2
33	BN	45	ASN	2.2
27	DE	162	ALA	2.2
58	Be	67	ALA	2.2
28	DF	90	PHE	2.2
1	AB	187	LEU	2.2
20	AY	221	ALA	2.2
58	De	67	ALA	2.2
58	Be	70	LYS	2.2
4	CE	122	GLU	2.2
20	CY	377	VAL	2.2
41	BV	20	LEU	2.2
56	D1	29	GLY	2.2
58	Be	94	GLU	2.2
56	B1	18	ILE	2.2
9	CJ	21	GLN	2.2
25	DC	46	ALA	2.2
46	D0	41	ARG	2.2
18	AS	42	PRO	2.2
18	AS	15	LEU	2.2
34	BO	2	ILE	2.2
35	DP	70	GLN	2.2
56	B1	42	GLN	2.2
25	BC	58	ASN	2.2
29	DG	68	PRO	2.2
33	DN	4	TYR	2.2
11	CL	127	GLU	2.2
29	DG	144	ILE	2.2
32	BK	2	LYS	2.2
28	BF	157	VAL	2.2
38	DS	30	ARG	2.2
45	DZ	88	PHE	2.2
25	BC	104	ILE	2.2
11	AL	56	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
16	CQ	99	SER	2.2
25	BC	47	LYS	2.2
50	D6	25	LYS	2.2
21	AA	1028(D)	C	2.2
58	Be	52	ALA	2.2
59	BA	2793	G	2.2
60	DB	43	C	2.2
2	AC	177	THR	2.2
50	D6	26	ASN	2.2
29	DG	5	VAL	2.2
4	CE	120	THR	2.1
34	BO	62	VAL	2.1
51	D7	42	LEU	2.1
1	AB	119	GLU	2.1
13	AN	52	GLN	2.1
34	DO	2	ILE	2.1
41	DV	8	GLY	2.1
13	AN	49	HIS	2.1
25	BC	52	PRO	2.1
18	CS	51	VAL	2.1
42	BW	17	VAL	2.1
25	DC	133	GLY	2.1
58	De	51	ALA	2.1
20	AY	107	VAL	2.1
25	BC	99	GLU	2.1
34	BO	34	THR	2.1
20	AY	310	ALA	2.1
26	DD	246	PRO	2.1
33	DN	42	TRP	2.1
59	DA	2110	G	2.1
44	DY	41	GLY	2.1
56	B1	17	SER	2.1
2	CC	103	VAL	2.1
13	CN	47	LEU	2.1
28	DF	14	PRO	2.1
49	D5	32	PRO	2.1
58	Be	71	LYS	2.1
4	CE	27	ARG	2.1
20	AY	132	ARG	2.1
