



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 04:59 am BST

PDB ID : 4U26
Title : Crystal structure of the E. coli ribosome bound to dalbavancin and quinupristin.
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.
Deposited on : 2014-07-16
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

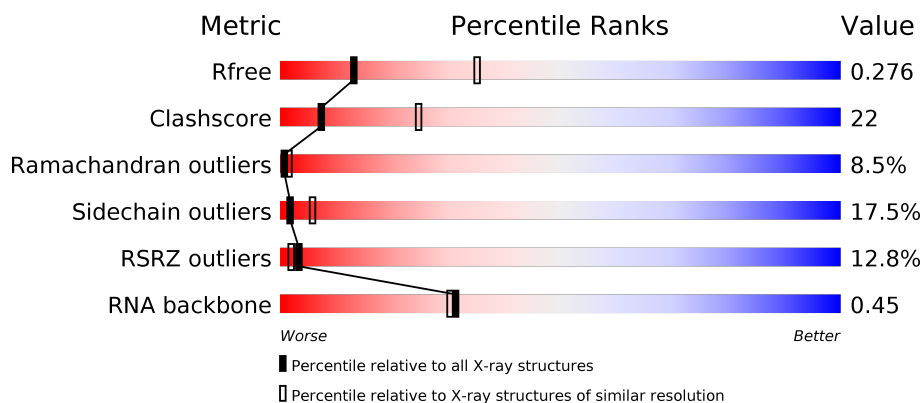
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	AA	1539	<div> <div>0%</div> <div> <div>34%</div> <div>50%</div> <div>15%</div> </div> </div>
1	CA	1539	<div> <div>4%</div> <div> <div>31%</div> <div>54%</div> <div>16%</div> </div> </div>
2	AB	218	<div> <div>13%</div> <div> <div>25%</div> <div>50%</div> <div>18%</div> <div>7%</div> </div> </div>
2	CB	218	<div> <div>21%</div> <div> <div>30%</div> <div>49%</div> <div>17%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	CC	206	
4	AD	205	
4	CD	205	
5	AE	150	
5	CE	150	
6	AF	100	
6	CF	100	
7	AG	151	
7	CG	151	
8	AH	129	
8	CH	129	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	117	
11	CK	117	
12	AL	123	
12	CL	123	
13	AM	114	
13	CM	114	
14	AN	100	
14	CN	100	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	82	
16	CP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	119	
23	DB	119	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	
27	DF	177	

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Mol	Chain	Length	Quality of chain
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	
31	BJ	142	
31	DJ	142	
32	BK	122	
32	DK	122	
33	BL	143	
33	DL	143	
34	BM	136	
34	DM	136	
35	BN	120	
35	DN	120	
36	BO	116	
36	DO	116	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	

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Mol	Chain	Length	Quality of chain
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	
44	BW	76	
44	DW	76	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	
52	B4	38	
52	D4	38	

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Mol	Chain	Length	Quality of chain
53	B5	228	
54	B6	8	
54	D6	8	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1659	-	-	-	X
55	MG	AM	201	-	-	-	X
55	MG	BA	3134	-	-	-	X
55	MG	DA	3003	-	-	-	X
55	MG	DA	3005	-	-	-	X
55	MG	DA	3026	-	-	-	X
55	MG	DA	3028	-	-	-	X
55	MG	DA	3041	-	-	-	X
55	MG	DA	3048	-	-	-	X
55	MG	DA	3056	-	-	-	X
55	MG	DA	3062	-	-	-	X
55	MG	DA	3071	-	-	-	X
55	MG	DA	3072	-	-	-	X
55	MG	DA	3077	-	-	-	X
55	MG	DA	3131	-	-	-	X
55	MG	DA	3133	-	-	-	X
55	MG	DA	3155	-	-	-	X
56	DOL	DA	3001	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 288423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	CA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	CB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			
5	CE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	CF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
12	CL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
14	CN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			
15	CO	88	Total	C	N	O	S	0	0	0
			710	437	143	129	1			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			
21	CU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
22	DA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	119	Total	C	N	O	P	0	0	0
			2549	1135	466	829	119			
23	DB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
25	DD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
30	DI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
31	DJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
32	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
33	DL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
34	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			
35	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BO	116	Total	C	N	O	0	0	0
			892	552	178	162			
36	DO	116	Total	C	N	O	0	0	0
			892	552	178	162			

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
37	DP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				
38	DQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
39	DR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
40	DS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
41	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BU	102	Total	C	N	O	S	0	0	0
			780	492	146	142				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	DU	102	Total	C	N	O	0	0	0
			780	492	146	142			

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
43	DV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BW	76	Total	C	N	O	S	0	0	0
			580	359	117	103	1			
44	DW	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
45	DX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BY	63	Total 509	C 313	N 99	O 95	S 2	0	0	0
46	DY	63	Total 509	C 313	N 99	O 95	S 2	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BZ	58	Total 449	C 281	N 87	O 79	S 2	0	0	0
47	DZ	58	Total 449	C 281	N 87	O 79	S 2	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
48	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B1	50	Total	C	N	O	0	0	0
			410	263	75	72			
49	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
50	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
51	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
52	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 53 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	B5	191	Total	C	N	O	0	0	1
			1142	691	221	230			

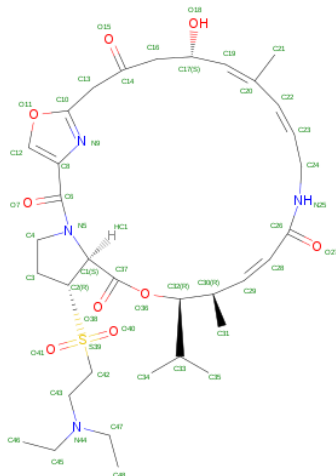
- Molecule 54 is a protein called Quinupristin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B6	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			
54	D6	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BB	4	Total	Mg	0	0
			4	4		
55	BA	194	Total	Mg	0	0
			194	194		
55	CA	56	Total	Mg	0	0
			56	56		
55	DQ	1	Total	Mg	0	0
			1	1		
55	D2	1	Total	Mg	0	0
			1	1		
55	AA	71	Total	Mg	0	0
			71	71		
55	BQ	1	Total	Mg	0	0
			1	1		
55	DA	166	Total	Mg	0	0
			166	166		
55	DB	3	Total	Mg	0	0
			3	3		
55	AM	1	Total	Mg	0	0
			1	1		

- Molecule 56 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula: C₃₄H₅₀N₄O₉S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
56	BA	1	Total 48	C 34	N 4	O 9	S 1	0	0
56	DA	1	Total 48	C 34	N 4	O 9	S 1	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B4	1	Total 1	Zn 1	0	0
57	D4	1	Total 1	Zn 1	0	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	194	Total 194	O 194	0	0
58	AE	2	Total 2	O 2	0	0
58	AL	1	Total 1	O 1	0	0
58	AN	3	Total 3	O 3	0	0
58	AT	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AU	1	Total 1	O 1	0	0
58	BA	617	Total 617	O 617	0	0
58	BB	14	Total 14	O 14	0	0
58	BC	6	Total 6	O 6	0	0
58	BD	4	Total 4	O 4	0	0
58	BE	1	Total 1	O 1	0	0
58	BF	1	Total 1	O 1	0	0
58	BG	1	Total 1	O 1	0	0
58	BJ	1	Total 1	O 1	0	0
58	BL	7	Total 7	O 7	0	0
58	BN	5	Total 5	O 5	0	0
58	BQ	1	Total 1	O 1	0	0
58	BS	1	Total 1	O 1	0	0
58	BT	2	Total 2	O 2	0	0
58	B3	3	Total 3	O 3	0	0
58	B4	1	Total 1	O 1	0	0
58	CA	192	Total 192	O 192	0	0
58	CL	1	Total 1	O 1	0	0
58	CN	2	Total 2	O 2	0	0
58	CT	2	Total 2	O 2	0	0
58	CU	1	Total 1	O 1	0	0

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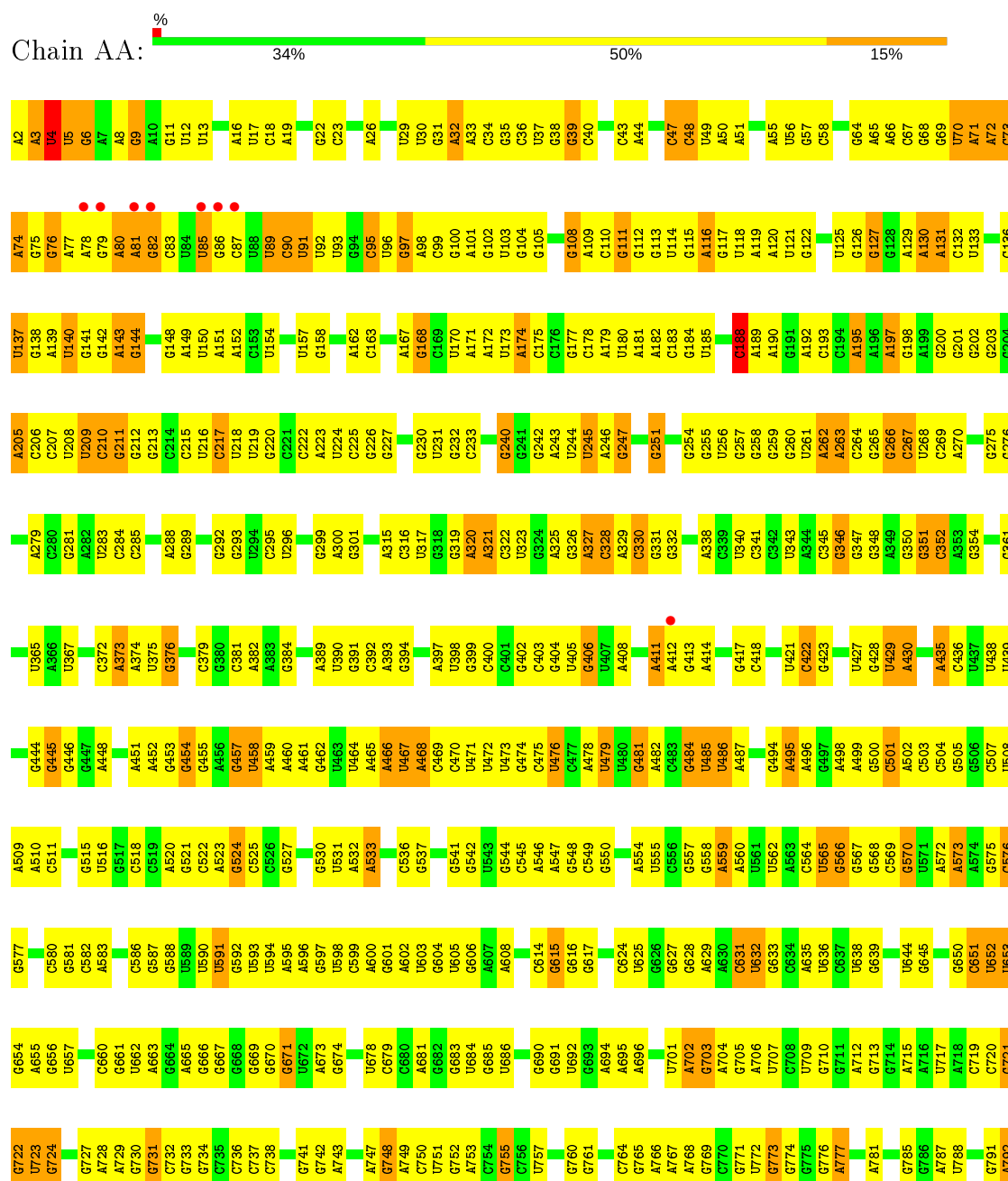
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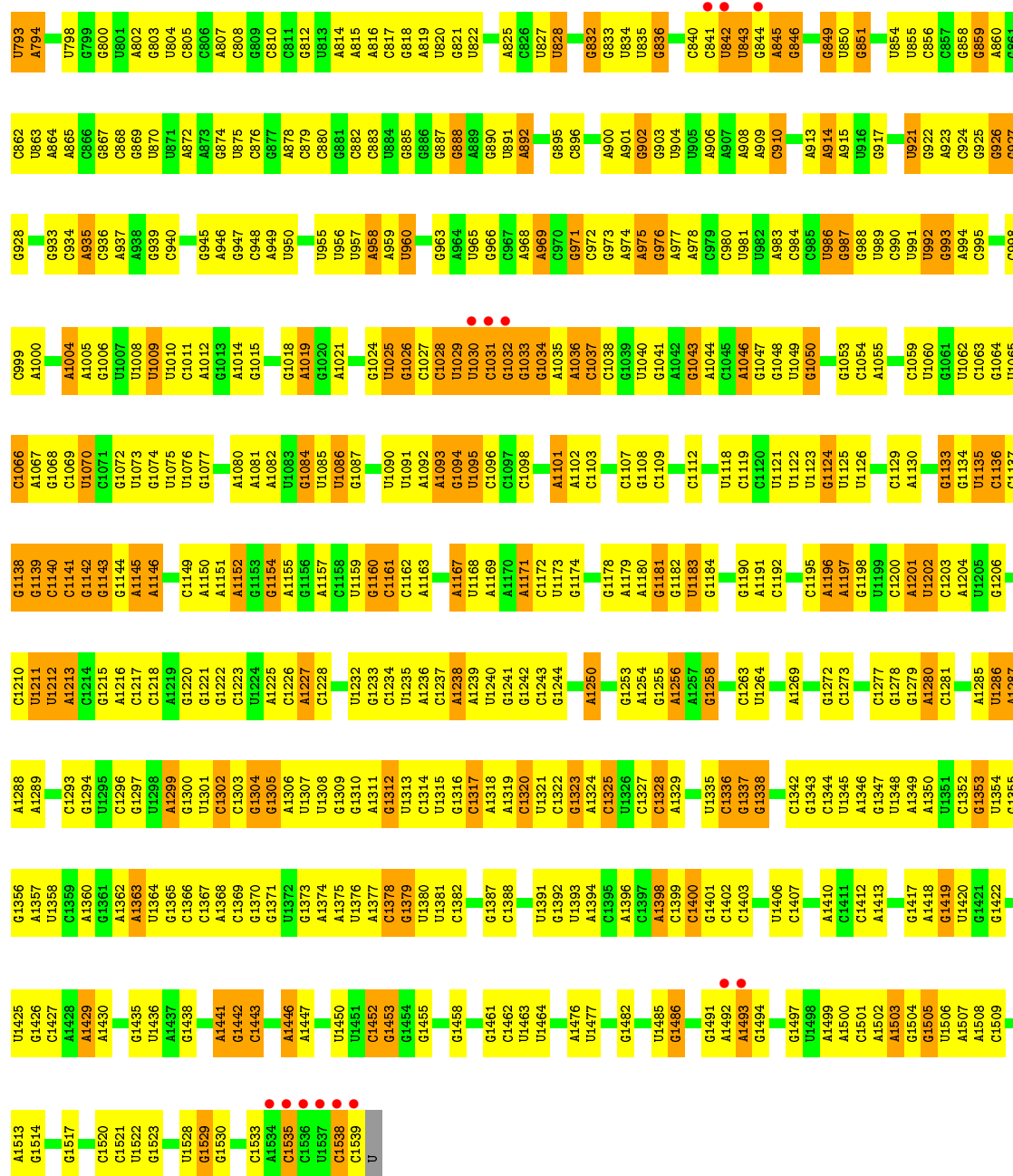
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DA	610	Total 610	O 610	0	0
58	DB	13	Total 13	O 13	0	0
58	DC	8	Total 8	O 8	0	0
58	DD	4	Total 4	O 4	0	0
58	DE	4	Total 4	O 4	0	0
58	DJ	1	Total 1	O 1	0	0
58	DL	4	Total 4	O 4	0	0
58	DN	2	Total 2	O 2	0	0
58	DS	2	Total 2	O 2	0	0
58	DT	3	Total 3	O 3	0	0
58	DU	1	Total 1	O 1	0	0
58	DV	1	Total 1	O 1	0	0
58	D2	1	Total 1	O 1	0	0
58	D3	1	Total 1	O 1	0	0
58	D4	1	Total 1	O 1	0	0

3 Residue-property plots

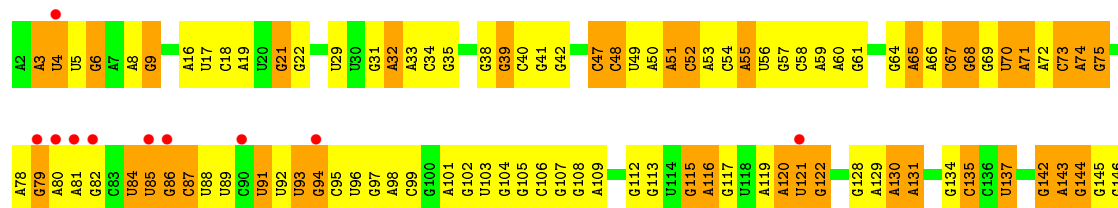
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S rRNA

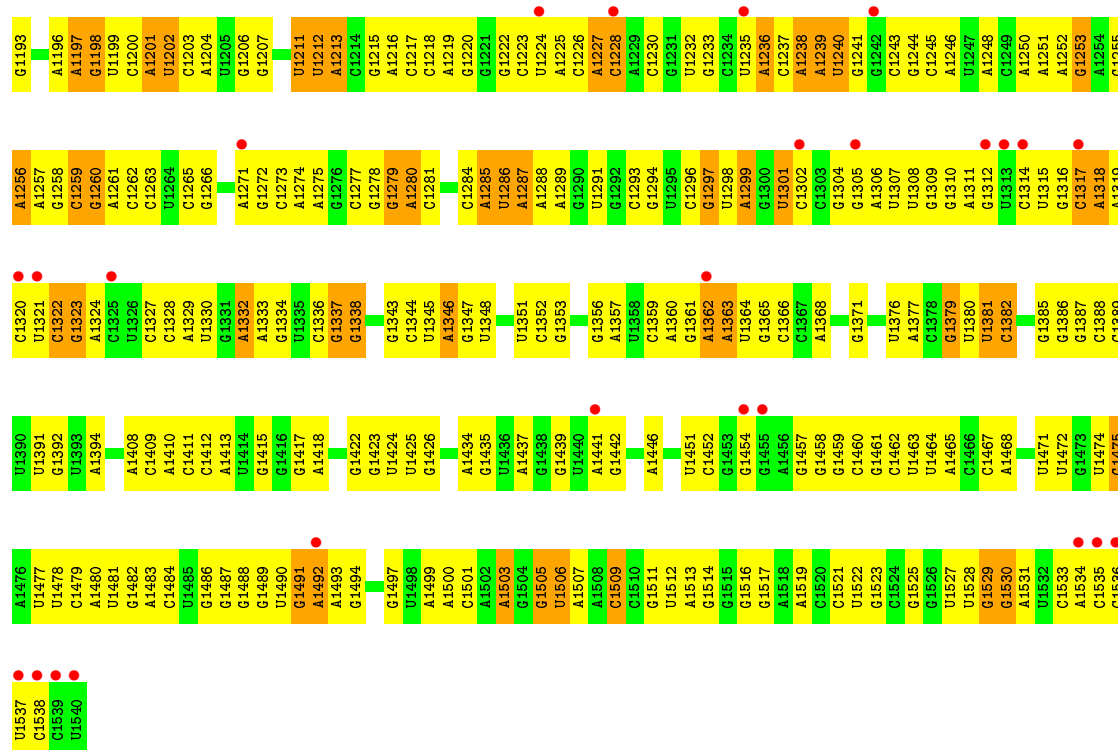




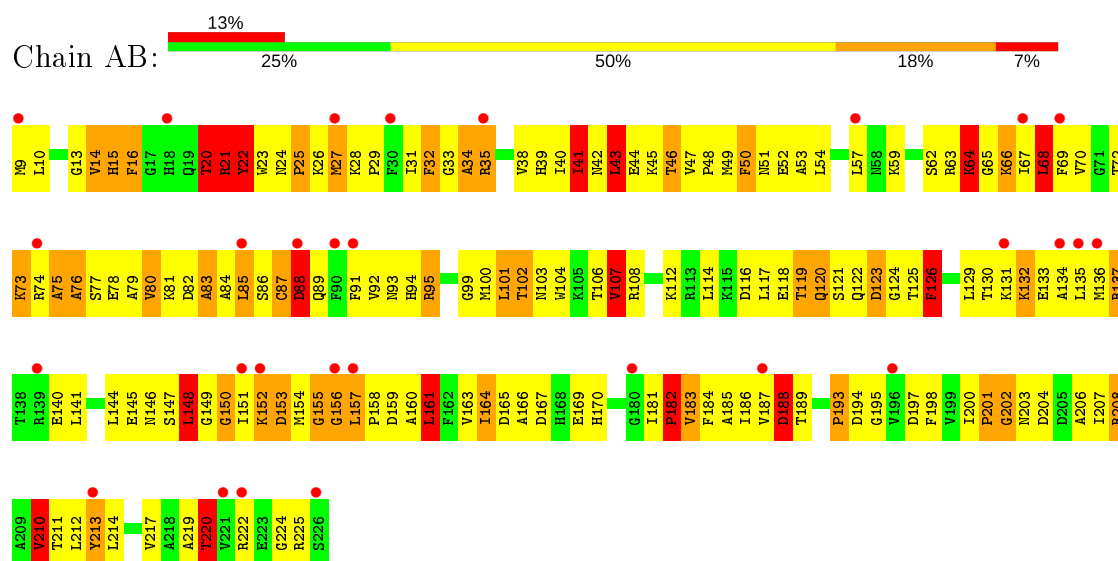
• Molecule 1: 16S rRNA



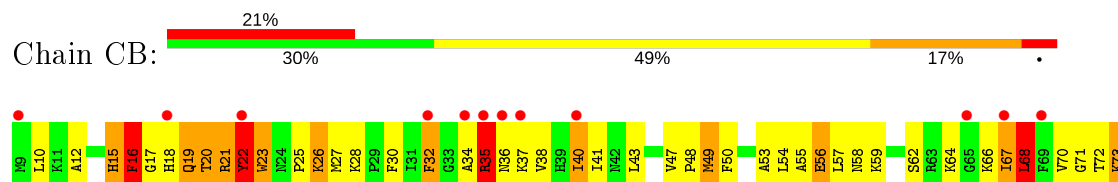


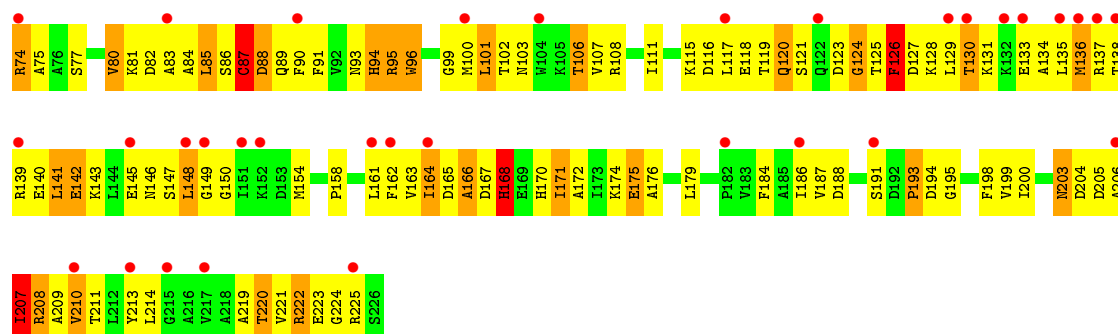


• Molecule 2: 30S ribosomal protein S2

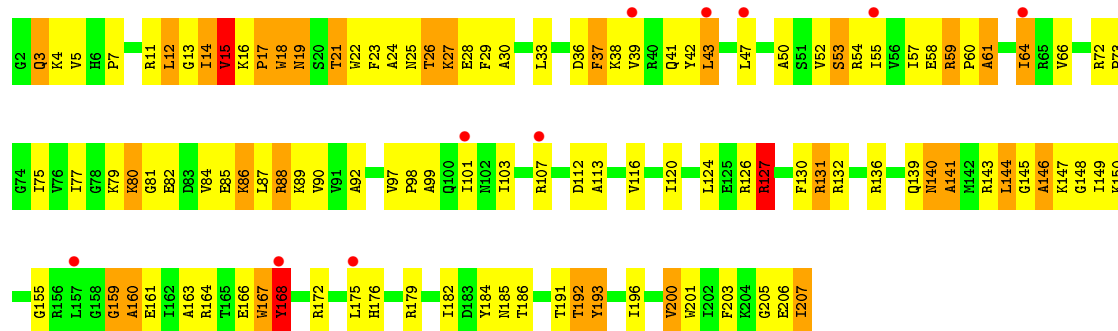


• Molecule 2: 30S ribosomal protein S2

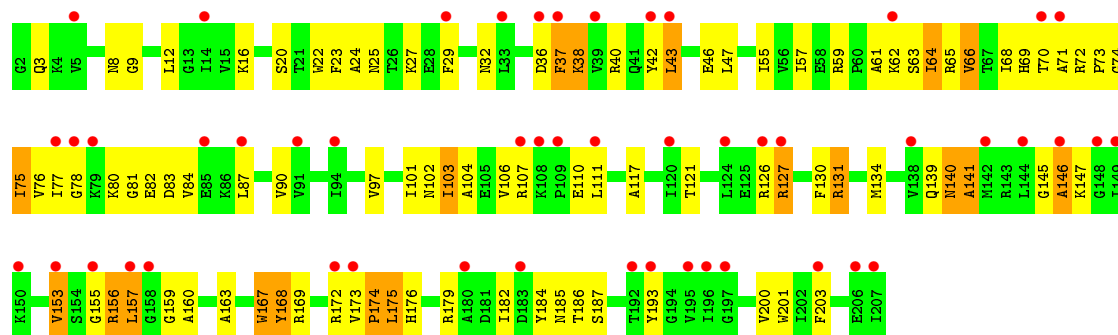




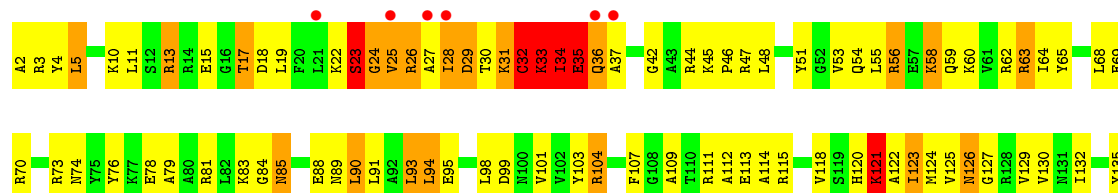
• Molecule 3: 30S ribosomal protein S3

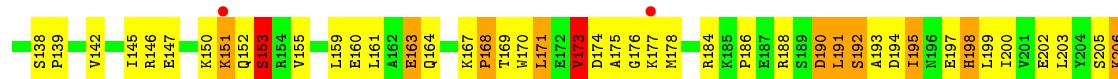


• Molecule 3: 30S ribosomal protein S3

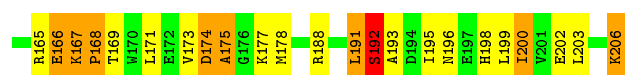
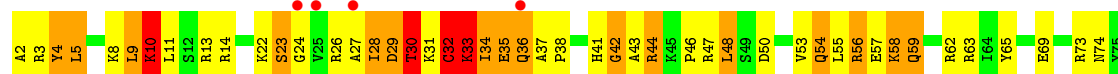
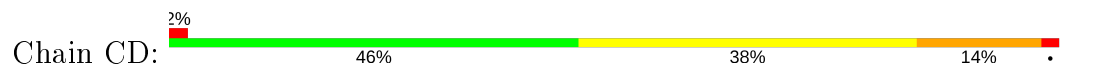