59	BA	2798	C	2.1
45	DZ	21	ALA	2.1
12	CM	87	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
50	D6	39	TYR	2.1
41	BV	24	LYS	2.1
44	DY	85	VAL	2.1
47	D2	14	ARG	2.1
51	D7	47	ARG	2.1
27	DE	24	THR	2.1
2	AC	202	ILE	2.1
53	B9	8	LYS	2.1
25	DC	137	LEU	2.1
2	AC	201	TYR	2.1
25	BC	45	HIS	2.1
25	DC	164	PHE	2.1
13	AN	29	ARG	2.1
29	DG	54	GLU	2.1
11	AL	93	LEU	2.1
32	BK	55	VAL	2.1
18	CS	74	PHE	2.1
25	DC	179	ALA	2.1
32	DK	120	LEU	2.1
2	CC	155	GLY	2.1
20	AY	162	VAL	2.1
20	CY	325	LEU	2.1
41	DV	75	PHE	2.1
29	BG	66	GLN	2.1
44	DY	101	LYS	2.1
2	CC	15	THR	2.1
20	AY	38	ARG	2.1
25	BC	151	GLY	2.1
25	BC	176	VAL	2.1
2	AC	181	ASN	2.1
12	CM	65	LYS	2.1
20	CY	17	ILE	2.1
20	CY	231	TYR	2.1
26	BD	64	ILE	2.1
13	CN	26	ARG	2.1
21	AA	68(L)	U	2.1
29	DG	102	PHE	2.1
51	B7	48	LYS	2.1
59	DA	2132	U	2.1
20	AY	260	LEU	2.1
20	CY	236	GLU	2.1
28	DF	11	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
17	AR	88	LYS	2.1
29	BG	157	ILE	2.1
25	DC	166	ASN	2.1
25	BC	68	GLY	2.1
41	DV	9	GLY	2.1
1	AB	80	ILE	2.0
20	AY	429	ALA	2.0
25	BC	139	PRO	2.0
7	AH	80	ILE	2.0
28	BF	5	ALA	2.0
32	DK	22	PRO	2.0
13	AN	3	ARG	2.0
13	CN	31	ARG	2.0
5	AF	10	LEU	2.0
29	DG	3	LEU	2.0
32	DK	3	LYS	2.0
40	DU	94	ASN	2.0
4	CE	82	VAL	2.0
4	CE	155	GLU	2.0
20	AY	134	ALA	2.0
32	DK	21	PRO	2.0
41	DV	93	GLU	2.0
58	Be	102	GLY	2.0
56	D1	40	ARG	2.0
20	AY	332	SER	2.0
30	DH	50	VAL	2.0
32	BK	27	LEU	2.0
33	DN	99	LEU	2.0
38	BS	51	ALA	2.0
25	DC	63	VAL	2.0
20	AY	176	GLY	2.0
25	BC	57	GLN	2.0
1	CB	97	TRP	2.0
33	DN	5	VAL	2.0
46	D0	63	VAL	2.0
18	CS	4	SER	2.0
29	DG	91	ARG	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, 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
24	KBE	CU	1	9/10	0.85	0.34	118,118,118,118	0
24	UAL	AU	5	9/10	0.88	0.16	114,114,114,114	0
24	KBE	AU	1	9/10	0.90	0.32	114,114,114,114	0
24	UAL	CU	5	9/10	0.90	0.13	118,118,118,118	0
24	DPP	CU	2	6/7	0.92	0.18	118,118,118,118	0
24	5OH	AU	6	12/13	0.93	0.29	99,101,102,102	0
24	5OH	CU	6	12/13	0.93	0.21	99,101,102,102	0
24	DPP	AU	2	6/7	0.97	0.23	114,114,114,114	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

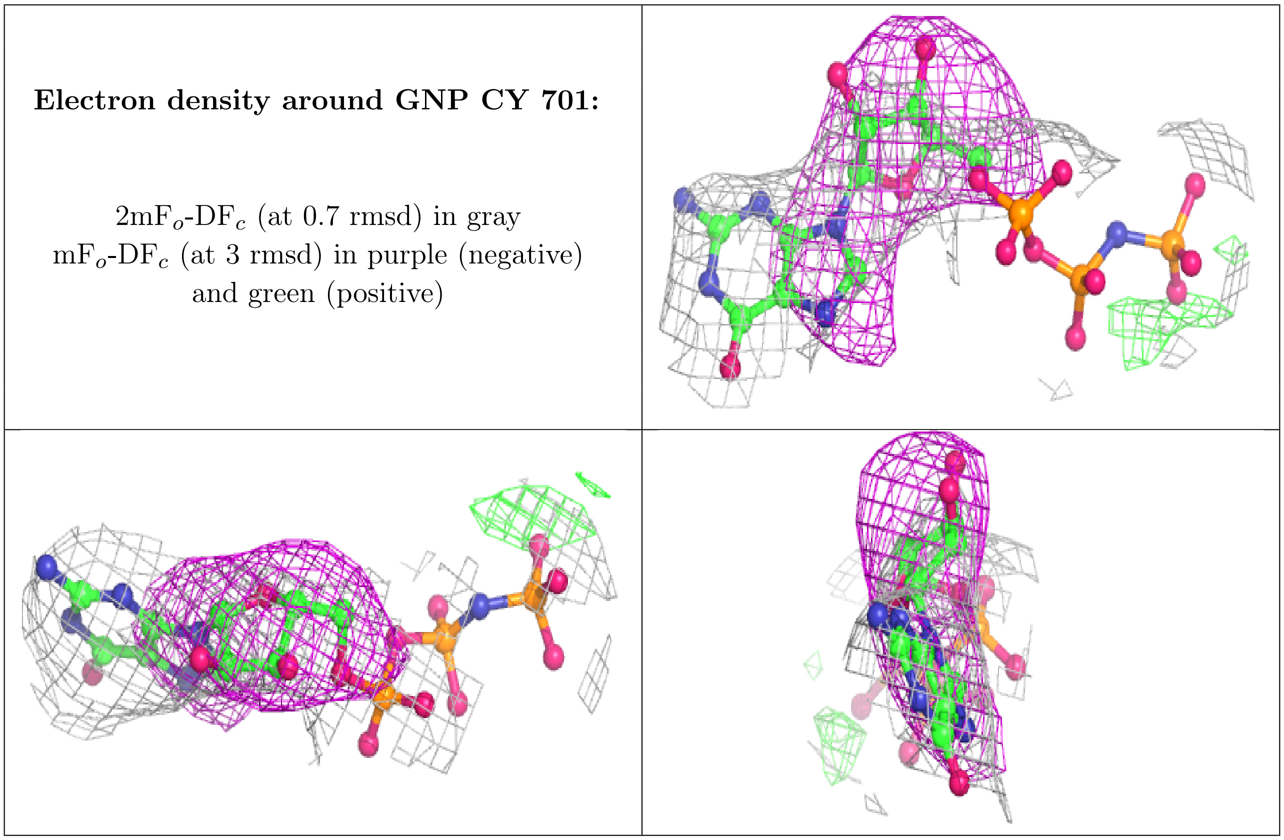
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
61	GNP	CY	701	32/32	0.91	0.23	58,71,81,83	0
61	GNP	AY	701	32/32	0.92	0.22	58,71,81,83	0
62	MG	CY	702	1/1	0.97	0.11	135,135,135,135	0
62	MG	AY	702	1/1	0.98	0.11	88,88,88,88	0

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

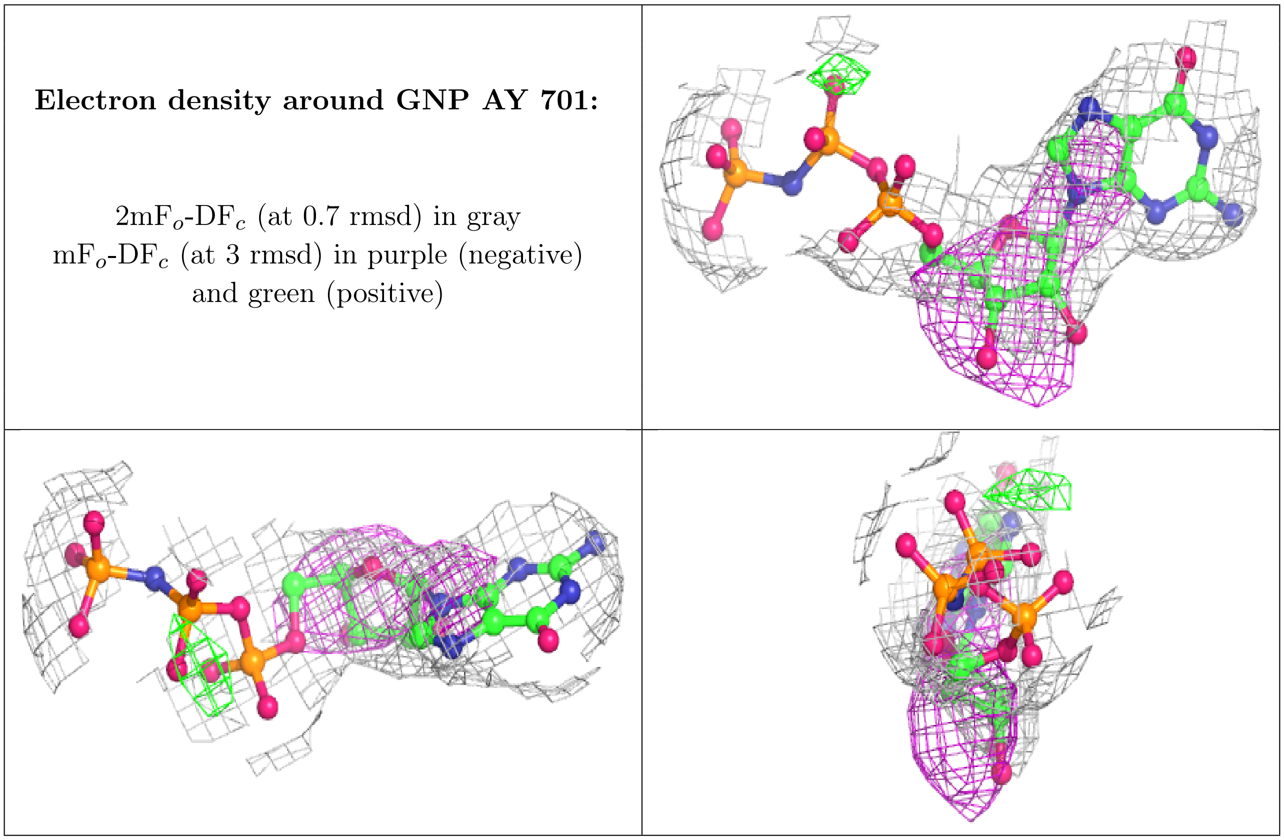
Electron density around GNP CY 701:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GNP AY 701:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.