• Molecule 4: 30S ribosomal protein S4

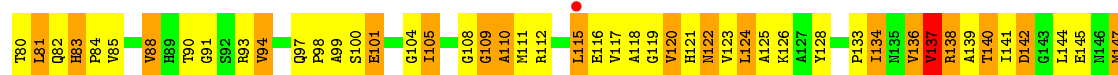
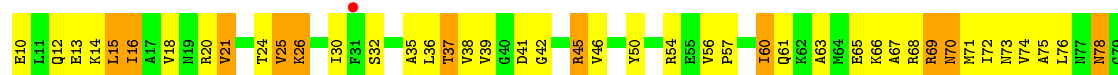




• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

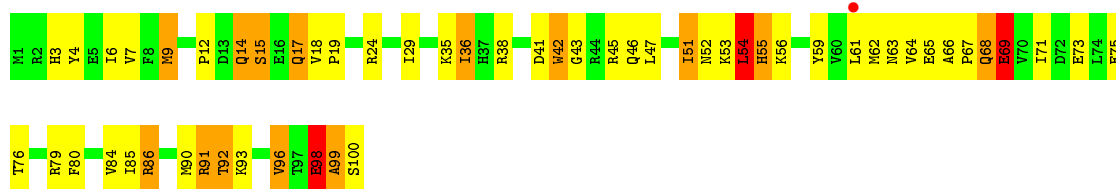


• Molecule 5: 30S ribosomal protein S5

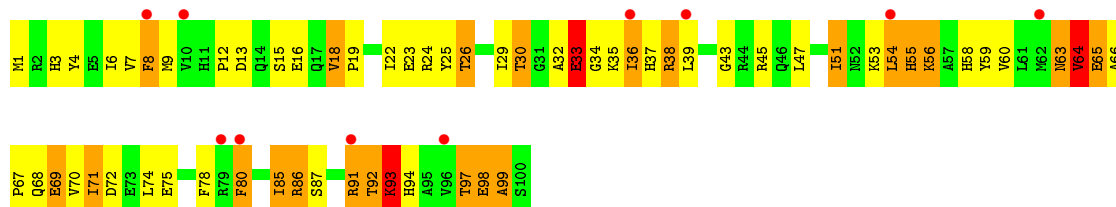


• Molecule 6: 30S ribosomal protein S6

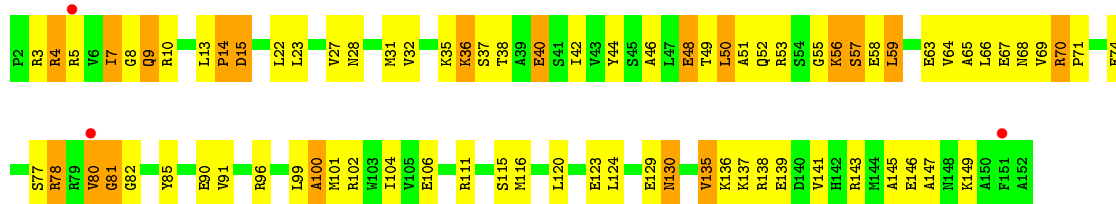




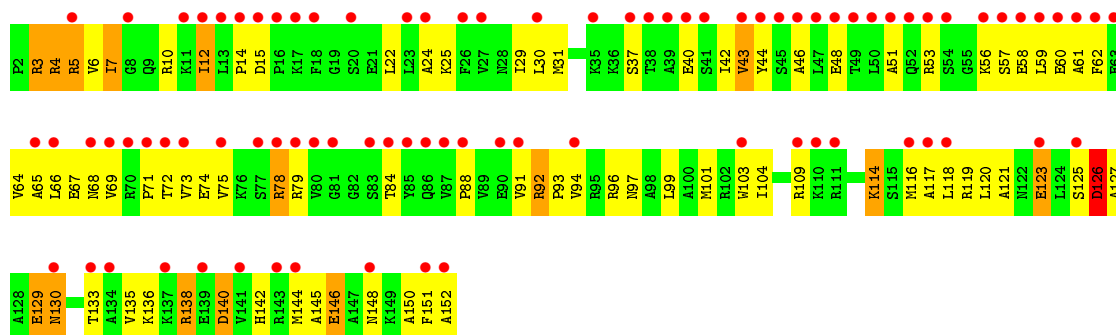
• Molecule 6: 30S ribosomal protein S6



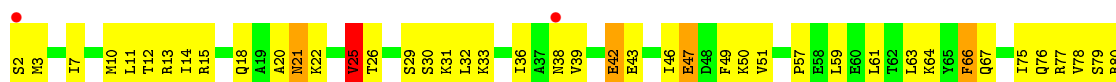
• Molecule 7: 30S ribosomal protein S7

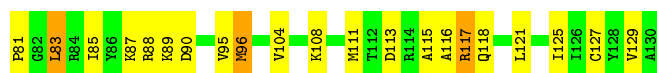


• Molecule 7: 30S ribosomal protein S7

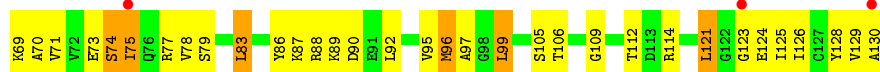
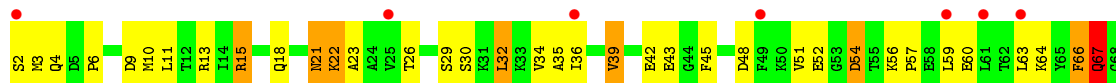


• Molecule 8: 30S ribosomal protein S8

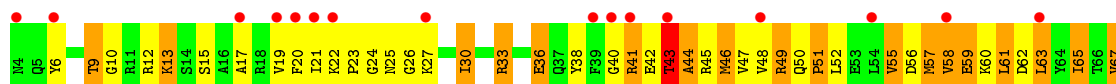




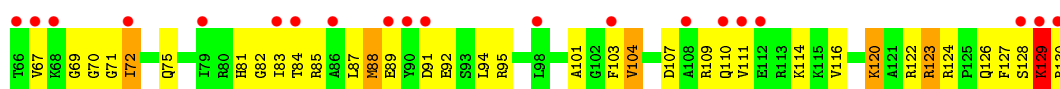
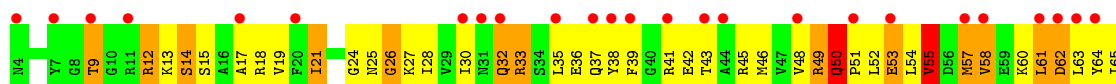
• Molecule 8: 30S ribosomal protein S8



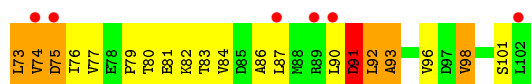
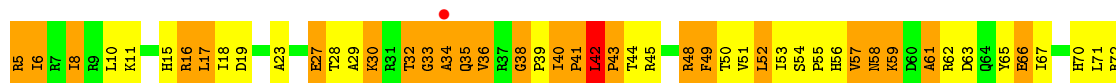
• Molecule 9: 30S ribosomal protein S9



• Molecule 9: 30S ribosomal protein S9

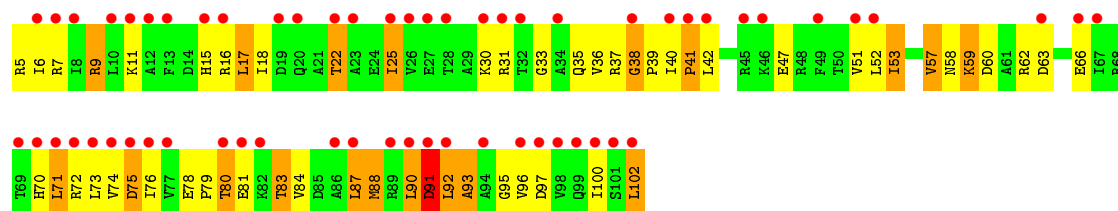


• Molecule 10: 30S ribosomal protein S10

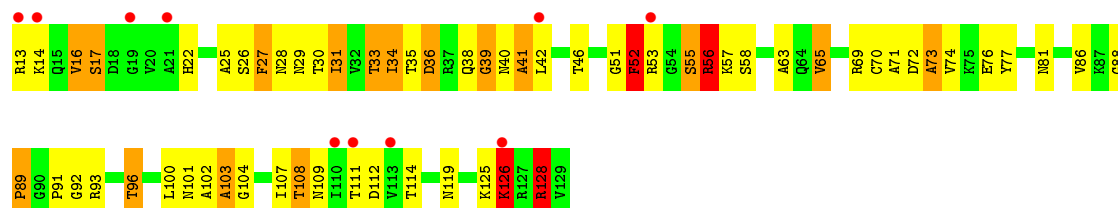


• Molecule 10: 30S ribosomal protein S10

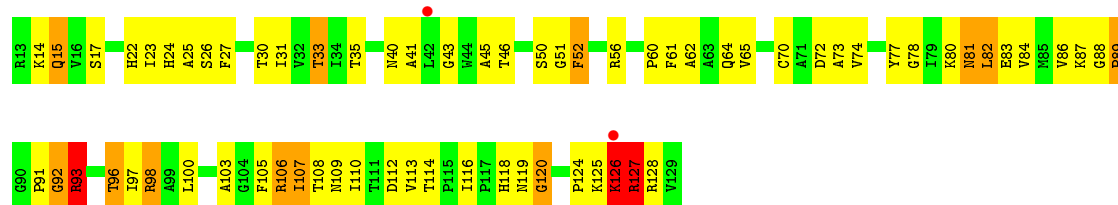
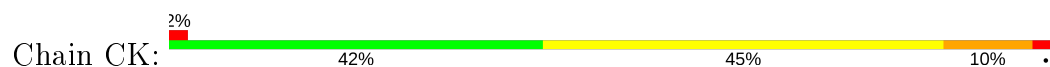




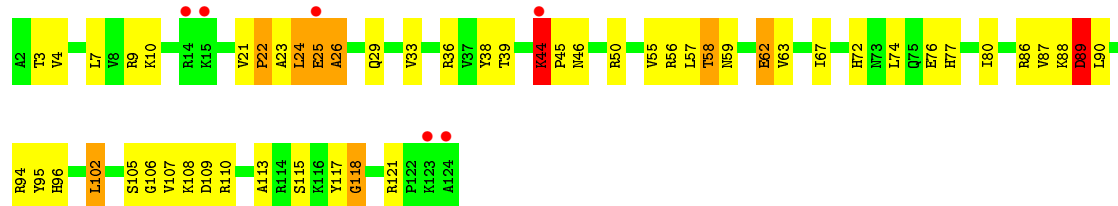
• Molecule 11: 30S ribosomal protein S11



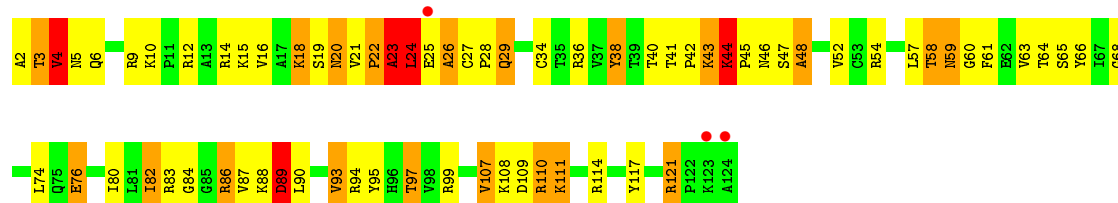
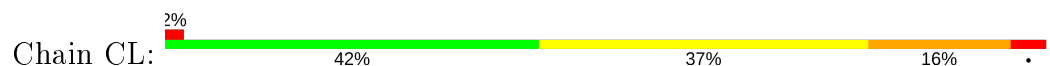
• Molecule 11: 30S ribosomal protein S11



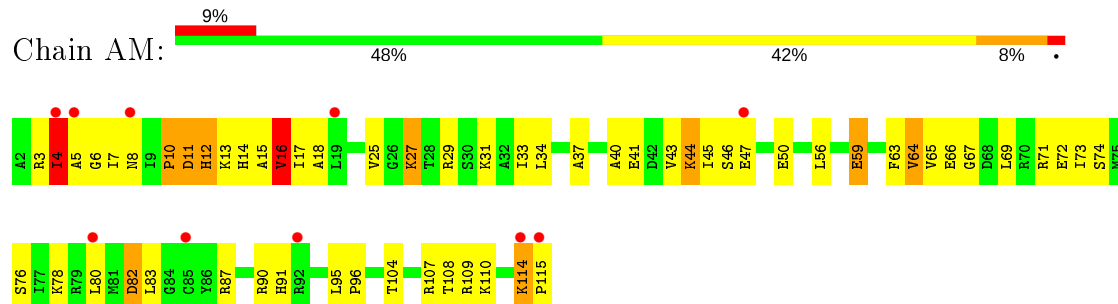
• Molecule 12: 30S ribosomal protein S12



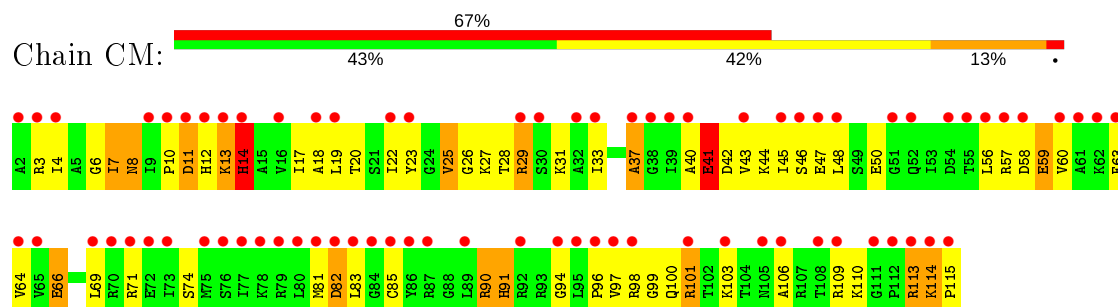
• Molecule 12: 30S ribosomal protein S12



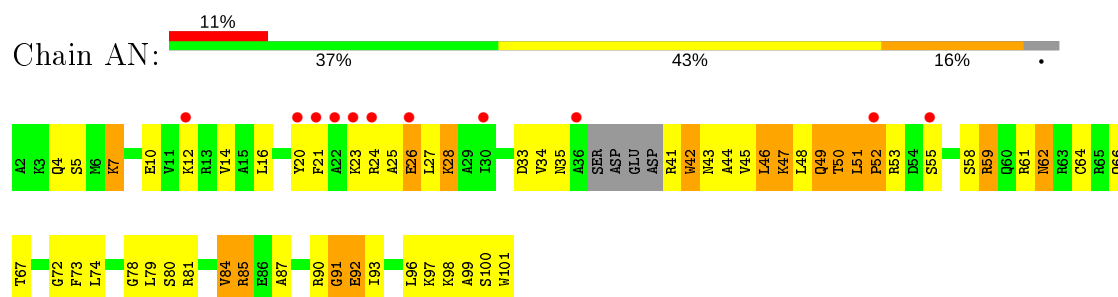
- Molecule 13: 30S ribosomal protein S13



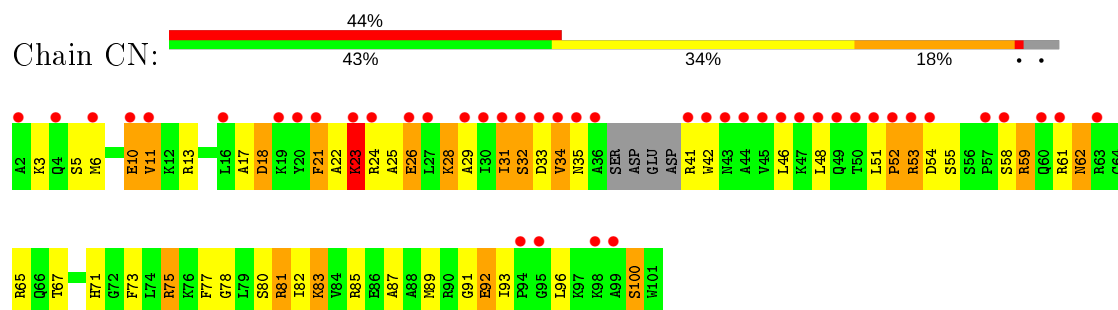
- Molecule 13: 30S ribosomal protein S13



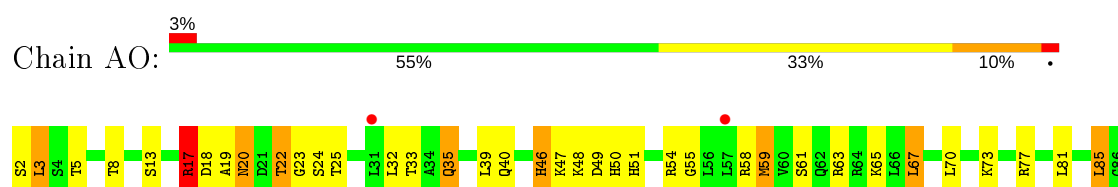
- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

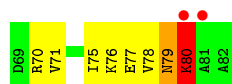
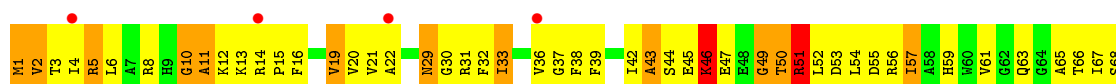




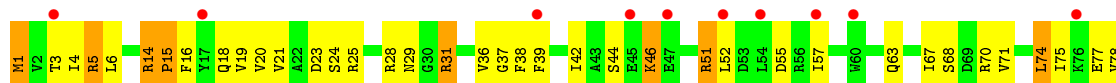
- Molecule 15: 30S ribosomal protein S15



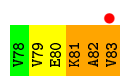
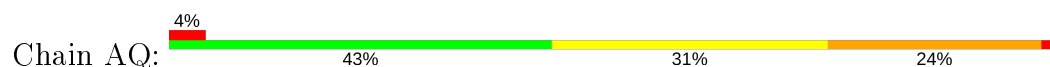
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17





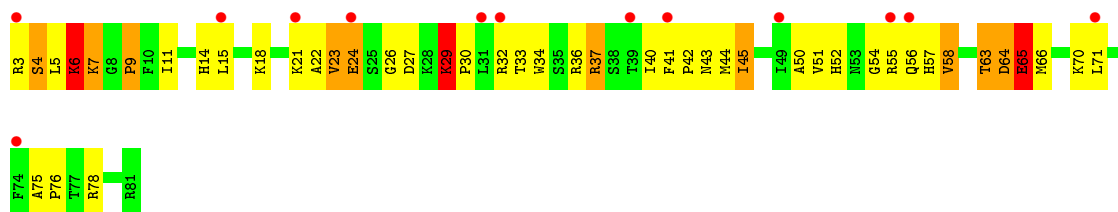
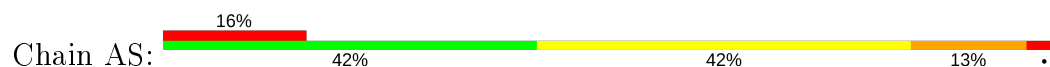
- Molecule 18: 30S ribosomal protein S18



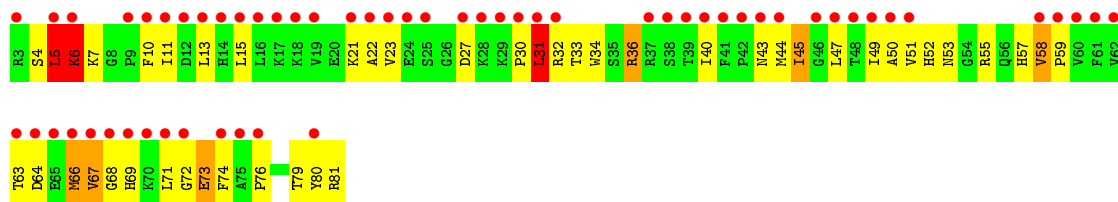
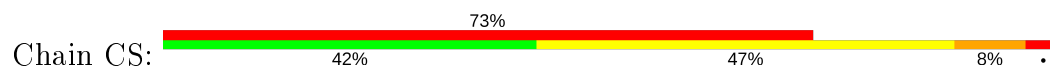
- Molecule 18: 30S ribosomal protein S18



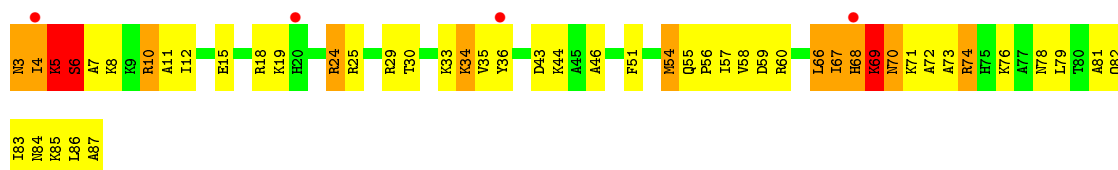
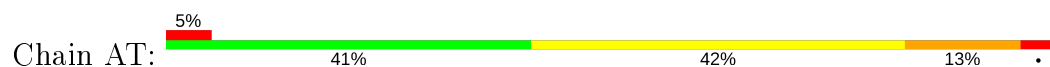
- Molecule 19: 30S ribosomal protein S19



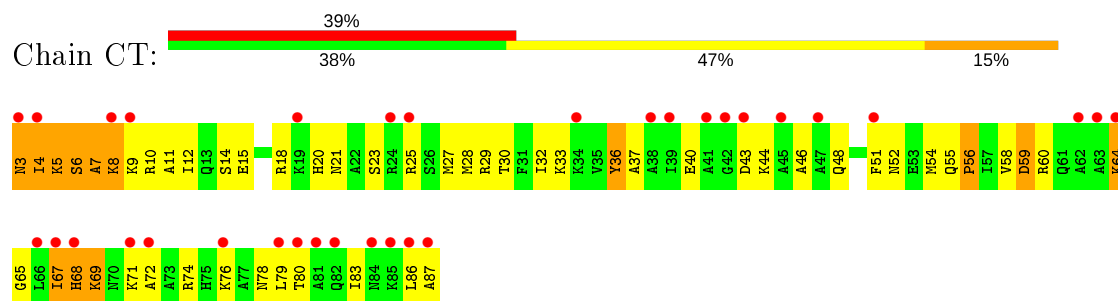
- Molecule 19: 30S ribosomal protein S19



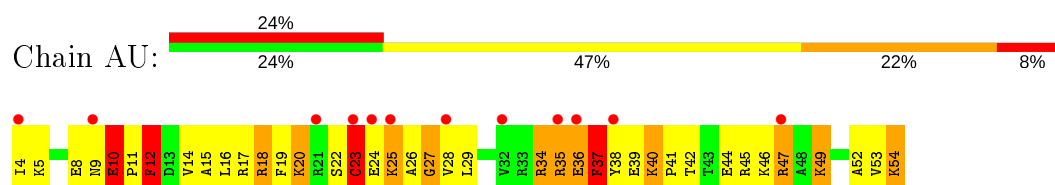
- Molecule 20: 30S ribosomal protein S20



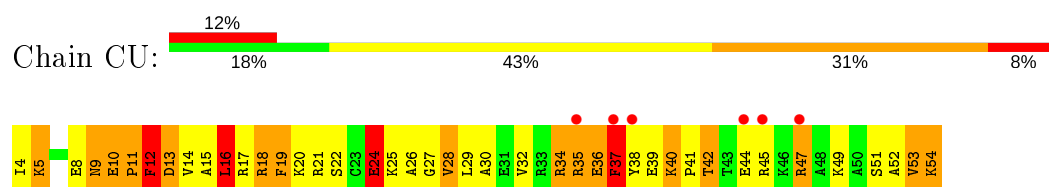
- Molecule 20: 30S ribosomal protein S20



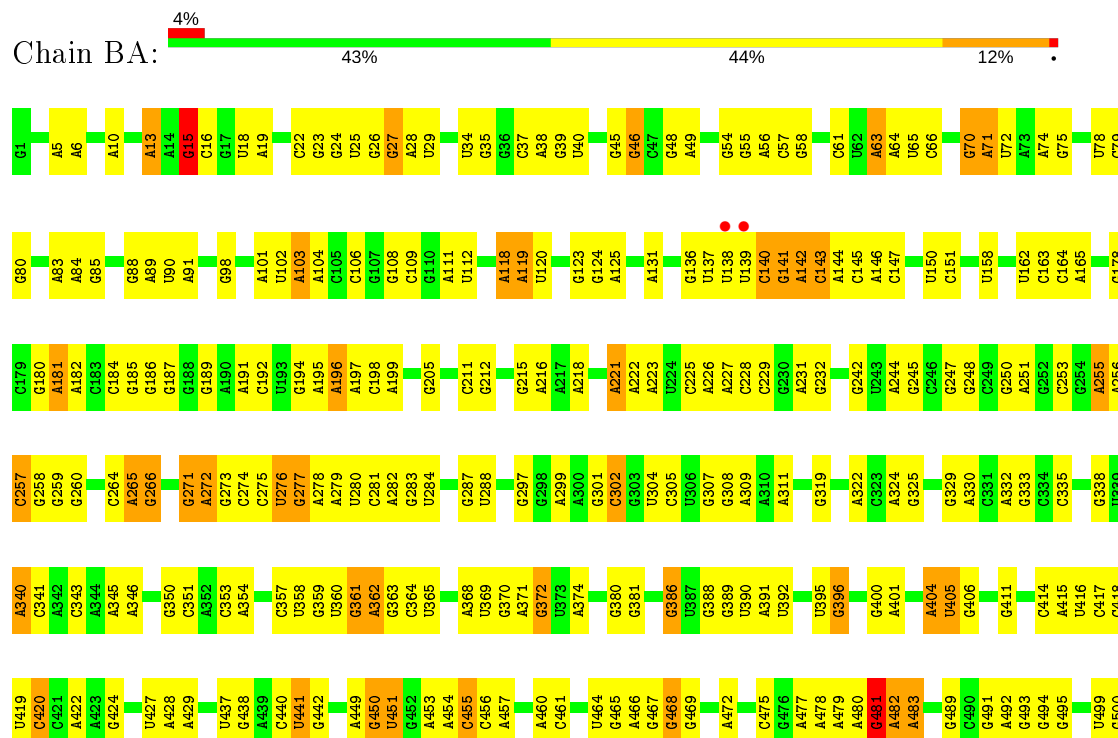
- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21

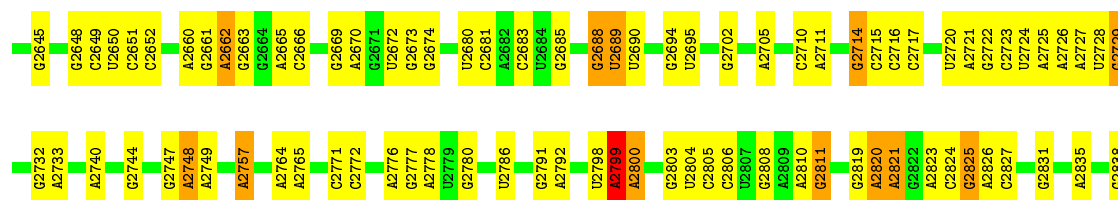


- Molecule 22: 23S rRNA

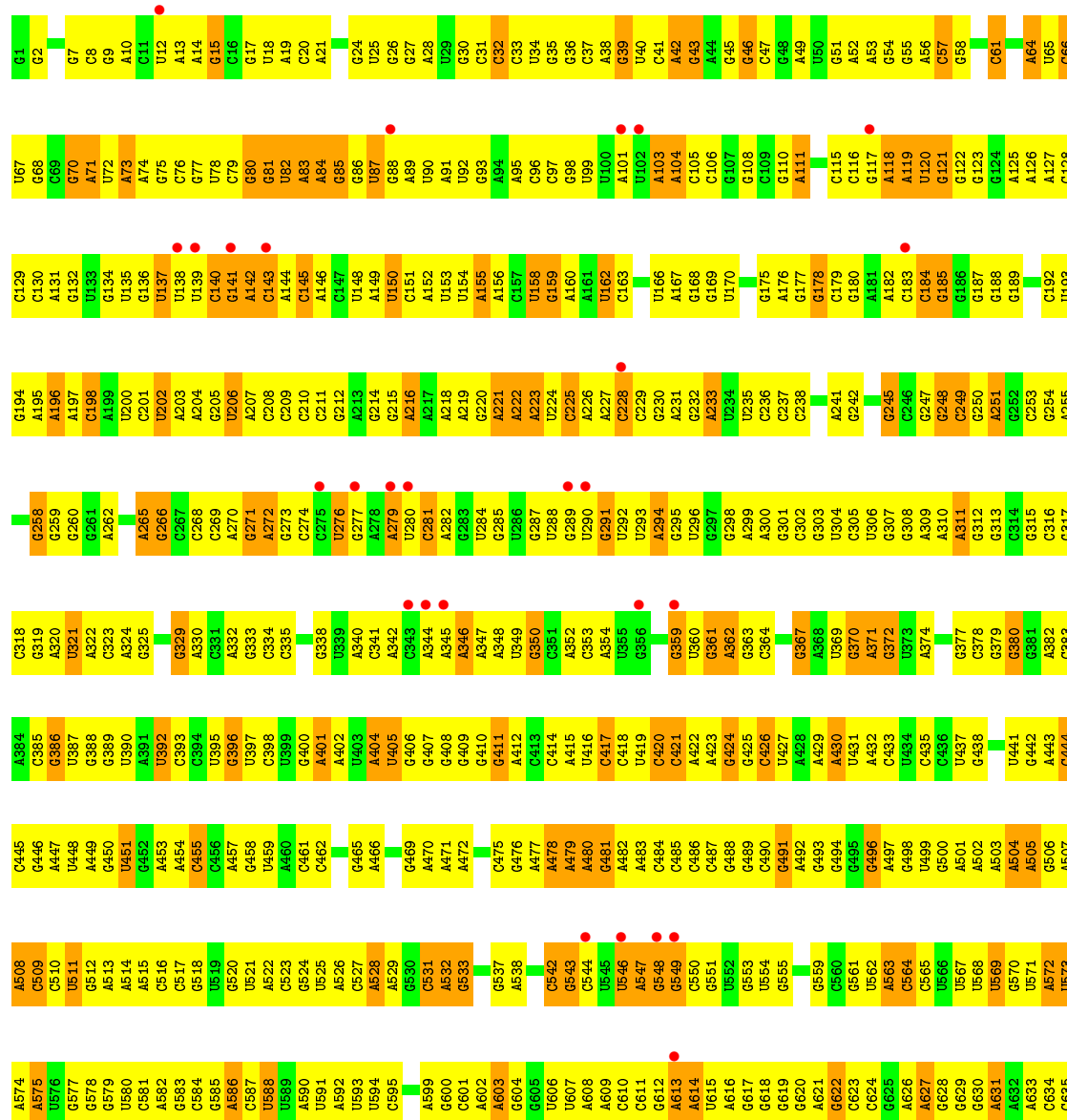


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G1501	A1432	G1356	A1276	G1187	A1103	U1033	C961	A	C812	C737	U653	A582	A502
A1502	A1433	C1357	G1277	U1188	C1104	U1033	C962	U	C813	C738	A654	C583	A503
A1503	A1434	G1358	A1189	A1189	U1105	U1035	U963	C	C814	A739	A655	C584	A504
A1504	G1435	A1359	G1283	G1190	A1039	A1039	U967	C	C815	C740	G656	C585	A505
C1507	G1436	G1360	A1284	G1191	A1040	A1040	U967	C	C816	U741	U657	A586	G506
A1508	C1437	A1285	A1285	A1194	C1045	C1045	C968	C	C817	A742	U658	C587	A507
A1509	U1438	A1365	A1286	A1195	A1046	A1046	C969	C	C818	A743	U658	A588	A508
A1510	A1439	A1366	A1287	G1195	A1046	U970	C971	C893	A819	U744	U659	C509	C509
G1510	U1440	A1367	G1288	C1196	G1112	G971	C971	C893	A819	U745	A590	C510	C510
G1511	G1441	C1289	C1289	U1199	G1120	A972	U894	U894	U894	U746	G664	U591	U511
C1512	U1442	G1371	U1294	U1199	G1120	A1050	A972	U895	U826	U747	U665	A592	G512
U1513	U1443	U1372	U1294	C1200	C1121	G1051	A973	A896	U827	C748	U666	A593	A513
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G1456	G1456	A1378	U1379	U1224	G1131	U1061	A981	A909	A833		C572	U598	C523
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	C1499	C1430	A1354	A1272	U1184	U1183	A1027	C959	C906		U646	U579	
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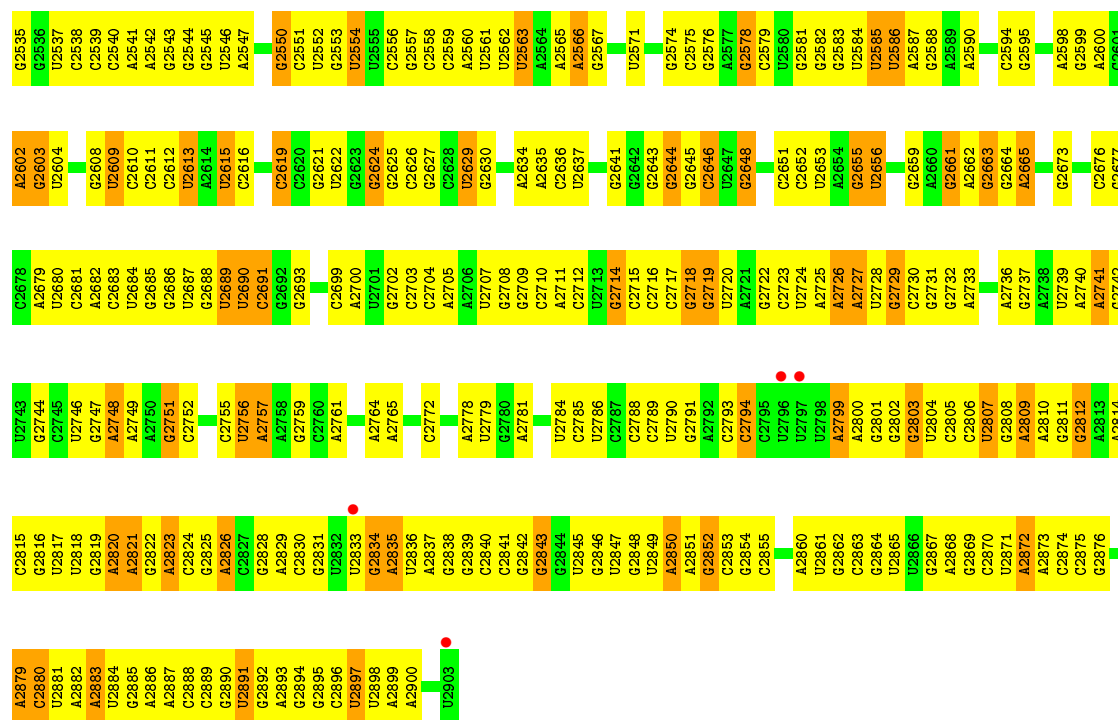


• Molecule 22: 23S rRNA



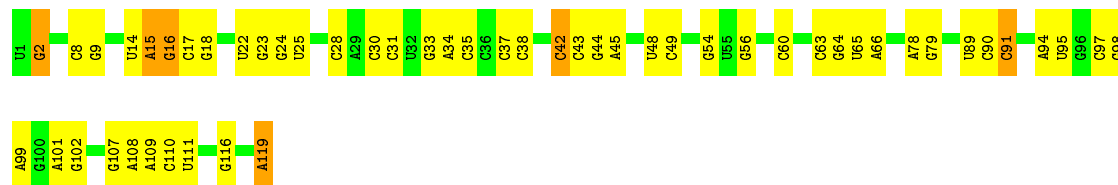


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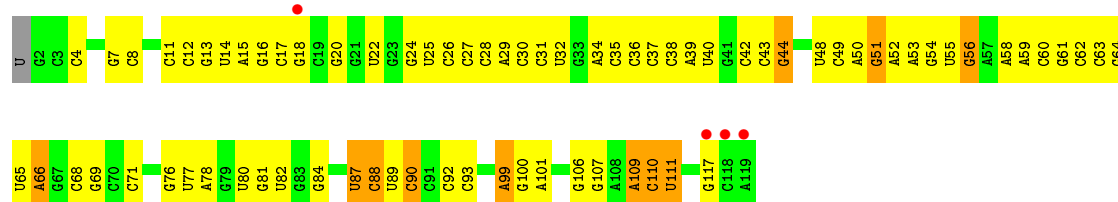
• Molecule 23: 5S rRNA

Chain BB: 56% 39% 5%



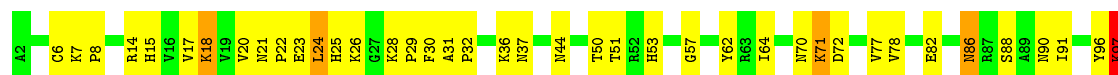
• Molecule 23: 5S rRNA

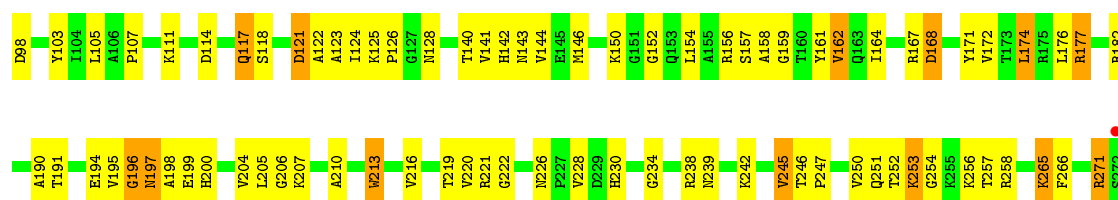
Chain DB: 3% 36% 54% 9%



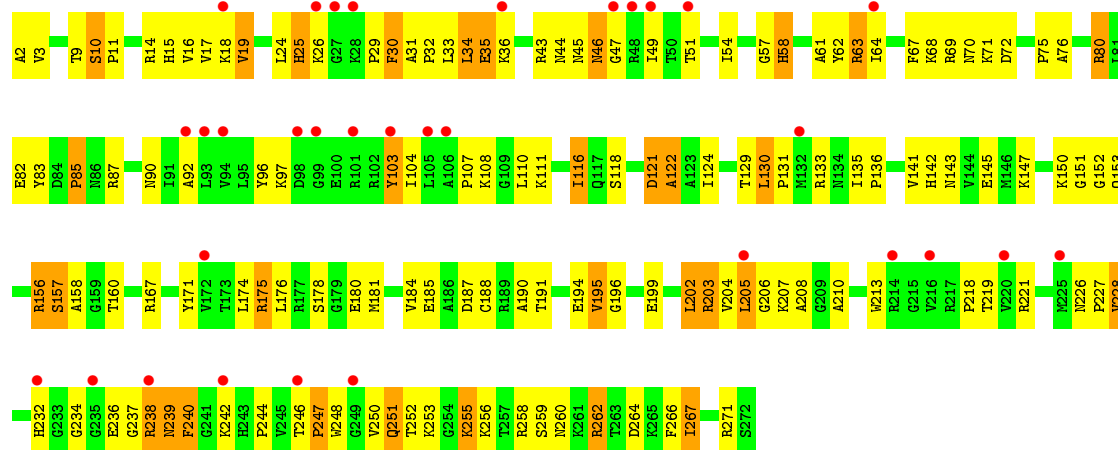
• Molecule 24: 50S ribosomal protein L2

Chain BC: 56% 38% 6%

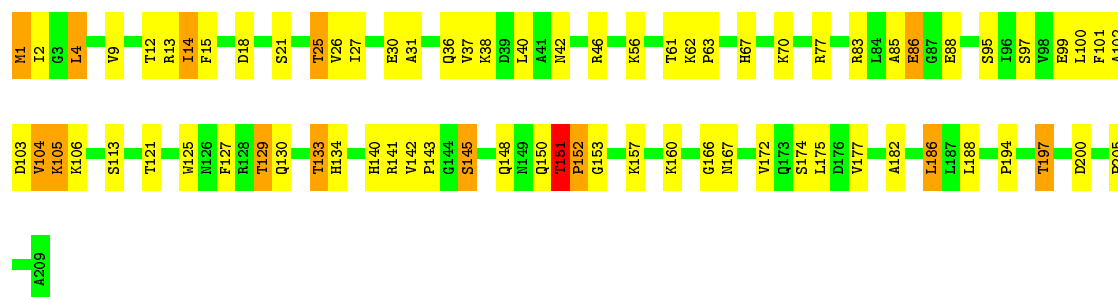




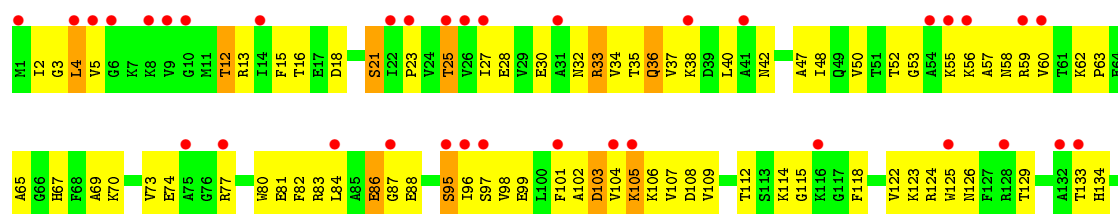
• Molecule 24: 50S ribosomal protein L2

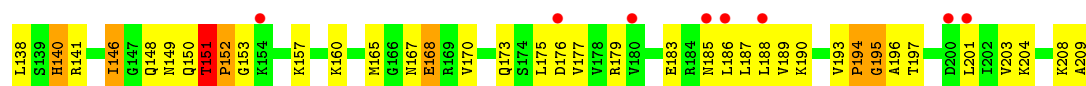


• Molecule 25: 50S ribosomal protein L3



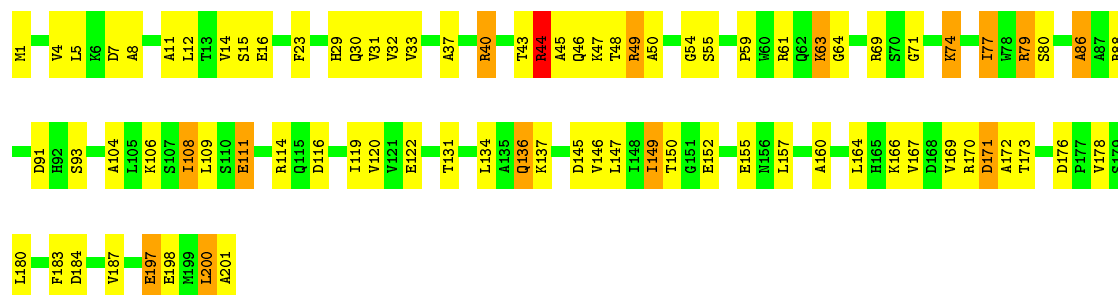
• Molecule 25: 50S ribosomal protein L3





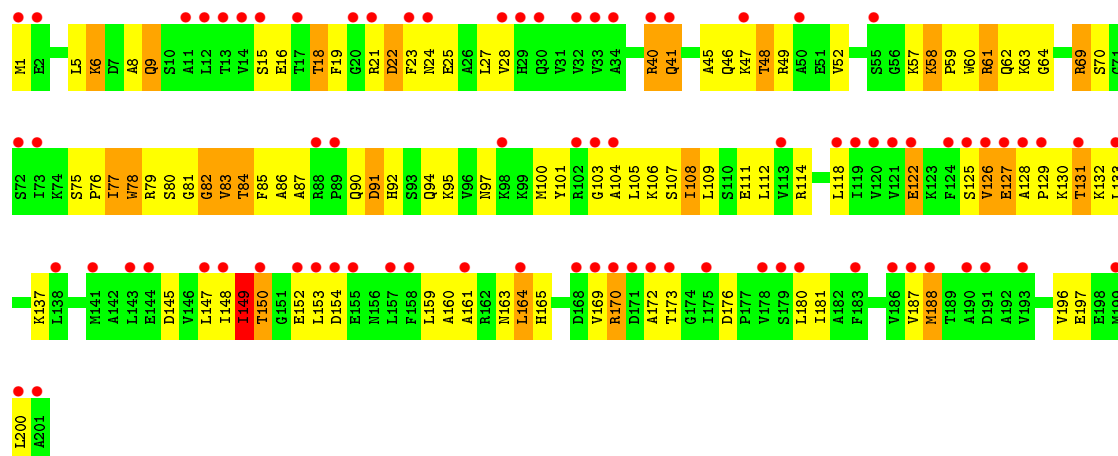
- Molecule 26: 50S ribosomal protein L4

Chain BE: 59% 34% 7%



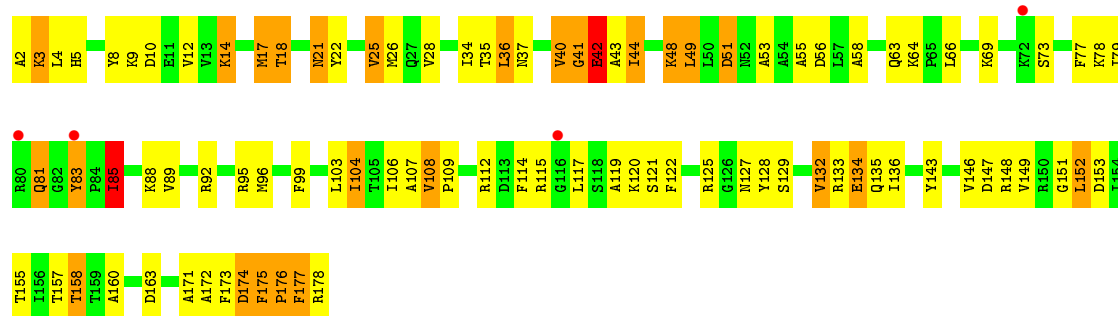
- Molecule 26: 50S ribosomal protein L4

Chain DE: 40% 49% 38% 12%

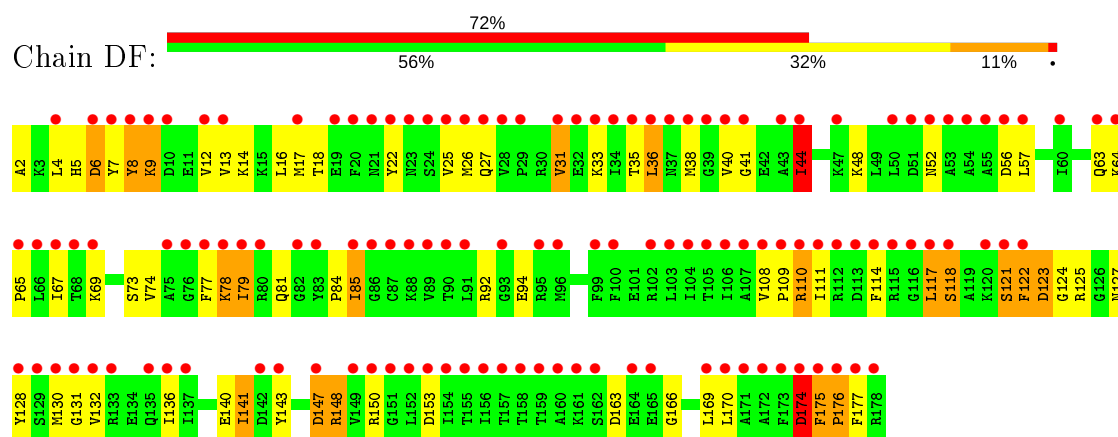


- Molecule 27: 50S ribosomal protein L5

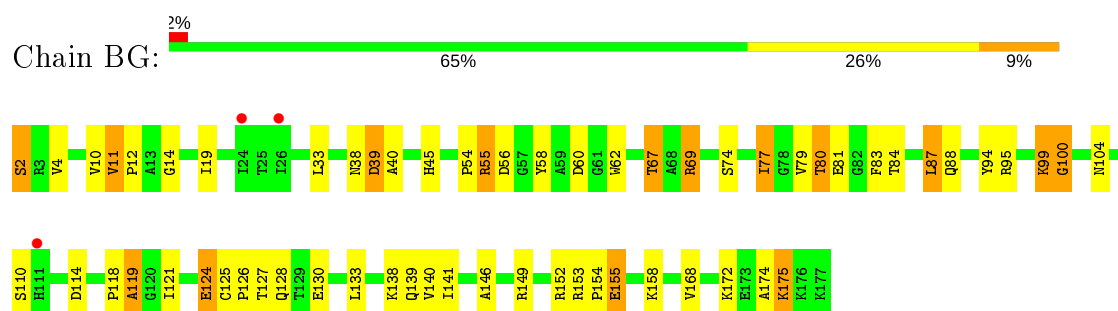
Chain BF: 2% 47% 37% 14%



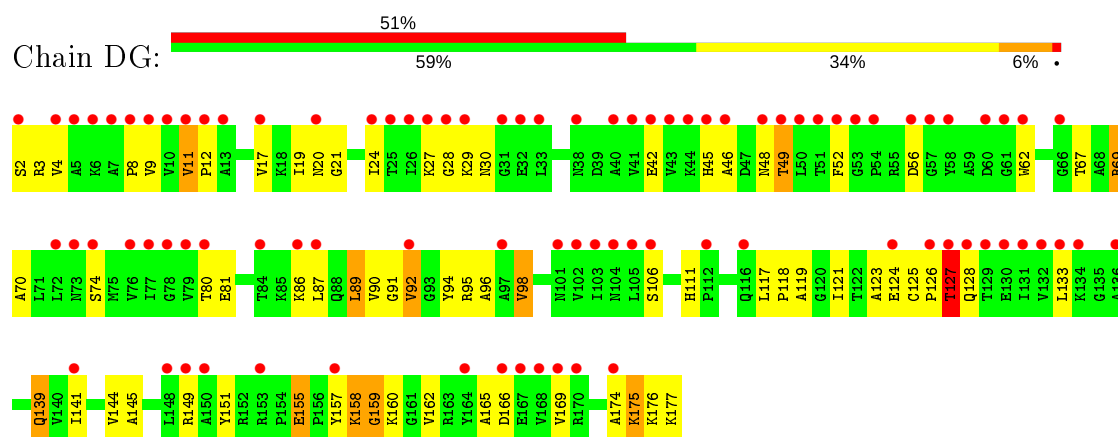
- Molecule 27: 50S ribosomal protein L5



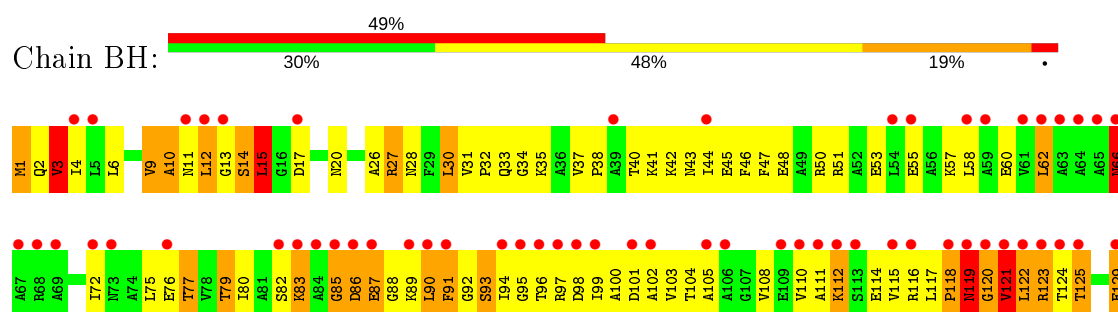
• Molecule 28: 50S ribosomal protein L6

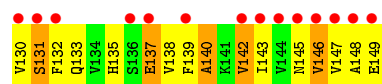


• Molecule 28: 50S ribosomal protein L6

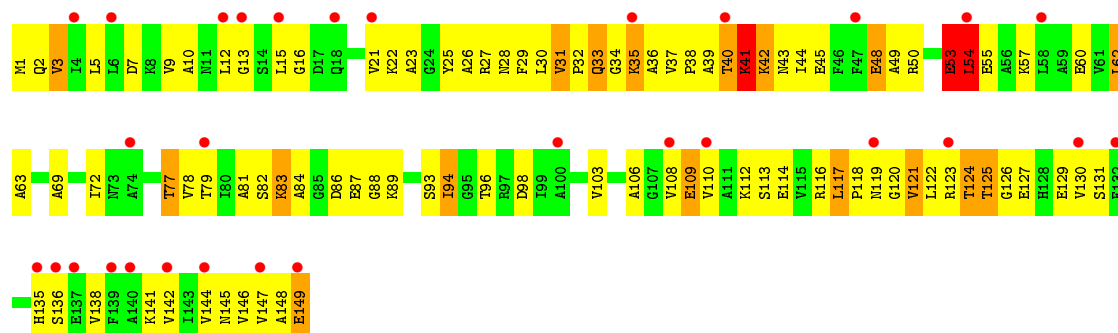


• Molecule 29: 50S ribosomal protein L9

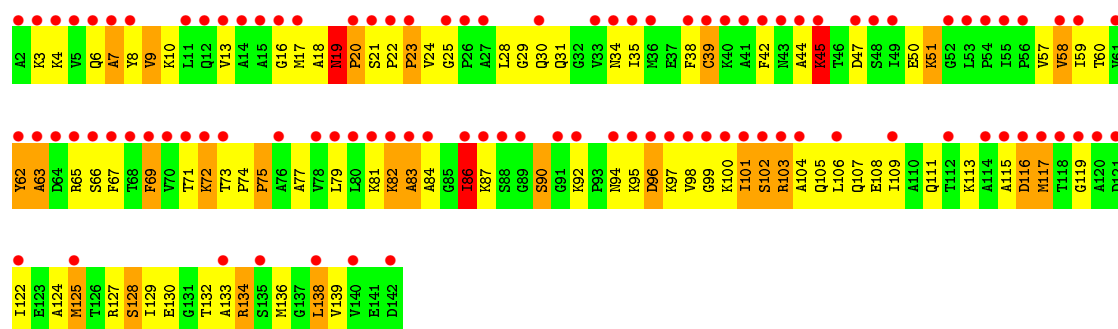




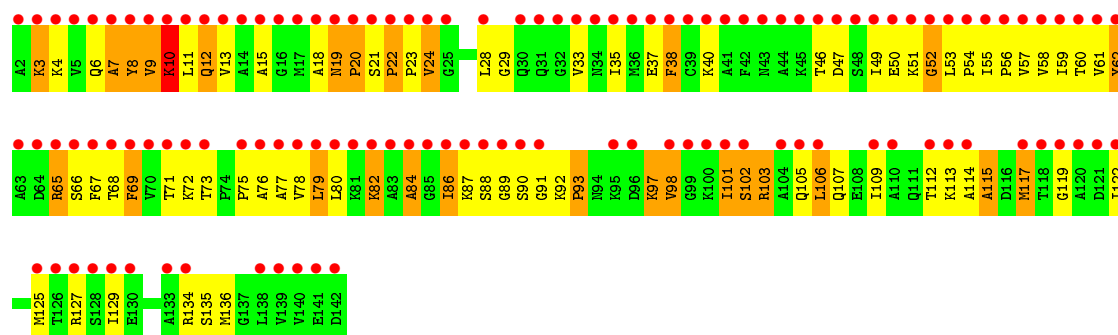
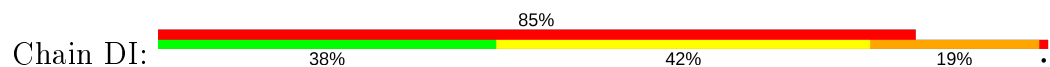
• Molecule 29: 50S ribosomal protein L9



• Molecule 30: 50S ribosomal protein L11

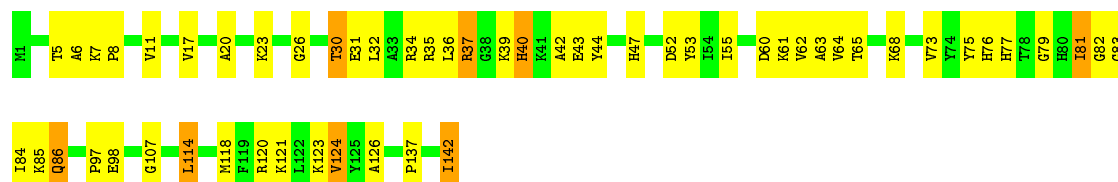


• Molecule 30: 50S ribosomal protein L11

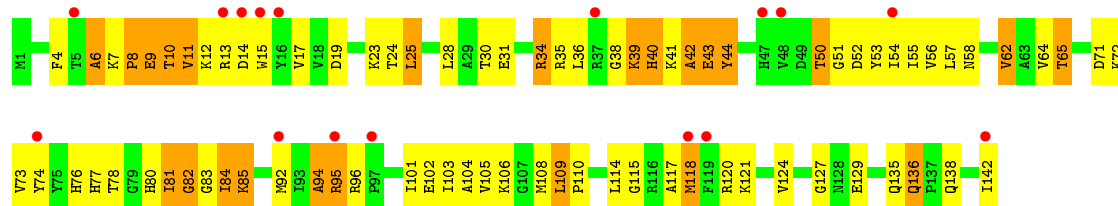


• Molecule 31: 50S ribosomal protein L13

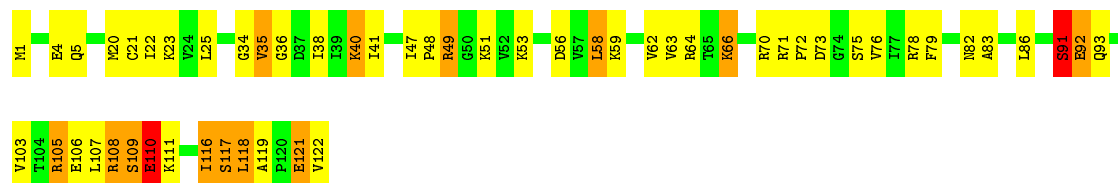




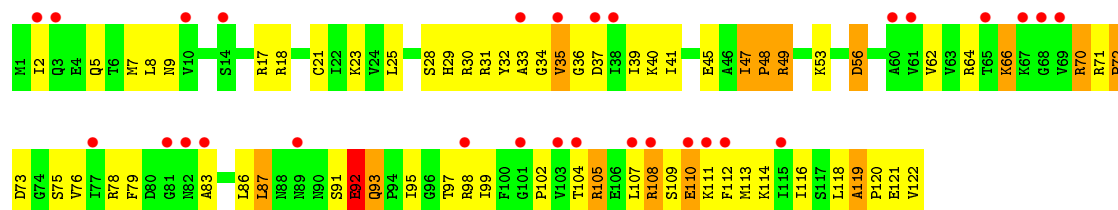
• Molecule 31: 50S ribosomal protein L13



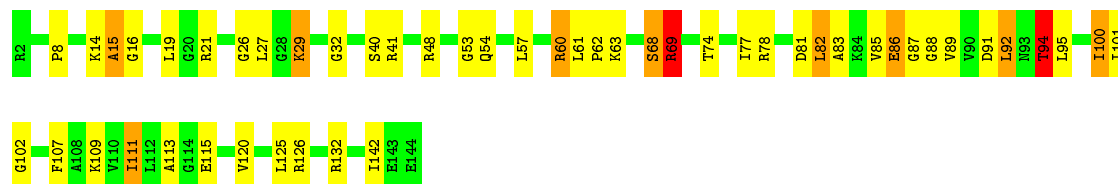
• Molecule 32: 50S ribosomal protein L14



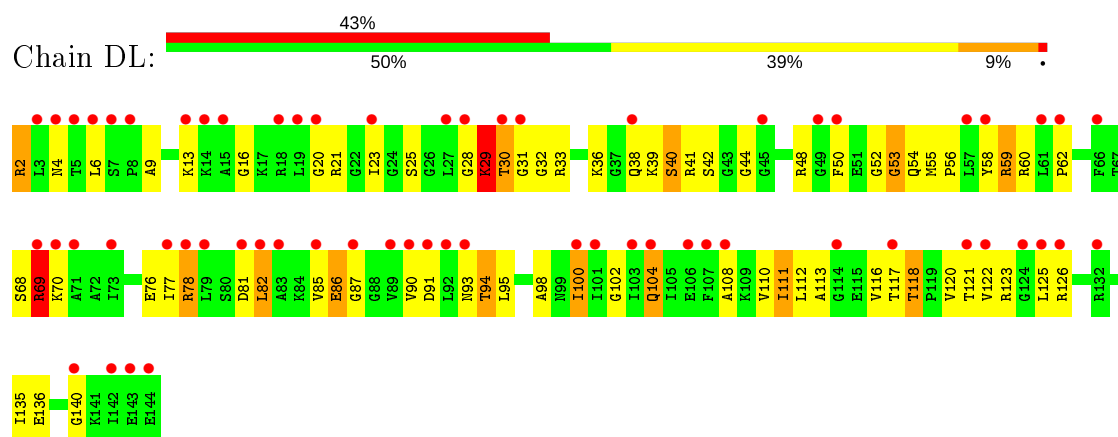
• Molecule 32: 50S ribosomal protein L14



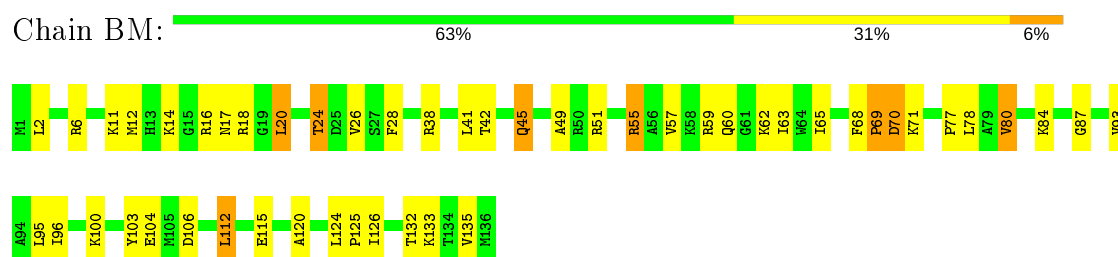
• Molecule 33: 50S ribosomal protein L15



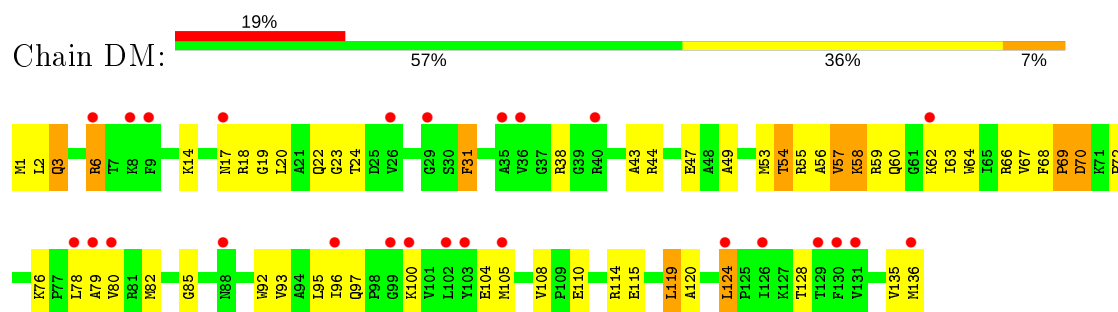
• Molecule 33: 50S ribosomal protein L15



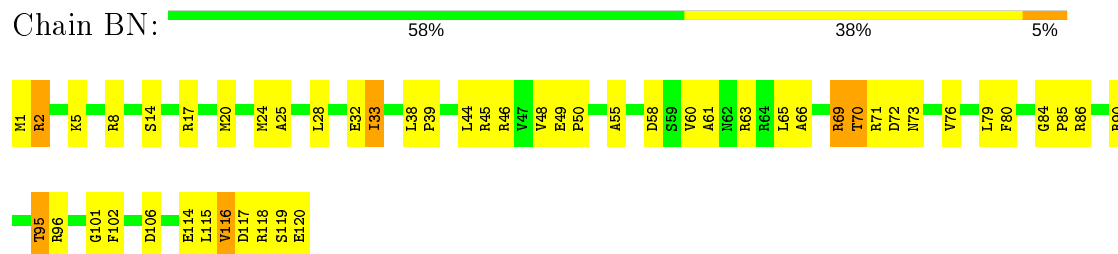
- Molecule 34: 50S ribosomal protein L16



- Molecule 34: 50S ribosomal protein L16



- Molecule 35: 50S ribosomal protein L17

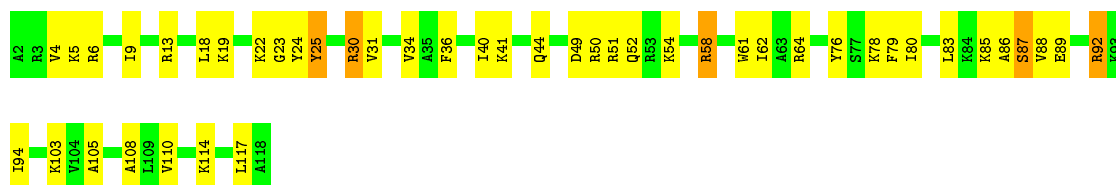


- Molecule 35: 50S ribosomal protein L17



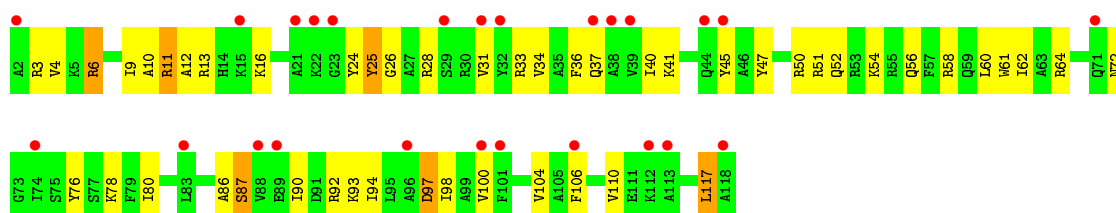
- Molecule 38: 50S ribosomal protein L20

Chain BQ: 



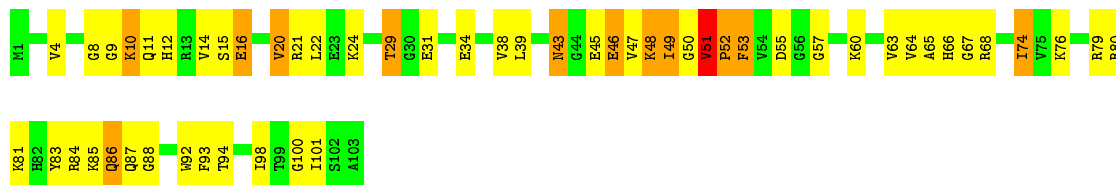
- Molecule 38: 50S ribosomal protein L20

Chain DQ: 



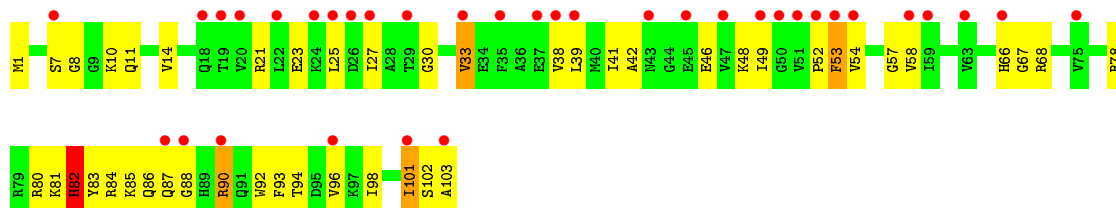
- Molecule 39: 50S ribosomal protein L21

Chain BR: 



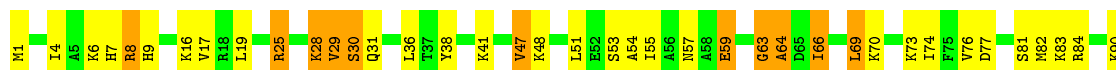
- Molecule 39: 50S ribosomal protein L21

Chain DR: 



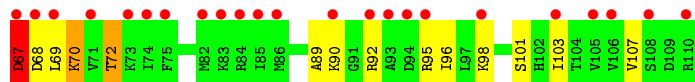
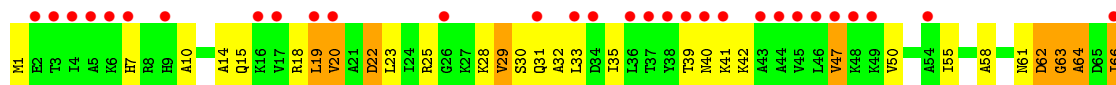
- Molecule 40: 50S ribosomal protein L22

Chain BS: 

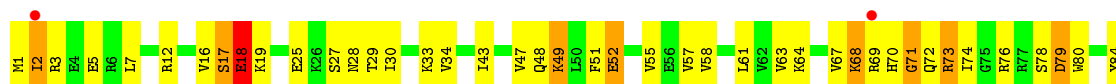




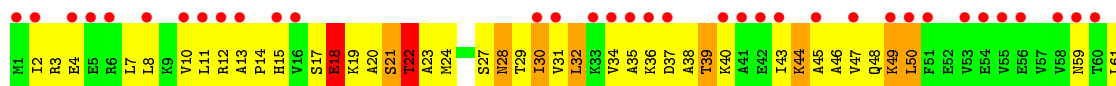
- Molecule 40: 50S ribosomal protein L22



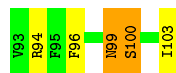
- Molecule 41: 50S ribosomal protein L23



- Molecule 41: 50S ribosomal protein L23

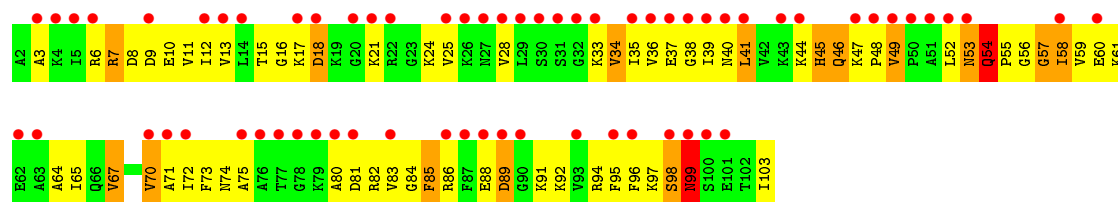


- Molecule 42: 50S ribosomal protein L24



- Molecule 42: 50S ribosomal protein L24

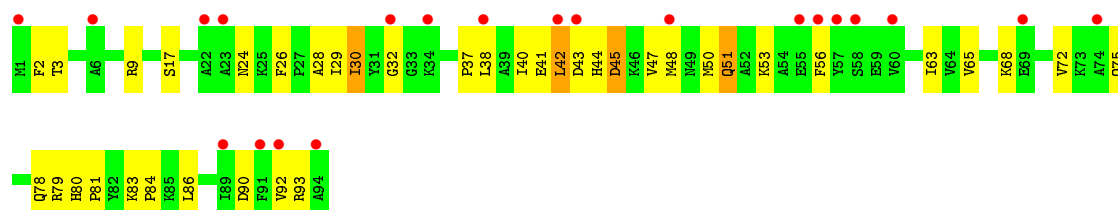




• Molecule 43: 50S ribosomal protein L25



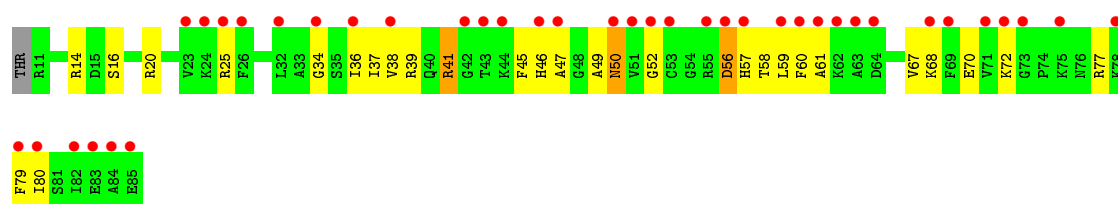
• Molecule 43: 50S ribosomal protein L25



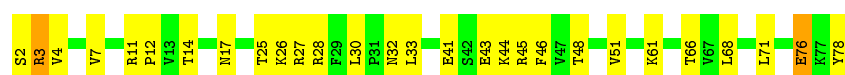
• Molecule 44: 50S ribosomal protein L27



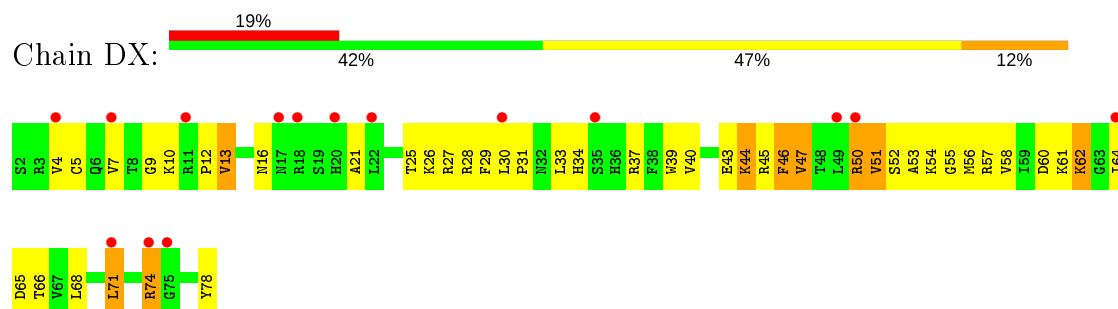
• Molecule 44: 50S ribosomal protein L27



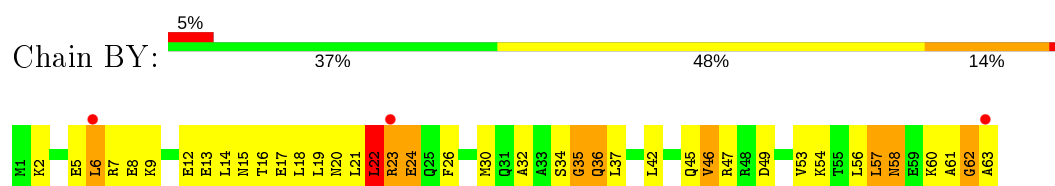
• Molecule 45: 50S ribosomal protein L28



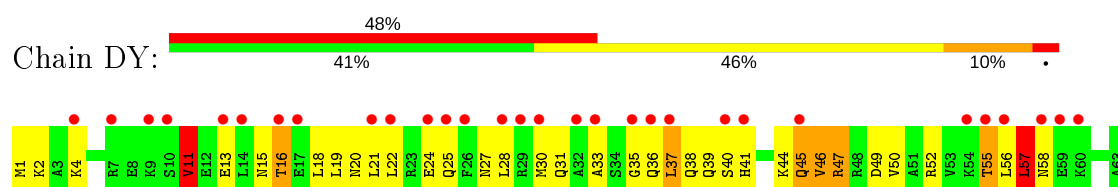
- Molecule 45: 50S ribosomal protein L28



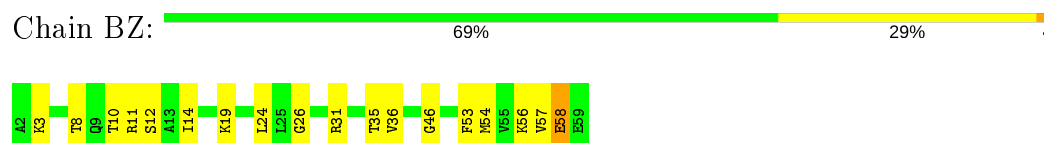
- Molecule 46: 50S ribosomal protein L29



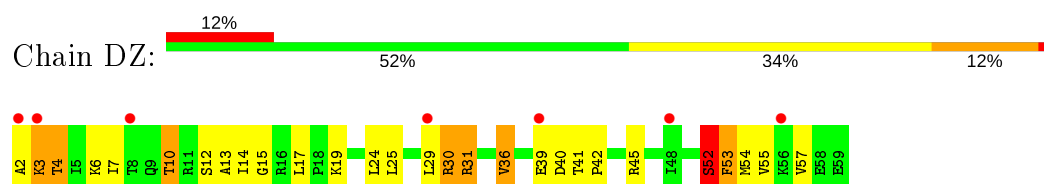
- Molecule 46: 50S ribosomal protein L29



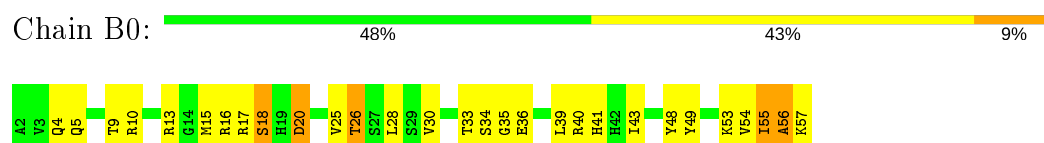
- Molecule 47: 50S ribosomal protein L30



- Molecule 47: 50S ribosomal protein L30



- Molecule 48: 50S ribosomal protein L32



- Molecule 48: 50S ribosomal protein L32

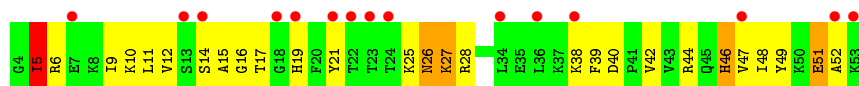




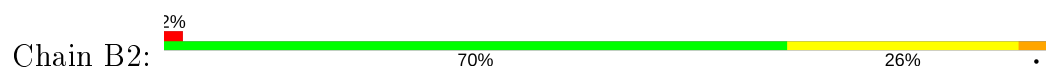
- Molecule 49: 50S ribosomal protein L33



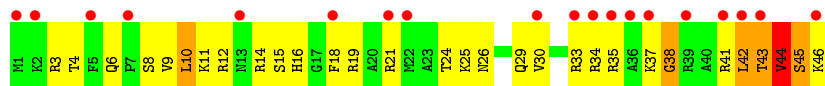
- Molecule 49: 50S ribosomal protein L33



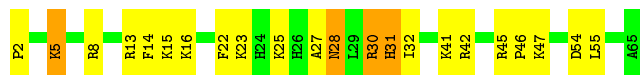
- Molecule 50: 50S ribosomal protein L34



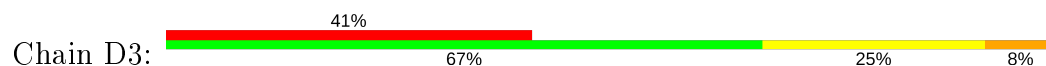
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L35



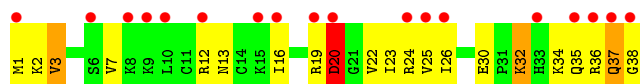
- Molecule 52: 50S ribosomal protein L36

Chain B4:  74% 24% .

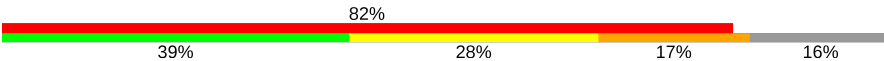


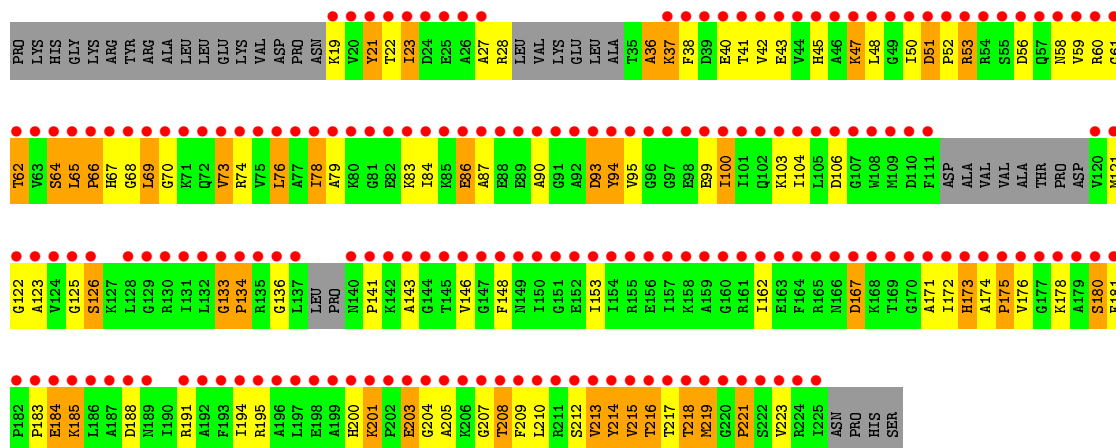
- Molecule 52: 50S ribosomal protein L36

Chain D4:  47% 45% 8% .



- Molecule 53: 50S ribosomal protein L1

Chain B5:  39% 82% 28% 17% 16%

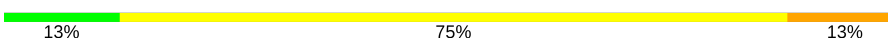


- Molecule 54: Quinupristin

Chain B6:  63% 38%



- Molecule 54: Quinupristin

Chain D6:  13% 75% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.26Å 432.34Å 621.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.08 – 2.80 69.08 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (69.08-2.80) 94.1 (69.08-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1160)	Depositor
R, R_{free}	0.225 , 0.271 0.230 , 0.276	Depositor DCC
R_{free} test set	5217 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	288423	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DOL, DBB, MG, 004, MHV, MHW, MHT, MHU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.34	0/36944	0.80	3/57632 (0.0%)
1	CA	0.28	0/36966	0.78	1/57666 (0.0%)
2	AB	0.28	0/1736	0.56	0/2338
2	CB	0.26	0/1736	0.50	0/2338
3	AC	0.28	0/1652	0.53	0/2225
3	CC	0.25	0/1652	0.48	0/2225
4	AD	0.29	0/1665	0.55	0/2227
4	CD	0.31	0/1665	0.55	0/2227
5	AE	0.31	0/1119	0.61	0/1504
5	CE	0.29	0/1119	0.59	0/1504
6	AF	0.30	0/836	0.55	0/1128
6	CF	0.27	0/836	0.57	1/1128 (0.1%)
7	AG	0.26	0/1196	0.48	0/1602
7	CG	0.25	0/1196	0.49	0/1602
8	AH	0.31	0/989	0.50	0/1326
8	CH	0.25	0/989	0.48	0/1326
9	AI	0.26	0/1034	0.54	0/1375
9	CI	0.26	0/1034	0.52	0/1375
10	AJ	0.29	0/797	0.55	0/1077
10	CJ	0.25	0/797	0.50	0/1077
11	AK	0.29	0/893	0.63	1/1205 (0.1%)
11	CK	0.26	0/893	0.52	0/1205
12	AL	0.31	0/969	0.58	0/1300
12	CL	0.29	0/969	0.60	0/1300
13	AM	0.27	0/893	0.55	0/1193
13	CM	0.26	0/893	0.50	0/1193
14	AN	0.28	0/785	0.55	0/1043
14	CN	0.25	0/785	0.46	0/1043
15	AO	0.28	0/718	0.53	0/959
15	CO	0.26	0/718	0.46	0/959
16	AP	0.30	0/659	0.66	1/884 (0.1%)
16	CP	0.27	0/659	0.49	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.30	0/658	0.58	0/881
17	CQ	0.28	0/658	0.51	0/881
18	AR	0.26	0/463	0.53	0/621
18	CR	0.26	0/463	0.49	0/621
19	AS	0.27	0/653	0.50	0/877
19	CS	0.27	0/653	0.54	0/877
20	AT	0.31	0/671	0.55	0/888
20	CT	0.25	0/671	0.50	0/888
21	AU	0.36	0/431	0.62	0/570
21	CU	0.33	0/431	0.56	0/570
22	BA	0.59	5/69659 (0.0%)	0.99	92/108672 (0.1%)
22	DA	0.27	0/69659	0.79	4/108672 (0.0%)
23	BB	0.52	0/2850	0.93	0/4444
23	DB	0.23	0/2828	0.76	0/4410
24	BC	0.38	0/2122	0.60	0/2852
24	DC	0.27	0/2122	0.52	0/2852
25	BD	0.42	0/1586	0.63	1/2134 (0.0%)
25	DD	0.26	0/1586	0.51	0/2134
26	BE	0.37	0/1571	0.60	0/2113
26	DE	0.26	0/1571	0.51	0/2113
27	BF	0.30	0/1435	0.52	0/1926
27	DF	0.24	0/1435	0.46	0/1926
28	BG	0.30	0/1343	0.53	0/1816
28	DG	0.25	0/1343	0.46	0/1816
29	BH	0.36	0/1121	0.66	1/1515 (0.1%)
29	DH	0.35	0/1121	0.56	0/1515
30	BI	0.29	0/1046	0.54	0/1410
30	DI	0.28	0/1046	0.52	0/1410
31	BJ	0.42	0/1152	0.58	0/1551
31	DJ	0.25	0/1152	0.51	0/1551
32	BK	0.41	0/948	0.64	0/1268
32	DK	0.27	0/948	0.51	0/1268
33	BL	0.39	0/1054	0.64	0/1403
33	DL	0.26	0/1054	0.51	0/1403
34	BM	0.42	0/1093	0.63	0/1460
34	DM	0.25	0/1093	0.46	0/1460
35	BN	0.43	0/974	0.68	0/1301
35	DN	0.27	0/974	0.56	1/1301 (0.1%)
36	BO	0.34	0/902	0.55	0/1209
36	DO	0.24	0/902	0.45	0/1209
37	BP	0.42	0/929	0.69	2/1242 (0.2%)
37	DP	0.26	0/929	0.47	0/1242
38	BQ	0.50	0/960	0.66	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.26	0/960	0.47	0/1278
39	BR	0.47	0/829	0.73	1/1107 (0.1%)
39	DR	0.25	0/829	0.50	0/1107
40	BS	0.51	0/864	0.64	0/1156
40	DS	0.26	0/864	0.50	0/1156
41	BT	0.36	0/745	0.60	0/994
41	DT	0.25	0/745	0.49	0/994
42	BU	0.36	0/788	0.57	0/1051
42	DU	0.28	0/788	0.52	0/1051
43	BV	0.37	0/766	0.58	0/1025
43	DV	0.24	0/766	0.44	0/1025
44	BW	0.44	0/587	0.71	2/776 (0.3%)
44	DW	0.25	0/576	0.47	0/762
45	BX	0.34	0/635	0.57	0/848
45	DX	0.28	0/635	0.53	0/848
46	BY	0.32	0/510	0.63	0/677
46	DY	0.25	0/510	0.50	0/677
47	BZ	0.43	0/453	0.61	0/605
47	DZ	0.26	0/453	0.48	0/605
48	B0	0.44	0/450	0.64	0/599
48	D0	0.27	0/450	0.50	0/599
49	B1	0.37	0/417	0.53	0/554
49	D1	0.28	0/417	0.49	0/554
50	B2	0.44	0/380	0.69	0/498
50	D2	0.28	0/380	0.51	0/498
51	B3	0.38	0/513	0.57	0/676
51	D3	0.25	0/513	0.44	0/676
52	B4	0.43	0/303	0.63	0/397
52	D4	0.25	0/303	0.49	0/397
53	B5	0.25	0/1145	0.49	0/1556
54	B6	1.77	0/13	2.40	1/15 (6.7%)
54	D6	1.44	0/13	2.02	1/15 (6.7%)
All	All	0.39	5/310652 (0.0%)	0.79	113/464396 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	CF	0	1
11	AK	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	CL	0	2
25	BD	0	1
25	DD	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	984	A	N9-C4	-8.33	1.32	1.37
22	BA	1142	A	N9-C4	-7.64	1.33	1.37
22	BA	1936	A	N9-C4	-7.63	1.33	1.37
22	BA	528	A	N9-C4	-7.62	1.33	1.37
22	BA	528	A	N3-C4	-5.47	1.31	1.34

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	974	G	C4-C5-N7	10.83	115.13	110.80
22	BA	974	G	C6-C5-N7	-10.21	124.27	130.40
25	BD	151	THR	C-N-CD	-9.98	98.64	120.60
22	BA	984	A	C2-N3-C4	-9.95	105.62	110.60
22	BA	974	G	C5-N7-C8	-9.65	99.48	104.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
25	BD	151	THR	Peptide
6	CF	54	LEU	Peptide
12	CL	23	ALA	Peptide
12	CL	24	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	962	0
1	CA	33015	0	16617	1107	1
2	AB	1705	0	1732	164	0
2	CB	1705	0	1732	135	0
3	AC	1625	0	1696	78	0
3	CC	1625	0	1696	69	0
4	AD	1643	0	1707	116	0
4	CD	1643	0	1707	116	0
5	AE	1106	0	1148	88	0
5	CE	1106	0	1148	99	0
6	AF	818	0	808	47	0
6	CF	818	0	808	60	0
7	AG	1182	0	1238	58	0
7	CG	1182	0	1238	66	0
8	AH	979	0	1031	49	0
8	CH	979	0	1031	52	0
9	AI	1022	0	1070	87	0
9	CI	1022	0	1070	66	0
10	AJ	787	0	828	81	0
10	CJ	787	0	828	56	0
11	AK	877	0	887	68	0
11	CK	877	0	887	55	0
12	AL	955	0	1016	44	0
12	CL	955	0	1016	74	0
13	AM	884	0	941	44	0
13	CM	884	0	941	51	0
14	AN	774	0	824	58	0
14	CN	774	0	824	51	0
15	AO	710	0	728	31	0
15	CO	710	0	728	29	0
16	AP	649	0	666	53	0
16	CP	649	0	666	36	0
17	AQ	649	0	691	63	0
17	CQ	649	0	691	53	0
18	AR	456	0	478	17	0
18	CR	456	0	478	25	0
19	AS	638	0	665	39	0
19	CS	638	0	665	42	0
20	AT	665	0	714	65	0
20	CT	665	0	714	46	0
21	AU	426	0	449	52	0
21	CU	426	0	449	53	0
22	BA	62195	0	31280	1486	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	62195	0	31280	2451	1
23	BB	2549	0	1291	37	0
23	DB	2529	0	1281	66	0
24	BC	2083	0	2154	102	0
24	DC	2083	0	2154	128	0
25	BD	1565	0	1616	66	0
25	DD	1565	0	1616	97	0
26	BE	1552	0	1619	67	0
26	DE	1552	0	1619	91	0
27	BF	1411	0	1444	84	0
27	DF	1411	0	1444	54	0
28	BG	1323	0	1371	41	0
28	DG	1323	0	1371	42	0
29	BH	1110	0	1147	139	0
29	DH	1110	0	1148	87	0
30	BI	1032	0	1085	76	0
30	DI	1032	0	1085	85	0
31	BJ	1129	0	1162	48	0
31	DJ	1129	0	1162	62	0
32	BK	939	0	1012	45	0
32	DK	939	0	1012	53	0
33	BL	1045	0	1117	54	0
33	DL	1045	0	1117	75	0
34	BM	1074	0	1157	43	0
34	DM	1074	0	1157	41	0
35	BN	961	0	1000	39	0
35	DN	961	0	1000	71	0
36	BO	892	0	923	38	0
36	DO	892	0	923	41	0
37	BP	917	0	962	45	0
37	DP	917	0	962	42	0
38	BQ	947	0	1019	39	0
38	DQ	947	0	1019	47	0
39	BR	816	0	839	66	0
39	DR	816	0	839	36	0
40	BS	857	0	922	33	0
40	DS	857	0	922	37	0
41	BT	739	0	807	41	0
41	DT	739	0	807	60	0
42	BU	780	0	831	37	0
42	DU	780	0	831	68	0
43	BV	753	0	780	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DV	753	0	780	21	0
44	BW	580	0	594	20	0
44	DW	569	0	581	23	0
45	BX	625	0	652	15	0
45	DX	625	0	652	46	0
46	BY	509	0	543	34	0
46	DY	509	0	543	26	0
47	BZ	449	0	488	9	0
47	DZ	449	0	488	24	0
48	B0	444	0	458	27	0
48	D0	444	0	458	23	0
49	B1	410	0	440	19	0
49	D1	410	0	440	22	0
50	B2	377	0	418	10	0
50	D2	377	0	418	31	0
51	B3	504	0	572	28	0
51	D3	504	0	572	22	0
52	B4	302	0	340	7	0
52	D4	302	0	340	15	0
53	B5	1142	0	865	69	0
54	B6	73	0	64	3	0
54	D6	73	0	65	12	0
55	AA	71	0	0	0	0
55	AM	1	0	0	0	0
55	BA	194	0	0	0	0
55	BB	4	0	0	0	0
55	BQ	1	0	0	0	0
55	CA	56	0	0	0	0
55	D2	1	0	0	0	0
55	DA	166	0	0	0	0
55	DB	3	0	0	0	0
55	DQ	1	0	0	0	0
56	BA	48	0	50	15	0
56	DA	48	0	50	25	0
57	B4	1	0	0	0	0
57	D4	1	0	0	0	0
58	AA	194	0	0	18	0
58	AE	2	0	0	0	0
58	AL	1	0	0	0	0
58	AN	3	0	0	0	0
58	AT	2	0	0	0	0
58	AU	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	B3	3	0	0	0	0
58	B4	1	0	0	0	0
58	BA	617	0	0	66	0
58	BB	14	0	0	1	0
58	BC	6	0	0	1	0
58	BD	4	0	0	2	0
58	BE	1	0	0	0	0
58	BF	1	0	0	1	0
58	BG	1	0	0	1	0
58	BJ	1	0	0	0	0
58	BL	7	0	0	0	0
58	BN	5	0	0	0	0
58	BQ	1	0	0	0	0
58	BS	1	0	0	0	0
58	BT	2	0	0	0	0
58	CA	192	0	0	12	0
58	CL	1	0	0	0	0
58	CN	2	0	0	0	0
58	CT	2	0	0	0	0
58	CU	1	0	0	1	0
58	D2	1	0	0	1	0
58	D3	1	0	0	0	0
58	D4	1	0	0	0	0
58	DA	610	0	0	84	0
58	DB	13	0	0	1	0
58	DC	8	0	0	1	0
58	DD	4	0	0	2	0
58	DE	4	0	0	0	0
58	DJ	1	0	0	0	0
58	DL	4	0	0	1	0
58	DN	2	0	0	0	0
58	DS	2	0	0	0	0
58	DT	3	0	0	1	0
58	DU	1	0	0	0	0
58	DV	1	0	0	0	0
All	All	288423	0	193016	10587	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

The worst 5 of 10587 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BH:117:LEU:O	29:BH:121:VAL:HG23	1.34	1.22
22:BA:730:A:OP2	58:BA:3693:HOH:O	1.58	1.21
1:AA:533:A:OP1	58:AA:1848:HOH:O	1.65	1.15
29:BH:117:LEU:O	29:BH:121:VAL:CG2	1.95	1.14
22:BA:2498:C:OP2	58:BA:3684:HOH:O	1.64	1.13

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:204:G:OP1	22:DA:289:G:O2'[3_545]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	126 (58%)	45 (21%)	45 (21%)	0	0
2	CB	216/218 (99%)	140 (65%)	51 (24%)	25 (12%)	0	1
3	AC	204/206 (99%)	148 (72%)	35 (17%)	21 (10%)	0	1
3	CC	204/206 (99%)	154 (76%)	39 (19%)	11 (5%)	2	5
4	AD	203/205 (99%)	137 (68%)	39 (19%)	27 (13%)	0	0
4	CD	203/205 (99%)	152 (75%)	32 (16%)	19 (9%)	0	1
5	AE	148/150 (99%)	102 (69%)	27 (18%)	19 (13%)	0	1
5	CE	148/150 (99%)	100 (68%)	33 (22%)	15 (10%)	0	1
6	AF	98/100 (98%)	73 (74%)	15 (15%)	10 (10%)	0	1
6	CF	98/100 (98%)	68 (69%)	15 (15%)	15 (15%)	0	0
7	AG	149/151 (99%)	107 (72%)	29 (20%)	13 (9%)	1	1
7	CG	149/151 (99%)	119 (80%)	22 (15%)	8 (5%)	2	5
8	AH	127/129 (98%)	90 (71%)	28 (22%)	9 (7%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	CH	127/129 (98%)	98 (77%)	19 (15%)	10 (8%)	1	2
9	AI	125/127 (98%)	87 (70%)	24 (19%)	14 (11%)	0	1
9	CI	125/127 (98%)	89 (71%)	18 (14%)	18 (14%)	0	0
10	AJ	96/98 (98%)	64 (67%)	11 (12%)	21 (22%)	0	0
10	CJ	96/98 (98%)	73 (76%)	11 (12%)	12 (12%)	0	1
11	AK	115/117 (98%)	81 (70%)	17 (15%)	17 (15%)	0	0
11	CK	115/117 (98%)	82 (71%)	24 (21%)	9 (8%)	1	2
12	AL	121/123 (98%)	91 (75%)	21 (17%)	9 (7%)	1	2
12	CL	121/123 (98%)	92 (76%)	18 (15%)	11 (9%)	1	1
13	AM	112/114 (98%)	81 (72%)	21 (19%)	10 (9%)	1	1
13	CM	112/114 (98%)	80 (71%)	18 (16%)	14 (12%)	0	1
14	AN	92/100 (92%)	61 (66%)	21 (23%)	10 (11%)	0	1
14	CN	92/100 (92%)	58 (63%)	20 (22%)	14 (15%)	0	0
15	AO	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	2
15	CO	86/88 (98%)	64 (74%)	17 (20%)	5 (6%)	1	4
16	AP	80/82 (98%)	55 (69%)	15 (19%)	10 (12%)	0	1
16	CP	80/82 (98%)	59 (74%)	13 (16%)	8 (10%)	0	1
17	AQ	78/80 (98%)	53 (68%)	18 (23%)	7 (9%)	1	1
17	CQ	78/80 (98%)	56 (72%)	15 (19%)	7 (9%)	1	1
18	AR	53/55 (96%)	42 (79%)	11 (21%)	0	100	100
18	CR	53/55 (96%)	37 (70%)	12 (23%)	4 (8%)	1	2
19	AS	77/79 (98%)	57 (74%)	11 (14%)	9 (12%)	0	1
19	CS	77/79 (98%)	55 (71%)	11 (14%)	11 (14%)	0	0
20	AT	83/85 (98%)	59 (71%)	19 (23%)	5 (6%)	1	4
20	CT	83/85 (98%)	62 (75%)	12 (14%)	9 (11%)	0	1
21	AU	49/51 (96%)	26 (53%)	8 (16%)	15 (31%)	0	0
21	CU	49/51 (96%)	21 (43%)	16 (33%)	12 (24%)	0	0
24	BC	269/271 (99%)	218 (81%)	39 (14%)	12 (4%)	2	8
24	DC	269/271 (99%)	196 (73%)	48 (18%)	25 (9%)	0	1
25	BD	207/209 (99%)	180 (87%)	21 (10%)	6 (3%)	4	15
25	DD	207/209 (99%)	153 (74%)	43 (21%)	11 (5%)	2	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BE	199/201 (99%)	165 (83%)	30 (15%)	4 (2%)	7	24
26	DE	199/201 (99%)	154 (77%)	27 (14%)	18 (9%)	1	1
27	BF	175/177 (99%)	142 (81%)	24 (14%)	9 (5%)	2	6
27	DF	175/177 (99%)	135 (77%)	27 (15%)	13 (7%)	1	2
28	BG	174/176 (99%)	148 (85%)	16 (9%)	10 (6%)	1	5
28	DG	174/176 (99%)	127 (73%)	36 (21%)	11 (6%)	1	3
29	BH	147/149 (99%)	89 (60%)	37 (25%)	21 (14%)	0	0
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	0	1
30	BI	139/141 (99%)	78 (56%)	37 (27%)	24 (17%)	0	0
30	DI	139/141 (99%)	82 (59%)	38 (27%)	19 (14%)	0	0
31	BJ	140/142 (99%)	125 (89%)	14 (10%)	1 (1%)	22	53
31	DJ	140/142 (99%)	104 (74%)	23 (16%)	13 (9%)	0	1
32	BK	120/122 (98%)	97 (81%)	14 (12%)	9 (8%)	1	2
32	DK	120/122 (98%)	95 (79%)	15 (12%)	10 (8%)	1	2
33	BL	141/143 (99%)	112 (79%)	21 (15%)	8 (6%)	1	5
33	DL	141/143 (99%)	98 (70%)	31 (22%)	12 (8%)	1	1
34	BM	134/136 (98%)	120 (90%)	11 (8%)	3 (2%)	6	22
34	DM	134/136 (98%)	112 (84%)	17 (13%)	5 (4%)	3	11
35	BN	118/120 (98%)	95 (80%)	21 (18%)	2 (2%)	9	29
35	DN	118/120 (98%)	90 (76%)	18 (15%)	10 (8%)	1	1
36	BO	114/116 (98%)	96 (84%)	14 (12%)	4 (4%)	3	12
36	DO	114/116 (98%)	82 (72%)	24 (21%)	8 (7%)	1	3
37	BP	112/114 (98%)	99 (88%)	8 (7%)	5 (4%)	2	8
37	DP	112/114 (98%)	88 (79%)	18 (16%)	6 (5%)	2	5
38	BQ	115/117 (98%)	102 (89%)	12 (10%)	1 (1%)	17	46
38	DQ	115/117 (98%)	92 (80%)	22 (19%)	1 (1%)	17	46
39	BR	101/103 (98%)	81 (80%)	10 (10%)	10 (10%)	0	1
39	DR	101/103 (98%)	72 (71%)	23 (23%)	6 (6%)	1	4
40	BS	108/110 (98%)	94 (87%)	10 (9%)	4 (4%)	3	11
40	DS	108/110 (98%)	83 (77%)	17 (16%)	8 (7%)	1	2
41	BT	91/93 (98%)	74 (81%)	9 (10%)	8 (9%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	DT	91/93 (98%)	53 (58%)	28 (31%)	10 (11%)	0	1
42	BU	100/102 (98%)	77 (77%)	19 (19%)	4 (4%)	3	9
42	DU	100/102 (98%)	69 (69%)	19 (19%)	12 (12%)	0	1
43	BV	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	14	41
43	DV	92/94 (98%)	76 (83%)	14 (15%)	2 (2%)	6	22
44	BW	74/76 (97%)	68 (92%)	4 (5%)	2 (3%)	5	17
44	DW	73/76 (96%)	61 (84%)	12 (16%)	0	100	100
45	BX	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	12	36
45	DX	75/77 (97%)	58 (77%)	12 (16%)	5 (7%)	1	3
46	BY	61/63 (97%)	43 (70%)	10 (16%)	8 (13%)	0	1
46	DY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	2
47	BZ	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
47	DZ	56/58 (97%)	41 (73%)	10 (18%)	5 (9%)	1	1
48	B0	54/56 (96%)	46 (85%)	4 (7%)	4 (7%)	1	2
48	D0	54/56 (96%)	37 (68%)	12 (22%)	5 (9%)	0	1
49	B1	48/50 (96%)	40 (83%)	4 (8%)	4 (8%)	1	2
49	D1	48/50 (96%)	36 (75%)	8 (17%)	4 (8%)	1	2
50	B2	44/46 (96%)	37 (84%)	5 (11%)	2 (4%)	2	8
50	D2	44/46 (96%)	34 (77%)	6 (14%)	4 (9%)	1	1
51	B3	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	9	31
51	D3	62/64 (97%)	52 (84%)	6 (10%)	4 (6%)	1	3
52	B4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5	17
52	D4	36/38 (95%)	32 (89%)	2 (6%)	2 (6%)	2	5
53	B5	183/228 (80%)	87 (48%)	53 (29%)	43 (24%)	0	0
54	B6	2/8 (25%)	2 (100%)	0	0	100	100
54	D6	2/8 (25%)	0	2 (100%)	0	100	100
All	All	11422/11688 (98%)	8528 (75%)	1918 (17%)	976 (8%)	1	1

5 of 976 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	PHE
2	AB	20	THR

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Mol	Chain	Res	Type
2	AB	22	TYR
2	AB	25	PRO
2	AB	34	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	132 (73%)	48 (27%)	0	1
2	CB	180/180 (100%)	130 (72%)	50 (28%)	0	1
3	AC	170/170 (100%)	135 (79%)	35 (21%)	1	3
3	CC	170/170 (100%)	144 (85%)	26 (15%)	2	8
4	AD	172/172 (100%)	139 (81%)	33 (19%)	1	4
4	CD	172/172 (100%)	143 (83%)	29 (17%)	2	6
5	AE	113/113 (100%)	84 (74%)	29 (26%)	0	1
5	CE	113/113 (100%)	86 (76%)	27 (24%)	0	2
6	AF	87/87 (100%)	69 (79%)	18 (21%)	1	3
6	CF	87/87 (100%)	61 (70%)	26 (30%)	0	1
7	AG	124/124 (100%)	101 (82%)	23 (18%)	1	5
7	CG	124/124 (100%)	99 (80%)	25 (20%)	1	4
8	AH	104/104 (100%)	84 (81%)	20 (19%)	1	4
8	CH	104/104 (100%)	82 (79%)	22 (21%)	1	3
9	AI	105/105 (100%)	77 (73%)	28 (27%)	0	1
9	CI	105/105 (100%)	88 (84%)	17 (16%)	2	7
10	AJ	86/86 (100%)	67 (78%)	19 (22%)	1	3
10	CJ	86/86 (100%)	68 (79%)	18 (21%)	1	3
11	AK	90/90 (100%)	76 (84%)	14 (16%)	2	8
11	CK	90/90 (100%)	71 (79%)	19 (21%)	1	3
12	AL	103/103 (100%)	89 (86%)	14 (14%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	CL	103/103 (100%)	82 (80%)	21 (20%)	1	4
13	AM	92/92 (100%)	74 (80%)	18 (20%)	1	4
13	CM	92/92 (100%)	75 (82%)	17 (18%)	1	5
14	AN	79/83 (95%)	64 (81%)	15 (19%)	1	4
14	CN	79/83 (95%)	70 (89%)	9 (11%)	5	18
15	AO	75/76 (99%)	63 (84%)	12 (16%)	2	7
15	CO	75/76 (99%)	65 (87%)	10 (13%)	4	12
16	AP	65/65 (100%)	50 (77%)	15 (23%)	1	2
16	CP	65/65 (100%)	54 (83%)	11 (17%)	2	6
17	AQ	74/74 (100%)	50 (68%)	24 (32%)	0	0
17	CQ	74/74 (100%)	51 (69%)	23 (31%)	0	0
18	AR	48/48 (100%)	38 (79%)	10 (21%)	1	3
18	CR	48/48 (100%)	38 (79%)	10 (21%)	1	3
19	AS	70/70 (100%)	55 (79%)	15 (21%)	1	3
19	CS	70/70 (100%)	58 (83%)	12 (17%)	2	6
20	AT	65/65 (100%)	51 (78%)	14 (22%)	1	3
20	CT	65/65 (100%)	57 (88%)	8 (12%)	4	15
21	AU	44/44 (100%)	29 (66%)	15 (34%)	0	0
21	CU	44/44 (100%)	29 (66%)	15 (34%)	0	0
24	BC	216/216 (100%)	189 (88%)	27 (12%)	4	14
24	DC	216/216 (100%)	197 (91%)	19 (9%)	10	29
25	BD	164/164 (100%)	148 (90%)	16 (10%)	8	24
25	DD	164/164 (100%)	145 (88%)	19 (12%)	5	17
26	BE	165/165 (100%)	136 (82%)	29 (18%)	2	5
26	DE	165/165 (100%)	137 (83%)	28 (17%)	2	6
27	BF	148/148 (100%)	116 (78%)	32 (22%)	1	3
27	DF	148/148 (100%)	119 (80%)	29 (20%)	1	4
28	BG	137/137 (100%)	118 (86%)	19 (14%)	3	11
28	DG	137/137 (100%)	114 (83%)	23 (17%)	2	6
29	BH	114/114 (100%)	88 (77%)	26 (23%)	1	2
29	DH	114/114 (100%)	88 (77%)	26 (23%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BI	109/109 (100%)	82 (75%)	27 (25%)	0	2
30	DI	109/109 (100%)	80 (73%)	29 (27%)	0	1
31	BJ	116/116 (100%)	105 (90%)	11 (10%)	8	25
31	DJ	116/116 (100%)	94 (81%)	22 (19%)	1	4
32	BK	103/103 (100%)	89 (86%)	14 (14%)	3	11
32	DK	103/103 (100%)	90 (87%)	13 (13%)	4	14
33	BL	102/102 (100%)	91 (89%)	11 (11%)	6	19
33	DL	102/102 (100%)	86 (84%)	16 (16%)	2	8
34	BM	109/109 (100%)	99 (91%)	10 (9%)	9	27
34	DM	109/109 (100%)	95 (87%)	14 (13%)	4	13
35	BN	100/100 (100%)	94 (94%)	6 (6%)	19	48
35	DN	100/100 (100%)	76 (76%)	24 (24%)	0	2
36	BO	86/86 (100%)	65 (76%)	21 (24%)	0	2
36	DO	86/86 (100%)	70 (81%)	16 (19%)	1	5
37	BP	99/99 (100%)	81 (82%)	18 (18%)	1	5
37	DP	99/99 (100%)	90 (91%)	9 (9%)	9	27
38	BQ	89/89 (100%)	78 (88%)	11 (12%)	4	14
38	DQ	89/89 (100%)	78 (88%)	11 (12%)	4	14
39	BR	84/84 (100%)	74 (88%)	10 (12%)	5	16
39	DR	84/84 (100%)	76 (90%)	8 (10%)	8	25
40	BS	93/93 (100%)	76 (82%)	17 (18%)	1	5
40	DS	93/93 (100%)	83 (89%)	10 (11%)	6	19
41	BT	80/80 (100%)	68 (85%)	12 (15%)	3	9
41	DT	80/80 (100%)	66 (82%)	14 (18%)	2	6
42	BU	83/83 (100%)	72 (87%)	11 (13%)	4	12
42	DU	83/83 (100%)	68 (82%)	15 (18%)	1	5
43	BV	78/78 (100%)	63 (81%)	15 (19%)	1	4
43	DV	78/78 (100%)	65 (83%)	13 (17%)	2	6
44	BW	57/58 (98%)	47 (82%)	10 (18%)	2	6
44	DW	56/58 (97%)	50 (89%)	6 (11%)	6	20
45	BX	67/67 (100%)	61 (91%)	6 (9%)	9	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DX	67/67 (100%)	58 (87%)	9 (13%)	4	12
46	BY	55/55 (100%)	50 (91%)	5 (9%)	9	27
46	DY	55/55 (100%)	43 (78%)	12 (22%)	1	3
47	BZ	48/48 (100%)	41 (85%)	7 (15%)	3	9
47	DZ	48/48 (100%)	38 (79%)	10 (21%)	1	3
48	B0	47/47 (100%)	42 (89%)	5 (11%)	6	20
48	D0	47/47 (100%)	43 (92%)	4 (8%)	10	31
49	B1	45/45 (100%)	42 (93%)	3 (7%)	16	43
49	D1	45/45 (100%)	39 (87%)	6 (13%)	4	12
50	B2	38/38 (100%)	34 (90%)	4 (10%)	7	20
50	D2	38/38 (100%)	31 (82%)	7 (18%)	1	5
51	B3	51/51 (100%)	45 (88%)	6 (12%)	5	16
51	D3	51/51 (100%)	46 (90%)	5 (10%)	8	24
52	B4	34/34 (100%)	32 (94%)	2 (6%)	19	49
52	D4	34/34 (100%)	26 (76%)	8 (24%)	1	2
53	B5	61/180 (34%)	48 (79%)	13 (21%)	1	3
54	B6	2/2 (100%)	2 (100%)	0	100	100
54	D6	2/2 (100%)	2 (100%)	0	100	100
All	All	9390/9522 (99%)	7747 (82%)	1643 (18%)	2	6

5 of 1643 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BU	72	ILE
4	CD	155	VAL
39	DR	41	ILE
44	BW	39	ARG
2	CB	43	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
5	CE	122	ASN
17	CQ	31	HIS
49	D1	26	ASN

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Mol	Chain	Res	Type
7	CG	97	ASN
15	CO	42	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	324 (21%)	11 (0%)
1	CA	1538/1539 (99%)	342 (22%)	10 (0%)
22	BA	2895/2903 (99%)	579 (20%)	24 (0%)
22	DA	2895/2903 (99%)	704 (24%)	32 (1%)
23	BB	118/119 (99%)	16 (13%)	0
23	DB	117/119 (98%)	20 (17%)	0
All	All	9100/9122 (99%)	1985 (21%)	77 (0%)

5 of 1985 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	3	A
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G

5 of 77 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2873	A
1	CA	1279	G
22	DA	2326	C
1	CA	85	U
1	CA	484	G

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

10 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$
54	MHV	B6	6	54	7,9,10	1.59	1 (14%)	7,11,13	3.44	4 (57%)
54	004	D6	7	54	9,10,11	0.78	0	9,12,14	0.60	0
54	DBB	B6	3	54	4,5,6	1.31	0	1,5,7	2.61	1 (100%)
54	MHW	D6	1	54	9,9,10	1.95	1 (11%)	10,11,13	3.07	4 (40%)
54	MHW	B6	1	54	9,9,10	1.64	1 (11%)	10,11,13	2.86	4 (40%)
54	MHU	D6	5	54	14,15,16	1.63	3 (21%)	18,19,21	1.15	2 (11%)
54	DBB	D6	3	54	4,5,6	1.18	0	1,5,7	1.37	0
54	004	B6	7	54	9,10,11	1.52	1 (11%)	9,12,14	2.03	3 (33%)
54	MHV	D6	6	54	7,9,10	1.19	0	7,11,13	3.21	4 (57%)
54	MHU	B6	5	54	14,15,16	1.80	3 (21%)	18,19,21	1.27	3 (16%)

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
54	MHV	B6	6	54	-	0/1/12/14	0/1/1/1
54	004	D6	7	54	-	2/4/6/8	0/1/1/1
54	DBB	B6	3	54	-	1/3/4/6	-
54	MHW	D6	1	54	-	0/2/2/4	0/1/1/1
54	MHW	B6	1	54	-	0/2/2/4	0/1/1/1
54	MHU	D6	5	54	-	0/9/12/14	0/1/1/1
54	DBB	D6	3	54	-	0/3/4/6	-
54	004	B6	7	54	-	1/4/6/8	0/1/1/1
54	MHV	D6	6	54	-	0/1/12/14	0/1/1/1
54	MHU	B6	5	54	-	0/9/12/14	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	D6	1	MHW	CA-C	5.22	1.54	1.48
54	B6	5	MHU	CZ-NZ	5.22	1.49	1.37
54	D6	5	MHU	CZ-NZ	4.69	1.48	1.37
54	B6	7	004	CB-CA	-4.30	1.48	1.52
54	B6	1	MHW	CA-C	3.99	1.52	1.48

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	D6	1	MHW	CD-CE-N	6.55	134.13	123.43
54	B6	1	MHW	CD-CE-N	5.89	133.04	123.43
54	B6	6	MHV	CD2-CG-CB	5.52	124.11	115.89
54	D6	6	MHV	CD2-CE-N	-5.22	98.62	110.03
54	D6	6	MHV	CD2-CG-CB	5.13	123.53	115.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	B6	3	DBB	N-CA-CB-CG
54	D6	7	004	C-CA-CB-CG1
54	D6	7	004	C-CA-CB-CG2
54	B6	7	004	C-CA-CB-CG1

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	D6	7	004	4	0
54	D6	1	MHW	2	0
54	D6	5	MHU	3	0
54	D6	3	DBB	1	0
54	B6	7	004	1	0
54	D6	6	MHV	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 502 ligands modelled in this entry, 500 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
56	DOL	DA	3001	-	43,50,50	2.90	13 (30%)	51,70,70	2.81	13 (25%)
56	DOL	BA	3001	-	43,50,50	2.86	13 (30%)	51,70,70	2.88	14 (27%)

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
56	DOL	DA	3001	-	-	10/58/77/77	0/2/3/3
56	DOL	BA	3001	-	-	18/58/77/77	0/2/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	DA	3001	DOL	O15-C14	9.27	1.37	1.21
56	BA	3001	DOL	O15-C14	8.90	1.36	1.21
56	DA	3001	DOL	C22-C23	8.04	1.53	1.32
56	BA	3001	DOL	C22-C23	7.76	1.52	1.32
56	DA	3001	DOL	O38-C37	6.42	1.37	1.21

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DA	3001	DOL	O40-S39-O41	-15.45	100.57	118.19
56	BA	3001	DOL	O40-S39-O41	-14.66	101.47	118.19
56	BA	3001	DOL	C8-C6-N5	6.55	127.31	119.76
56	BA	3001	DOL	C29-C28-C26	-5.90	107.93	122.69
56	DA	3001	DOL	C4-N5-C1	-5.06	106.22	112.45

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

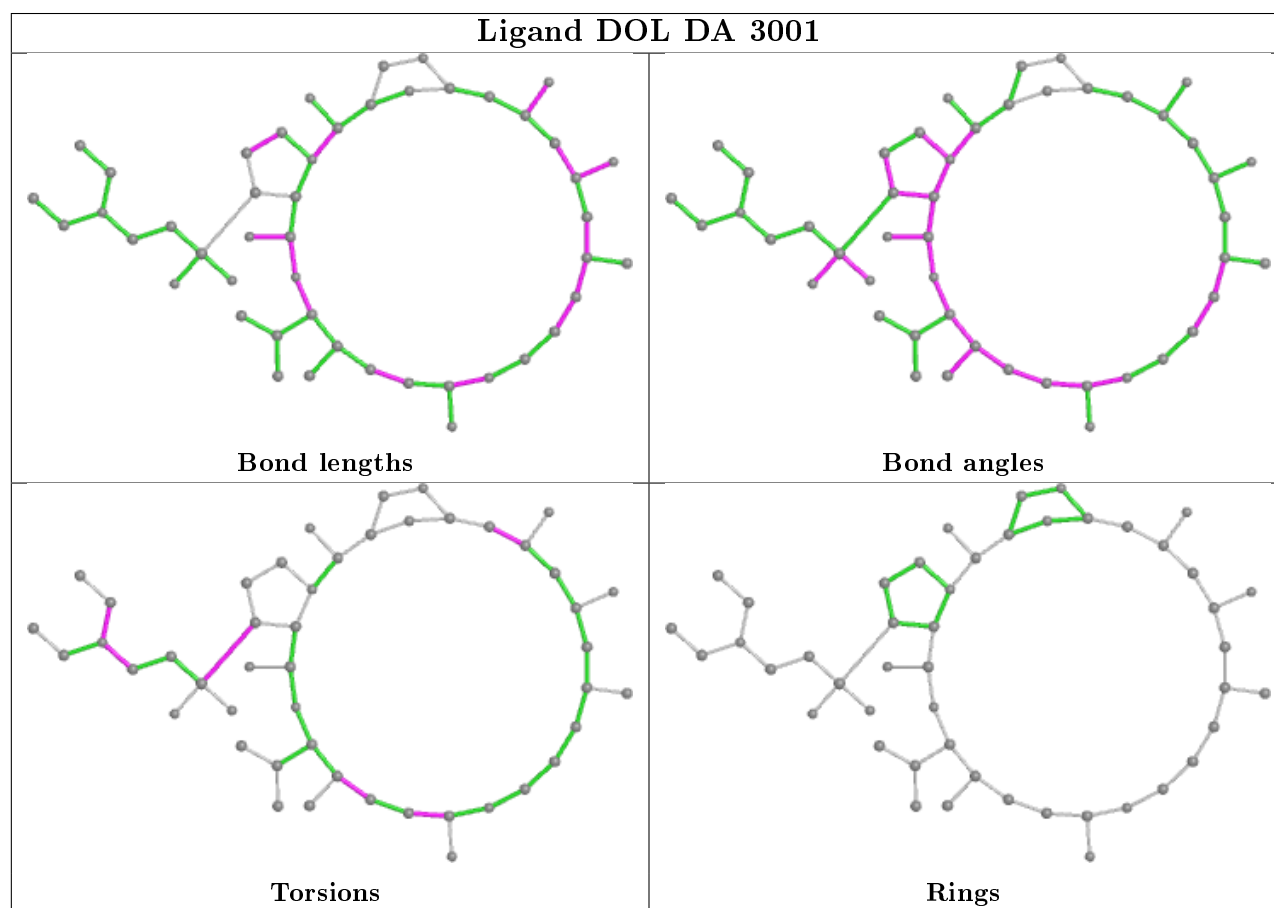
Mol	Chain	Res	Type	Atoms
56	BA	3001	DOL	C1-C2-S39-O40
56	BA	3001	DOL	C1-C2-S39-C42
56	BA	3001	DOL	S39-C42-C43-N44
56	BA	3001	DOL	C14-C16-C17-O18
56	BA	3001	DOL	C17-C19-C20-C22

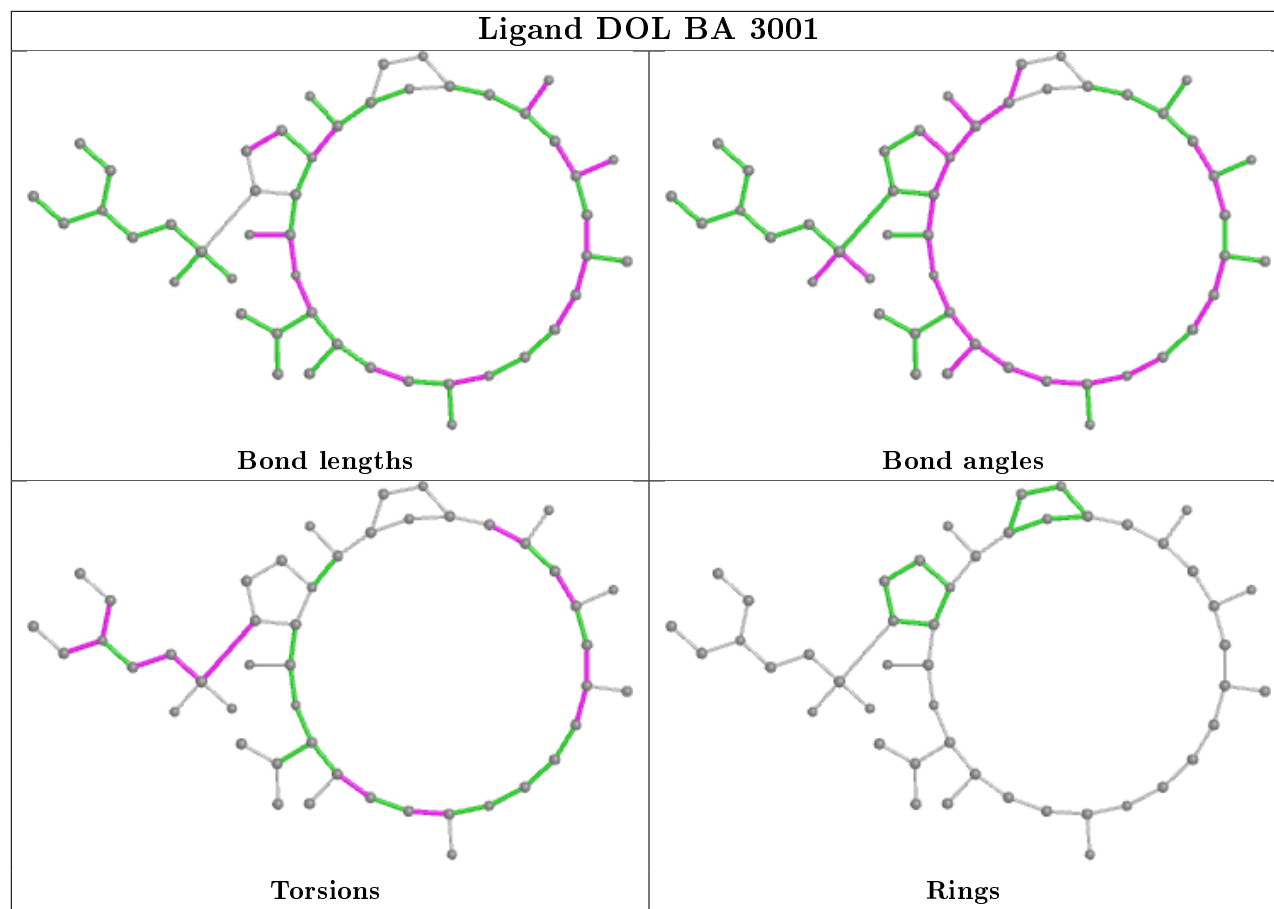
There are no ring outliers.

2 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DA	3001	DOL	25	0
56	BA	3001	DOL	15	0

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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1538/1539 (99%)	-0.16	22 (1%) 75 70	10, 49, 132, 182	0
1	CA	1539/1539 (100%)	0.16	55 (3%) 42 32	22, 70, 146, 178	0
2	AB	218/218 (100%)	0.80	29 (13%) 3 2	36, 73, 100, 117	0
2	CB	218/218 (100%)	1.05	45 (20%) 1 0	57, 86, 108, 121	0
3	AC	206/206 (100%)	0.15	10 (4%) 29 20	33, 57, 78, 95	0
3	CC	206/206 (100%)	1.19	50 (24%) 0 0	55, 80, 96, 107	0
4	AD	205/205 (100%)	0.36	8 (3%) 39 29	31, 56, 79, 99	0
4	CD	205/205 (100%)	-0.03	5 (2%) 59 49	13, 35, 60, 82	0
5	AE	150/150 (100%)	0.10	2 (1%) 77 72	26, 47, 78, 93	0
5	CE	150/150 (100%)	0.18	1 (0%) 87 84	25, 52, 84, 104	0
6	AF	100/100 (100%)	-0.18	1 (1%) 82 77	32, 54, 73, 77	0
6	CF	100/100 (100%)	0.53	10 (10%) 7 4	41, 74, 92, 103	0
7	AG	151/151 (100%)	0.26	3 (1%) 65 56	51, 75, 92, 100	0
7	CG	151/151 (100%)	2.56	85 (56%) 0 0	82, 106, 114, 118	0
8	AH	129/129 (100%)	0.18	2 (1%) 72 66	29, 46, 67, 79	0
8	CH	129/129 (100%)	0.45	10 (7%) 13 7	46, 64, 80, 94	0
9	AI	127/127 (100%)	0.93	22 (17%) 1 1	40, 74, 98, 107	0
9	CI	127/127 (100%)	1.84	45 (35%) 0 0	79, 96, 112, 121	0
10	AJ	98/98 (100%)	0.64	7 (7%) 16 9	38, 66, 86, 116	0
10	CJ	98/98 (100%)	2.70	59 (60%) 0 0	72, 97, 115, 123	0
11	AK	117/117 (100%)	0.49	10 (8%) 10 5	25, 61, 89, 119	0
11	CK	117/117 (100%)	0.23	2 (1%) 70 63	35, 68, 79, 90	0
12	AL	123/123 (100%)	0.15	6 (4%) 29 20	20, 34, 65, 97	0
12	CL	123/123 (100%)	0.32	3 (2%) 59 49	30, 50, 74, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.42	10 (8%)	10	5	47, 69, 91, 103	0
13	CM	114/114 (100%)	3.11	76 (66%)	0	0	93, 113, 122, 125	0
14	AN	96/100 (96%)	0.67	11 (11%)	4	2	36, 60, 96, 105	0
14	CN	96/100 (96%)	2.16	44 (45%)	0	0	70, 96, 115, 122	0
15	AO	88/88 (100%)	0.35	3 (3%)	45	35	29, 47, 64, 91	0
15	CO	88/88 (100%)	0.32	3 (3%)	45	35	36, 64, 80, 102	0
16	AP	82/82 (100%)	0.69	6 (7%)	15	8	34, 47, 83, 109	0
16	CP	82/82 (100%)	0.98	11 (13%)	3	1	45, 62, 91, 112	0
17	AQ	80/80 (100%)	0.26	3 (3%)	40	30	27, 48, 75, 111	0
17	CQ	80/80 (100%)	1.14	19 (23%)	0	0	42, 77, 97, 99	0
18	AR	55/55 (100%)	0.22	3 (5%)	25	16	40, 52, 77, 102	0
18	CR	55/55 (100%)	0.28	4 (7%)	15	8	36, 54, 78, 108	0
19	AS	79/79 (100%)	0.70	13 (16%)	1	1	54, 70, 88, 97	0
19	CS	79/79 (100%)	3.96	58 (73%)	0	0	95, 114, 122, 128	0
20	AT	85/85 (100%)	0.43	4 (4%)	31	22	35, 48, 68, 96	0
20	CT	85/85 (100%)	1.81	33 (38%)	0	0	53, 78, 96, 101	0
21	AU	51/51 (100%)	1.26	12 (23%)	0	0	41, 74, 95, 105	0
21	CU	51/51 (100%)	0.68	6 (11%)	4	2	42, 69, 98, 102	0
22	BA	2897/2903 (99%)	0.14	106 (3%)	41	31	0, 14, 129, 195	0
22	DA	2897/2903 (99%)	0.40	129 (4%)	33	23	41, 85, 148, 181	0
23	BB	119/119 (100%)	-0.36	0	100	100	2, 23, 46, 81	0
23	DB	118/119 (99%)	0.19	4 (3%)	45	35	69, 115, 134, 142	0
24	BC	271/271 (100%)	-0.18	1 (0%)	92	91	2, 18, 35, 55	0
24	DC	271/271 (100%)	0.73	32 (11%)	4	2	46, 64, 77, 95	0
25	BD	209/209 (100%)	-0.25	0	100	100	0, 9, 34, 65	0
25	DD	209/209 (100%)	1.16	44 (21%)	1	0	53, 72, 87, 97	0
26	BE	201/201 (100%)	-0.30	0	100	100	1, 23, 54, 88	0
26	DE	201/201 (100%)	1.86	80 (39%)	0	0	52, 89, 105, 113	0
27	BF	177/177 (100%)	0.19	4 (2%)	60	51	21, 40, 74, 88	0
27	DF	177/177 (100%)	3.27	128 (72%)	0	0	94, 113, 124, 131	0
28	BG	176/176 (100%)	0.04	3 (1%)	70	63	15, 35, 58, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	2.22	89 (50%) 0 0	78, 96, 110, 121	0
29	BH	149/149 (100%)	3.01	73 (48%) 0 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	1.18	30 (20%) 1 0	25, 92, 107, 115	0
30	BI	141/141 (100%)	3.56	100 (70%) 0 0	89, 116, 126, 134	0
30	DI	141/141 (100%)	4.83	120 (85%) 0 0	105, 124, 135, 142	0
31	BJ	142/142 (100%)	-0.27	0 100 100	1, 6, 26, 35	0
31	DJ	142/142 (100%)	0.84	16 (11%) 5 3	49, 69, 83, 91	0
32	BK	122/122 (100%)	-0.34	0 100 100	3, 11, 28, 60	0
32	DK	122/122 (100%)	1.12	29 (23%) 0 0	48, 66, 84, 95	0
33	BL	143/143 (100%)	-0.13	0 100 100	1, 18, 42, 65	0
33	DL	143/143 (100%)	1.95	62 (43%) 0 0	43, 87, 98, 115	0
34	BM	136/136 (100%)	-0.38	0 100 100	1, 10, 24, 85	0
34	DM	136/136 (100%)	1.01	26 (19%) 1 1	44, 70, 85, 99	0
35	BN	120/120 (100%)	-0.25	0 100 100	2, 7, 17, 65	0
35	DN	120/120 (100%)	1.29	28 (23%) 0 0	58, 78, 92, 112	0
36	BO	116/116 (100%)	-0.21	0 100 100	14, 24, 42, 54	0
36	DO	116/116 (100%)	2.77	75 (64%) 0 0	85, 99, 110, 117	0
37	BP	114/114 (100%)	-0.22	1 (0%) 84 80	6, 16, 41, 71	0
37	DP	114/114 (100%)	1.07	27 (23%) 0 0	61, 74, 86, 94	0
38	BQ	117/117 (100%)	-0.31	0 100 100	0, 3, 12, 30	0
38	DQ	117/117 (100%)	1.15	25 (21%) 0 0	55, 70, 81, 89	0
39	BR	103/103 (100%)	-0.29	0 100 100	0, 11, 31, 56	0
39	DR	103/103 (100%)	1.66	35 (33%) 0 0	57, 80, 92, 103	0
40	BS	110/110 (100%)	-0.22	0 100 100	1, 4, 21, 68	0
40	DS	110/110 (100%)	2.12	53 (48%) 0 0	60, 79, 94, 105	0
41	BT	93/93 (100%)	0.19	3 (3%) 47 37	10, 24, 68, 99	0
41	DT	93/93 (100%)	2.71	57 (61%) 0 0	73, 91, 106, 115	0
42	BU	102/102 (100%)	-0.22	2 (1%) 65 56	10, 25, 58, 77	0
42	DU	102/102 (100%)	3.20	65 (63%) 0 0	77, 95, 109, 120	0
43	BV	94/94 (100%)	-0.27	0 100 100	4, 18, 39, 52	0
43	DV	94/94 (100%)	1.14	21 (22%) 0 0	72, 86, 98, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.15	2 (2%) 56 46	4, 11, 27, 57	0
44	DW	75/76 (98%)	2.04	39 (52%) 0 0	58, 83, 93, 104	0
45	BX	77/77 (100%)	-0.24	0 100 100	8, 22, 48, 68	0
45	DX	77/77 (100%)	1.11	15 (19%) 1 0	47, 72, 87, 91	0
46	BY	63/63 (100%)	0.23	3 (4%) 30 21	18, 38, 71, 94	0
46	DY	63/63 (100%)	1.95	30 (47%) 0 0	81, 99, 106, 109	0
47	BZ	58/58 (100%)	-0.22	0 100 100	2, 6, 25, 34	0
47	DZ	58/58 (100%)	0.83	7 (12%) 4 2	60, 73, 85, 103	0
48	B0	56/56 (100%)	-0.30	0 100 100	0, 7, 33, 60	0
48	D0	56/56 (100%)	1.49	17 (30%) 0 0	51, 82, 95, 103	0
49	B1	50/50 (100%)	-0.23	1 (2%) 65 56	13, 25, 49, 57	0
49	D1	50/50 (100%)	1.73	15 (30%) 0 0	73, 89, 94, 106	0
50	B2	46/46 (100%)	-0.14	1 (2%) 62 52	4, 8, 15, 79	0
50	D2	46/46 (100%)	1.94	19 (41%) 0 0	58, 72, 86, 101	0
51	B3	64/64 (100%)	-0.18	0 100 100	4, 9, 17, 29	0
51	D3	64/64 (100%)	1.69	26 (40%) 0 0	60, 75, 84, 94	0
52	B4	38/38 (100%)	-0.13	0 100 100	5, 15, 29, 52	0
52	D4	38/38 (100%)	2.23	18 (47%) 0 0	62, 77, 88, 98	0
53	B5	191/228 (83%)	6.24	186 (97%) 0 0	100, 121, 133, 141	0
54	B6	2/8 (25%)	0.45	0 100 100	1, 1, 1, 1	0
54	D6	2/8 (25%)	-0.02	0 100 100	46, 46, 46, 51	0
All	All	20738/20810 (99%)	0.62	2658 (12%) 3 2	0, 63, 124, 195	0

The worst 5 of 2658 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	BI	53	LEU	25.2
53	B5	55	SER	19.9
22	BA	2101	A	17.4
22	BA	2184	A	17.4
53	B5	207	GLY	16.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MHW	D6	1	9/10	0.87	0.20	40,52,59,59	0
54	DBB	D6	3	6/7	0.91	0.30	36,38,47,51	0
54	MHU	D6	5	15/16	0.92	0.32	44,54,60,61	0
54	004	D6	7	10/11	0.94	0.21	42,47,58,59	0
54	MHW	B6	1	9/10	0.94	0.18	0,0,2,9	0
54	MHV	D6	6	9/10	0.94	0.14	45,51,58,60	0
54	DBB	B6	3	6/7	0.96	0.19	0,1,1,2	0
54	MHU	B6	5	15/16	0.96	0.20	0,0,1,2	0
54	MHV	B6	6	9/10	0.97	0.16	0,0,1,1	0
54	004	B6	7	10/11	0.97	0.23	0,0,2,3	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3111	1/1	0.18	0.32	107,107,107,107	0
55	MG	DA	3048	1/1	0.20	0.44	127,127,127,127	0
55	MG	DA	3135	1/1	0.24	0.32	101,101,101,101	0
55	MG	DA	3084	1/1	0.35	0.23	105,105,105,105	0
55	MG	DA	3100	1/1	0.36	0.20	77,77,77,77	0
55	MG	DA	3041	1/1	0.38	0.42	68,68,68,68	0
55	MG	DA	3017	1/1	0.38	0.25	98,98,98,98	0
55	MG	DA	3026	1/1	0.43	0.48	101,101,101,101	0
55	MG	BA	3134	1/1	0.46	0.42	54,54,54,54	0
55	MG	DA	3093	1/1	0.46	0.11	86,86,86,86	0
55	MG	CA	1630	1/1	0.48	0.36	120,120,120,120	0
55	MG	AA	1619	1/1	0.50	0.31	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1636	1/1	0.51	0.14	126,126,126,126	0
55	MG	DA	3148	1/1	0.51	0.29	65,65,65,65	0
55	MG	DA	3062	1/1	0.51	0.61	82,82,82,82	0
55	MG	DA	3113	1/1	0.52	0.29	66,66,66,66	0
55	MG	DA	3133	1/1	0.52	0.78	100,100,100,100	0
55	MG	DA	3144	1/1	0.52	0.10	68,68,68,68	0
55	MG	DA	3045	1/1	0.53	0.12	94,94,94,94	0
55	MG	DA	3042	1/1	0.54	0.19	87,87,87,87	0
55	MG	DA	3057	1/1	0.54	0.29	95,95,95,95	0
55	MG	CA	1635	1/1	0.54	0.13	124,124,124,124	0
55	MG	BA	3090	1/1	0.55	0.10	19,19,19,19	0
55	MG	DA	3099	1/1	0.57	0.38	86,86,86,86	0
55	MG	DA	3075	1/1	0.57	0.16	91,91,91,91	0
55	MG	DA	3067	1/1	0.59	0.13	58,58,58,58	0
55	MG	DA	3029	1/1	0.59	0.22	73,73,73,73	0
55	MG	BA	3100	1/1	0.60	0.28	52,52,52,52	0
55	MG	CA	1608	1/1	0.61	0.22	84,84,84,84	0
55	MG	CA	1627	1/1	0.61	0.20	89,89,89,89	0
55	MG	DA	3028	1/1	0.61	0.87	103,103,103,103	0
55	MG	AA	1614	1/1	0.61	0.22	69,69,69,69	0
55	MG	DA	3027	1/1	0.62	0.17	91,91,91,91	0
55	MG	DA	3071	1/1	0.63	0.49	92,92,92,92	0
55	MG	DA	3131	1/1	0.64	1.04	99,99,99,99	0
55	MG	CA	1606	1/1	0.64	0.19	89,89,89,89	0
55	MG	DA	3002	1/1	0.64	0.10	78,78,78,78	0
55	MG	DA	3127	1/1	0.64	0.15	71,71,71,71	0
55	MG	D2	101	1/1	0.65	0.15	83,83,83,83	0
55	MG	DA	3090	1/1	0.65	0.14	90,90,90,90	0
55	MG	DA	3010	1/1	0.65	0.12	80,80,80,80	0
55	MG	DA	3070	1/1	0.65	0.17	108,108,108,108	0
55	MG	CA	1629	1/1	0.66	0.12	91,91,91,91	0
55	MG	AA	1639	1/1	0.67	0.07	65,65,65,65	0
55	MG	DA	3126	1/1	0.67	0.23	80,80,80,80	0
55	MG	AA	1665	1/1	0.67	0.40	37,37,37,37	0
55	MG	AA	1658	1/1	0.67	0.35	62,62,62,62	0
55	MG	DA	3078	1/1	0.68	0.14	106,106,106,106	0
55	MG	DA	3103	1/1	0.69	0.24	73,73,73,73	0
55	MG	DA	3034	1/1	0.69	0.16	69,69,69,69	0
55	MG	DQ	201	1/1	0.69	0.30	45,45,45,45	0
55	MG	DA	3077	1/1	0.69	0.70	113,113,113,113	0
55	MG	CA	1632	1/1	0.69	0.12	73,73,73,73	0
55	MG	DA	3019	1/1	0.69	0.18	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3044	1/1	0.70	0.40	112,112,112,112	0
55	MG	DA	3155	1/1	0.71	0.45	62,62,62,62	0
55	MG	DA	3088	1/1	0.72	0.10	74,74,74,74	0
55	MG	DA	3012	1/1	0.72	0.10	73,73,73,73	0
55	MG	DA	3060	1/1	0.72	0.31	77,77,77,77	0
55	MG	CA	1602	1/1	0.72	0.11	88,88,88,88	0
55	MG	DA	3098	1/1	0.72	0.16	66,66,66,66	0
55	MG	DA	3013	1/1	0.73	0.16	44,44,44,44	0
55	MG	DA	3064	1/1	0.73	0.20	48,48,48,48	0
55	MG	AA	1620	1/1	0.73	0.12	69,69,69,69	0
55	MG	DA	3134	1/1	0.73	0.14	58,58,58,58	0
55	MG	DB	201	1/1	0.73	0.06	116,116,116,116	0
55	MG	BA	3050	1/1	0.74	0.07	27,27,27,27	0
55	MG	AA	1648	1/1	0.74	0.20	47,47,47,47	0
55	MG	DA	3136	1/1	0.74	0.16	91,91,91,91	0
55	MG	CA	1631	1/1	0.74	0.13	95,95,95,95	0
55	MG	DA	3147	1/1	0.74	0.39	54,54,54,54	0
55	MG	BA	3186	1/1	0.75	0.30	29,29,29,29	0
55	MG	DA	3005	1/1	0.75	0.43	102,102,102,102	0
55	MG	AA	1651	1/1	0.76	0.32	61,61,61,61	0
55	MG	BA	3049	1/1	0.76	0.13	44,44,44,44	0
55	MG	BA	3093	1/1	0.76	0.09	58,58,58,58	0
55	MG	DA	3046	1/1	0.76	0.16	62,62,62,62	0
55	MG	DA	3037	1/1	0.76	0.08	93,93,93,93	0
55	MG	CA	1617	1/1	0.76	0.12	39,39,39,39	0
55	MG	DA	3072	1/1	0.76	0.52	90,90,90,90	0
55	MG	CA	1605	1/1	0.76	0.19	86,86,86,86	0
55	MG	BA	3153	1/1	0.76	0.23	31,31,31,31	0
55	MG	DA	3163	1/1	0.77	0.32	54,54,54,54	0
55	MG	DA	3125	1/1	0.77	0.22	62,62,62,62	0
55	MG	AA	1626	1/1	0.77	0.17	23,23,23,23	0
55	MG	BA	3038	1/1	0.77	0.16	42,42,42,42	0
55	MG	DB	203	1/1	0.78	0.08	85,85,85,85	0
55	MG	DA	3121	1/1	0.78	0.10	52,52,52,52	0
55	MG	AA	1659	1/1	0.78	0.76	50,50,50,50	0
55	MG	BA	3167	1/1	0.78	0.18	25,25,25,25	0
55	MG	DA	3056	1/1	0.78	0.41	93,93,93,93	0
55	MG	DA	3107	1/1	0.78	0.16	75,75,75,75	0
55	MG	AA	1635	1/1	0.79	0.17	66,66,66,66	0
55	MG	BA	3077	1/1	0.79	0.17	8,8,8,8	0
55	MG	BA	3057	1/1	0.79	0.35	73,73,73,73	0
55	MG	BA	3058	1/1	0.79	0.29	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3108	1/1	0.79	0.17	59,59,59,59	0
55	MG	AM	201	1/1	0.79	0.86	62,62,62,62	0
55	MG	AA	1652	1/1	0.79	0.19	49,49,49,49	0
55	MG	DA	3003	1/1	0.79	0.47	99,99,99,99	0
55	MG	AA	1667	1/1	0.79	0.19	49,49,49,49	0
55	MG	BA	3059	1/1	0.80	0.25	38,38,38,38	0
55	MG	DA	3006	1/1	0.80	0.13	93,93,93,93	0
55	MG	AA	1657	1/1	0.80	0.63	64,64,64,64	0
55	MG	AA	1662	1/1	0.80	0.38	57,57,57,57	0
55	MG	CA	1621	1/1	0.80	0.09	64,64,64,64	0
55	MG	CA	1609	1/1	0.80	0.15	89,89,89,89	0
55	MG	DA	3152	1/1	0.80	0.29	52,52,52,52	0
55	MG	DA	3115	1/1	0.80	0.19	111,111,111,111	0
55	MG	DA	3022	1/1	0.81	0.10	52,52,52,52	0
55	MG	BA	3137	1/1	0.81	0.42	49,49,49,49	0
55	MG	BA	3103	1/1	0.81	0.17	0,0,0,0	0
55	MG	DA	3089	1/1	0.81	0.33	83,83,83,83	0
55	MG	DA	3092	1/1	0.81	0.58	113,113,113,113	0
55	MG	DA	3097	1/1	0.81	0.25	91,91,91,91	0
55	MG	CA	1638	1/1	0.81	0.10	76,76,76,76	0
55	MG	DA	3149	1/1	0.81	0.29	35,35,35,35	0
55	MG	AA	1601	1/1	0.81	0.09	58,58,58,58	0
55	MG	DA	3009	1/1	0.81	0.37	90,90,90,90	0
55	MG	DA	3073	1/1	0.81	0.11	60,60,60,60	0
55	MG	BA	3180	1/1	0.82	0.19	32,32,32,32	0
55	MG	BA	3146	1/1	0.82	0.19	30,30,30,30	0
55	MG	BA	3119	1/1	0.82	0.07	20,20,20,20	0
55	MG	BA	3151	1/1	0.82	0.27	12,12,12,12	0
55	MG	BA	3075	1/1	0.82	0.16	29,29,29,29	0
55	MG	BA	3189	1/1	0.82	0.24	45,45,45,45	0
55	MG	DA	3120	1/1	0.82	0.11	79,79,79,79	0
55	MG	CA	1626	1/1	0.82	0.08	48,48,48,48	0
55	MG	CA	1646	1/1	0.82	0.24	92,92,92,92	0
55	MG	DA	3129	1/1	0.83	0.18	45,45,45,45	0
55	MG	DA	3033	1/1	0.83	0.10	71,71,71,71	0
55	MG	BA	3021	1/1	0.83	0.19	1,1,1,1	0
55	MG	CA	1637	1/1	0.83	0.10	64,64,64,64	0
55	MG	DA	3038	1/1	0.83	0.13	63,63,63,63	0
55	MG	DA	3040	1/1	0.83	0.18	83,83,83,83	0
55	MG	DA	3091	1/1	0.83	0.09	77,77,77,77	0
55	MG	DA	3114	1/1	0.83	0.14	65,65,65,65	0
55	MG	AA	1628	1/1	0.83	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3089	1/1	0.84	0.07	33,33,33,33	0
55	MG	CA	1603	1/1	0.84	0.15	44,44,44,44	0
55	MG	BA	3046	1/1	0.84	0.09	17,17,17,17	0
55	MG	DA	3094	1/1	0.84	0.18	84,84,84,84	0
55	MG	AA	1623	1/1	0.84	0.05	46,46,46,46	0
55	MG	BA	3054	1/1	0.84	0.09	9,9,9,9	0
55	MG	DA	3016	1/1	0.84	0.14	62,62,62,62	0
55	MG	AA	1638	1/1	0.84	0.10	87,87,87,87	0
55	MG	CA	1655	1/1	0.84	0.10	44,44,44,44	0
55	MG	DA	3153	1/1	0.84	0.26	53,53,53,53	0
55	MG	AA	1644	1/1	0.84	0.39	44,44,44,44	0
55	MG	DA	3151	1/1	0.85	0.52	59,59,59,59	0
55	MG	CA	1601	1/1	0.85	0.09	39,39,39,39	0
55	MG	DA	3154	1/1	0.85	0.17	40,40,40,40	0
55	MG	BA	3027	1/1	0.85	0.34	46,46,46,46	0
55	MG	DA	3119	1/1	0.85	0.44	106,106,106,106	0
55	MG	DA	3145	1/1	0.85	0.17	71,71,71,71	0
55	MG	DA	3124	1/1	0.85	0.23	89,89,89,89	0
55	MG	BA	3069	1/1	0.85	0.15	4,4,4,4	0
55	MG	AA	1631	1/1	0.85	0.10	46,46,46,46	0
55	MG	CA	1624	1/1	0.85	0.10	45,45,45,45	0
55	MG	DA	3080	1/1	0.85	0.15	95,95,95,95	0
55	MG	CA	1604	1/1	0.85	0.13	95,95,95,95	0
55	MG	BA	3120	1/1	0.85	0.20	37,37,37,37	0
55	MG	DA	3104	1/1	0.85	0.08	79,79,79,79	0
55	MG	BA	3170	1/1	0.85	0.35	38,38,38,38	0
55	MG	DA	3047	1/1	0.85	0.13	73,73,73,73	0
55	MG	BA	3016	1/1	0.85	0.43	58,58,58,58	0
55	MG	CA	1651	1/1	0.86	0.30	44,44,44,44	0
55	MG	DA	3143	1/1	0.86	0.24	60,60,60,60	0
55	MG	DA	3008	1/1	0.86	0.26	100,100,100,100	0
55	MG	CA	1654	1/1	0.86	0.36	56,56,56,56	0
55	MG	BA	3178	1/1	0.86	0.68	30,30,30,30	0
55	MG	BA	3154	1/1	0.86	0.33	25,25,25,25	0
55	MG	CA	1615	1/1	0.86	0.30	58,58,58,58	0
55	MG	DA	3061	1/1	0.86	1.12	96,96,96,96	0
55	MG	BA	3104	1/1	0.86	0.17	17,17,17,17	0
55	MG	DA	3157	1/1	0.86	0.30	58,58,58,58	0
55	MG	DA	3039	1/1	0.86	0.18	57,57,57,57	0
55	MG	AA	1605	1/1	0.86	0.22	23,23,23,23	0
55	MG	AA	1612	1/1	0.86	0.10	47,47,47,47	0
55	MG	DA	3024	1/1	0.87	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3081	1/1	0.87	0.10	60,60,60,60	0
55	MG	CA	1628	1/1	0.87	0.18	98,98,98,98	0
55	MG	BB	202	1/1	0.87	0.10	16,16,16,16	0
55	MG	AA	1664	1/1	0.87	0.14	49,49,49,49	0
55	MG	BA	3125	1/1	0.87	0.54	37,37,37,37	0
55	MG	DA	3025	1/1	0.87	0.26	69,69,69,69	0
55	MG	AA	1661	1/1	0.87	0.29	29,29,29,29	0
55	MG	AA	1613	1/1	0.87	0.09	24,24,24,24	0
55	MG	AA	1671	1/1	0.87	0.52	59,59,59,59	0
55	MG	CA	1656	1/1	0.87	0.37	54,54,54,54	0
55	MG	DB	202	1/1	0.87	0.11	66,66,66,66	0
55	MG	DA	3165	1/1	0.87	0.22	42,42,42,42	0
55	MG	DA	3138	1/1	0.88	0.35	40,40,40,40	0
55	MG	DA	3052	1/1	0.88	0.07	56,56,56,56	0
55	MG	BA	3092	1/1	0.88	0.10	19,19,19,19	0
55	MG	DA	3049	1/1	0.88	0.25	84,84,84,84	0
55	MG	DA	3112	1/1	0.88	1.38	104,104,104,104	0
55	MG	AA	1632	1/1	0.88	0.10	55,55,55,55	0
55	MG	AA	1609	1/1	0.88	0.08	36,36,36,36	0
55	MG	BA	3179	1/1	0.88	0.33	26,26,26,26	0
55	MG	BA	3102	1/1	0.88	0.10	7,7,7,7	0
55	MG	DA	3160	1/1	0.88	0.24	43,43,43,43	0
56	DOL	DA	3001	48/48	0.88	0.26	26,45,58,63	0
55	MG	DA	3132	1/1	0.88	0.18	54,54,54,54	0
55	MG	BA	3141	1/1	0.88	0.15	17,17,17,17	0
55	MG	AA	1670	1/1	0.88	0.29	33,33,33,33	0
55	MG	AA	1650	1/1	0.88	0.32	36,36,36,36	0
55	MG	BA	3004	1/1	0.88	0.11	26,26,26,26	0
55	MG	DA	3036	1/1	0.88	0.15	62,62,62,62	0
55	MG	DA	3031	1/1	0.88	0.08	69,69,69,69	0
55	MG	AA	1634	1/1	0.88	0.13	35,35,35,35	0
55	MG	BA	3082	1/1	0.88	0.11	6,6,6,6	0
55	MG	AA	1643	1/1	0.88	0.14	28,28,28,28	0
55	MG	BA	3114	1/1	0.89	0.17	0,0,0,0	0
55	MG	AA	1630	1/1	0.89	0.18	73,73,73,73	0
55	MG	BA	3040	1/1	0.89	0.15	0,0,0,0	0
55	MG	BB	204	1/1	0.89	0.37	16,16,16,16	0
55	MG	DA	3020	1/1	0.89	0.15	54,54,54,54	0
55	MG	DA	3014	1/1	0.89	0.14	73,73,73,73	0
55	MG	DA	3110	1/1	0.89	0.23	33,33,33,33	0
55	MG	DA	3117	1/1	0.89	0.09	67,67,67,67	0
55	MG	DA	3011	1/1	0.89	0.08	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	1610	1/1	0.89	0.10	63,63,63,63	0
55	MG	BA	3157	1/1	0.89	0.19	24,24,24,24	0
55	MG	DA	3137	1/1	0.89	0.42	47,47,47,47	0
55	MG	AA	1637	1/1	0.89	0.10	15,15,15,15	0
55	MG	DA	3141	1/1	0.89	0.27	40,40,40,40	0
55	MG	CA	1650	1/1	0.89	0.22	35,35,35,35	0
55	MG	BA	3064	1/1	0.89	0.19	5,5,5,5	0
55	MG	CA	1649	1/1	0.89	0.18	52,52,52,52	0
55	MG	DA	3074	1/1	0.89	0.33	77,77,77,77	0
55	MG	CA	1613	1/1	0.89	0.14	19,19,19,19	0
55	MG	BA	3191	1/1	0.89	0.23	12,12,12,12	0
55	MG	DA	3146	1/1	0.90	0.10	43,43,43,43	0
55	MG	BA	3156	1/1	0.90	0.28	19,19,19,19	0
55	MG	DA	3007	1/1	0.90	0.44	121,121,121,121	0
55	MG	BA	3087	1/1	0.90	0.13	4,4,4,4	0
55	MG	BA	3002	1/1	0.90	0.06	18,18,18,18	0
55	MG	CA	1640	1/1	0.90	0.14	26,26,26,26	0
55	MG	BA	3112	1/1	0.90	0.08	20,20,20,20	0
55	MG	BA	3076	1/1	0.90	0.07	14,14,14,14	0
55	MG	DA	3096	1/1	0.90	0.08	57,57,57,57	0
55	MG	DA	3066	1/1	0.90	0.07	47,47,47,47	0
55	MG	AA	1602	1/1	0.90	0.13	46,46,46,46	0
55	MG	CA	1647	1/1	0.90	0.11	41,41,41,41	0
55	MG	DA	3058	1/1	0.90	1.10	109,109,109,109	0
55	MG	DA	3085	1/1	0.90	0.12	67,67,67,67	0
55	MG	CA	1648	1/1	0.90	0.20	22,22,22,22	0
55	MG	BA	3051	1/1	0.90	0.17	6,6,6,6	0
55	MG	BA	3182	1/1	0.90	0.25	33,33,33,33	0
55	MG	DA	3069	1/1	0.90	0.09	79,79,79,79	0
55	MG	BA	3169	1/1	0.90	0.16	35,35,35,35	0
55	MG	AA	1660	1/1	0.90	0.22	51,51,51,51	0
55	MG	BA	3171	1/1	0.90	0.20	24,24,24,24	0
55	MG	AA	1629	1/1	0.91	0.14	61,61,61,61	0
55	MG	DA	3054	1/1	0.91	0.10	55,55,55,55	0
55	MG	DA	3164	1/1	0.91	0.18	57,57,57,57	0
55	MG	DA	3068	1/1	0.91	0.13	65,65,65,65	0
55	MG	DA	3030	1/1	0.91	0.24	60,60,60,60	0
55	MG	DA	3015	1/1	0.91	0.06	55,55,55,55	0
55	MG	BA	3008	1/1	0.91	0.14	37,37,37,37	0
55	MG	DA	3159	1/1	0.91	0.30	43,43,43,43	0
55	MG	DA	3050	1/1	0.91	0.10	56,56,56,56	0
55	MG	CA	1616	1/1	0.91	0.10	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3150	1/1	0.91	0.20	56,56,56,56	0
55	MG	DA	3032	1/1	0.91	0.26	68,68,68,68	0
55	MG	DA	3123	1/1	0.91	0.12	57,57,57,57	0
55	MG	BA	3193	1/1	0.91	0.15	38,38,38,38	0
55	MG	DA	3021	1/1	0.91	0.18	63,63,63,63	0
55	MG	BA	3015	1/1	0.91	0.07	2,2,2,2	0
55	MG	CA	1614	1/1	0.91	0.08	50,50,50,50	0
55	MG	BA	3081	1/1	0.91	0.12	24,24,24,24	0
55	MG	BA	3006	1/1	0.91	0.14	50,50,50,50	0
55	MG	DA	3065	1/1	0.91	0.12	36,36,36,36	0
55	MG	AA	1641	1/1	0.91	0.15	19,19,19,19	0
55	MG	BA	3195	1/1	0.91	0.56	23,23,23,23	0
55	MG	BA	3132	1/1	0.91	0.09	23,23,23,23	0
55	MG	DA	3106	1/1	0.91	0.14	52,52,52,52	0
55	MG	DA	3087	1/1	0.91	0.09	54,54,54,54	0
55	MG	BA	3168	1/1	0.91	0.12	35,35,35,35	0
55	MG	DA	3105	1/1	0.91	0.18	80,80,80,80	0
55	MG	BA	3003	1/1	0.91	0.06	17,17,17,17	0
55	MG	BA	3116	1/1	0.91	0.26	34,34,34,34	0
55	MG	BA	3033	1/1	0.91	0.12	11,11,11,11	0
55	MG	BA	3005	1/1	0.91	0.07	34,34,34,34	0
55	MG	BA	3078	1/1	0.91	0.72	79,79,79,79	0
55	MG	CA	1607	1/1	0.92	0.08	54,54,54,54	0
55	MG	AA	1625	1/1	0.92	0.07	47,47,47,47	0
55	MG	AA	1654	1/1	0.92	0.14	43,43,43,43	0
55	MG	CA	1639	1/1	0.92	0.10	43,43,43,43	0
55	MG	BA	3071	1/1	0.92	0.07	60,60,60,60	0
55	MG	BA	3098	1/1	0.92	0.12	2,2,2,2	0
55	MG	BA	3042	1/1	0.92	0.38	0,0,0,0	0
55	MG	DA	3158	1/1	0.92	0.19	70,70,70,70	0
55	MG	BA	3133	1/1	0.92	0.10	32,32,32,32	0
55	MG	DA	3082	1/1	0.92	0.13	60,60,60,60	0
55	MG	BA	3152	1/1	0.92	0.19	6,6,6,6	0
55	MG	BA	3127	1/1	0.92	0.12	9,9,9,9	0
55	MG	AA	1646	1/1	0.92	0.20	49,49,49,49	0
55	MG	CA	1622	1/1	0.92	0.13	51,51,51,51	0
55	MG	DA	3004	1/1	0.92	0.11	76,76,76,76	0
55	MG	DA	3116	1/1	0.92	0.36	76,76,76,76	0
55	MG	DA	3023	1/1	0.92	0.05	69,69,69,69	0
55	MG	BA	3066	1/1	0.92	0.15	0,0,0,0	0
55	MG	BA	3063	1/1	0.92	0.45	31,31,31,31	0
55	MG	AA	1606	1/1	0.92	0.11	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1603	1/1	0.92	0.10	44,44,44,44	0
55	MG	BA	3086	1/1	0.92	0.07	14,14,14,14	0
55	MG	BA	3091	1/1	0.92	0.09	3,3,3,3	0
55	MG	CA	1620	1/1	0.92	0.06	61,61,61,61	0
55	MG	DA	3095	1/1	0.92	0.41	91,91,91,91	0
55	MG	BA	3174	1/1	0.92	0.12	12,12,12,12	0
55	MG	BA	3113	1/1	0.92	0.17	22,22,22,22	0
55	MG	BA	3187	1/1	0.92	0.06	33,33,33,33	0
55	MG	BA	3131	1/1	0.92	0.18	1,1,1,1	0
55	MG	AA	1666	1/1	0.92	0.19	46,46,46,46	0
55	MG	BA	3047	1/1	0.92	0.10	4,4,4,4	0
55	MG	DA	3053	1/1	0.93	0.11	40,40,40,40	0
55	MG	AA	1610	1/1	0.93	0.23	65,65,65,65	0
55	MG	BA	3173	1/1	0.93	0.14	27,27,27,27	0
55	MG	BA	3013	1/1	0.93	0.21	0,0,0,0	0
55	MG	DA	3142	1/1	0.93	0.26	33,33,33,33	0
55	MG	BA	3030	1/1	0.93	0.14	9,9,9,9	0
55	MG	BA	3121	1/1	0.93	0.12	3,3,3,3	0
55	MG	BA	3181	1/1	0.93	0.20	24,24,24,24	0
55	MG	BA	3155	1/1	0.93	0.21	20,20,20,20	0
55	MG	BA	3190	1/1	0.93	0.10	31,31,31,31	0
55	MG	AA	1627	1/1	0.93	0.09	37,37,37,37	0
55	MG	CA	1633	1/1	0.93	0.32	64,64,64,64	0
55	MG	BA	3185	1/1	0.93	0.30	16,16,16,16	0
55	MG	CA	1643	1/1	0.93	0.24	50,50,50,50	0
55	MG	AA	1617	1/1	0.93	0.12	52,52,52,52	0
55	MG	BA	3031	1/1	0.93	0.07	14,14,14,14	0
55	MG	DA	3101	1/1	0.93	0.09	57,57,57,57	0
55	MG	BA	3126	1/1	0.93	0.12	6,6,6,6	0
55	MG	DA	3161	1/1	0.93	0.11	57,57,57,57	0
55	MG	AA	1669	1/1	0.93	0.42	51,51,51,51	0
55	MG	AA	1663	1/1	0.93	0.22	48,48,48,48	0
55	MG	AA	1618	1/1	0.93	0.08	37,37,37,37	0
55	MG	BA	3166	1/1	0.93	0.17	19,19,19,19	0
55	MG	BA	3034	1/1	0.93	0.10	6,6,6,6	0
55	MG	DA	3140	1/1	0.93	0.43	43,43,43,43	0
55	MG	BA	3056	1/1	0.93	0.08	5,5,5,5	0
55	MG	CA	1652	1/1	0.93	0.11	83,83,83,83	0
55	MG	DA	3130	1/1	0.93	0.10	81,81,81,81	0
55	MG	BA	3065	1/1	0.93	0.14	0,0,0,0	0
55	MG	BA	3085	1/1	0.93	0.22	27,27,27,27	0
55	MG	BA	3079	1/1	0.93	0.09	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3136	1/1	0.93	0.12	21,21,21,21	0
55	MG	BA	3149	1/1	0.93	0.12	38,38,38,38	0
55	MG	CA	1641	1/1	0.94	0.68	73,73,73,73	0
55	MG	DA	3079	1/1	0.94	0.13	96,96,96,96	0
55	MG	DA	3167	1/1	0.94	0.29	100,100,100,100	0
55	MG	AA	1607	1/1	0.94	0.09	44,44,44,44	0
55	MG	DA	3035	1/1	0.94	0.09	79,79,79,79	0
55	MG	BA	3150	1/1	0.94	0.20	37,37,37,37	0
55	MG	AA	1668	1/1	0.94	0.13	29,29,29,29	0
55	MG	CA	1625	1/1	0.94	0.15	22,22,22,22	0
55	MG	CA	1619	1/1	0.94	0.10	33,33,33,33	0
55	MG	BA	3160	1/1	0.94	0.10	10,10,10,10	0
55	MG	CA	1645	1/1	0.94	0.20	32,32,32,32	0
55	MG	BA	3043	1/1	0.94	0.13	16,16,16,16	0
55	MG	BA	3084	1/1	0.94	0.05	6,6,6,6	0
55	MG	BA	3140	1/1	0.94	0.39	0,0,0,0	0
55	MG	CA	1642	1/1	0.94	0.25	25,25,25,25	0
55	MG	DA	3102	1/1	0.94	0.22	62,62,62,62	0
55	MG	BA	3053	1/1	0.94	0.14	2,2,2,2	0
55	MG	AA	1649	1/1	0.94	0.14	32,32,32,32	0
55	MG	BA	3159	1/1	0.94	0.22	14,14,14,14	0
55	MG	DA	3055	1/1	0.94	0.13	72,72,72,72	0
55	MG	CA	1653	1/1	0.94	0.09	52,52,52,52	0
55	MG	BA	3164	1/1	0.94	0.14	4,4,4,4	0
55	MG	BA	3039	1/1	0.94	0.27	0,0,0,0	0
55	MG	BA	3115	1/1	0.94	0.12	20,20,20,20	0
55	MG	BA	3165	1/1	0.94	0.30	43,43,43,43	0
55	MG	BA	3025	1/1	0.94	0.10	2,2,2,2	0
55	MG	BA	3080	1/1	0.94	0.07	39,39,39,39	0
55	MG	BA	3192	1/1	0.94	0.21	22,22,22,22	0
55	MG	AA	1616	1/1	0.94	0.12	50,50,50,50	0
55	MG	BA	3130	1/1	0.94	0.12	0,0,0,0	0
55	MG	BA	3020	1/1	0.95	0.09	22,22,22,22	0
55	MG	BA	3172	1/1	0.95	0.17	31,31,31,31	0
55	MG	BA	3061	1/1	0.95	0.35	30,30,30,30	0
55	MG	BA	3036	1/1	0.95	0.12	11,11,11,11	0
55	MG	AA	1653	1/1	0.95	0.17	28,28,28,28	0
55	MG	AA	1608	1/1	0.95	0.14	17,17,17,17	0
55	MG	AA	1640	1/1	0.95	0.09	36,36,36,36	0
55	MG	BA	3017	1/1	0.95	0.06	2,2,2,2	0
55	MG	BB	203	1/1	0.95	0.06	7,7,7,7	0
55	MG	BA	3045	1/1	0.95	0.08	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1655	1/1	0.95	0.11	35,35,35,35	0
55	MG	BA	3118	1/1	0.95	0.12	1,1,1,1	0
55	MG	DA	3043	1/1	0.95	0.13	66,66,66,66	0
55	MG	BA	3145	1/1	0.95	0.29	28,28,28,28	0
55	MG	BA	3094	1/1	0.95	0.05	31,31,31,31	0
55	MG	AA	1624	1/1	0.95	0.04	41,41,41,41	0
55	MG	DA	3109	1/1	0.95	0.22	42,42,42,42	0
55	MG	DA	3051	1/1	0.95	0.09	28,28,28,28	0
55	MG	BA	3161	1/1	0.95	0.17	31,31,31,31	0
55	MG	BA	3138	1/1	0.95	0.45	1,1,1,1	0
55	MG	AA	1647	1/1	0.95	0.12	48,48,48,48	0
55	MG	BA	3062	1/1	0.95	0.36	50,50,50,50	0
55	MG	DA	3166	1/1	0.95	0.09	41,41,41,41	0
55	MG	BA	3035	1/1	0.95	0.18	0,0,0,0	0
55	MG	BA	3148	1/1	0.95	0.12	29,29,29,29	0
55	MG	BA	3088	1/1	0.95	0.23	2,2,2,2	0
55	MG	DA	3118	1/1	0.95	0.08	60,60,60,60	0
55	MG	BA	3188	1/1	0.95	0.14	10,10,10,10	0
55	MG	CA	1611	1/1	0.95	0.29	90,90,90,90	0
55	MG	CA	1644	1/1	0.96	0.15	42,42,42,42	0
55	MG	BA	3009	1/1	0.96	0.09	4,4,4,4	0
55	MG	DA	3122	1/1	0.96	0.15	41,41,41,41	0
55	MG	DA	3128	1/1	0.96	0.08	80,80,80,80	0
55	MG	BA	3147	1/1	0.96	0.31	9,9,9,9	0
55	MG	BA	3176	1/1	0.96	0.10	20,20,20,20	0
55	MG	BA	3024	1/1	0.96	0.17	0,0,0,0	0
55	MG	BA	3070	1/1	0.96	0.21	0,0,0,0	0
55	MG	DA	3083	1/1	0.96	0.10	69,69,69,69	0
55	MG	BA	3101	1/1	0.96	0.07	1,1,1,1	0
55	MG	BA	3124	1/1	0.96	0.09	11,11,11,11	0
55	MG	BA	3026	1/1	0.96	0.15	3,3,3,3	0
55	MG	CA	1623	1/1	0.96	0.16	50,50,50,50	0
55	MG	CA	1634	1/1	0.96	0.13	49,49,49,49	0
55	MG	BA	3029	1/1	0.96	0.08	21,21,21,21	0
55	MG	BA	3135	1/1	0.96	0.14	2,2,2,2	0
55	MG	BA	3175	1/1	0.96	0.11	27,27,27,27	0
55	MG	CA	1618	1/1	0.96	0.11	37,37,37,37	0
55	MG	BB	201	1/1	0.96	0.10	20,20,20,20	0
55	MG	BA	3014	1/1	0.96	0.18	0,0,0,0	0
55	MG	BA	3023	1/1	0.96	0.14	1,1,1,1	0
55	MG	DA	3018	1/1	0.96	0.12	60,60,60,60	0
55	MG	BA	3074	1/1	0.96	0.18	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	3022	1/1	0.96	0.08	2,2,2,2	0
55	MG	AA	1633	1/1	0.96	0.12	30,30,30,30	0
55	MG	BA	3110	1/1	0.96	0.20	3,3,3,3	0
55	MG	CA	1612	1/1	0.96	0.05	40,40,40,40	0
55	MG	BA	3095	1/1	0.96	0.09	21,21,21,21	0
55	MG	DA	3059	1/1	0.96	0.10	51,51,51,51	0
55	MG	BA	3108	1/1	0.96	0.24	0,0,0,0	0
55	MG	BA	3122	1/1	0.96	0.04	18,18,18,18	0
55	MG	BA	3044	1/1	0.96	0.14	3,3,3,3	0
55	MG	BA	3012	1/1	0.96	0.05	14,14,14,14	0
56	DOL	BA	3001	48/48	0.96	0.21	0,3,25,36	0
55	MG	BA	3060	1/1	0.97	0.06	15,15,15,15	0
55	MG	BA	3068	1/1	0.97	0.17	0,0,0,0	0
55	MG	DA	3076	1/1	0.97	0.12	69,69,69,69	0
55	MG	BA	3142	1/1	0.97	0.43	2,2,2,2	0
55	MG	AA	1615	1/1	0.97	0.06	47,47,47,47	0
55	MG	BA	3037	1/1	0.97	0.17	0,0,0,0	0
55	MG	BA	3158	1/1	0.97	0.12	19,19,19,19	0
55	MG	DA	3156	1/1	0.97	0.19	41,41,41,41	0
55	MG	BA	3117	1/1	0.97	0.17	1,1,1,1	0
55	MG	BA	3018	1/1	0.97	0.20	0,0,0,0	0
55	MG	DA	3063	1/1	0.97	0.22	54,54,54,54	0
55	MG	BA	3007	1/1	0.97	0.09	22,22,22,22	0
55	MG	BA	3052	1/1	0.97	0.06	11,11,11,11	0
55	MG	BA	3067	1/1	0.97	0.17	0,0,0,0	0
55	MG	BA	3073	1/1	0.97	0.07	7,7,7,7	0
55	MG	BA	3123	1/1	0.97	0.16	0,0,0,0	0
55	MG	BA	3184	1/1	0.97	0.20	6,6,6,6	0
55	MG	BA	3083	1/1	0.97	0.17	0,0,0,0	0
55	MG	AA	1604	1/1	0.97	0.06	48,48,48,48	0
55	MG	BA	3163	1/1	0.97	0.33	15,15,15,15	0
55	MG	BA	3032	1/1	0.97	0.16	4,4,4,4	0
55	MG	BA	3111	1/1	0.97	0.20	6,6,6,6	0
55	MG	DA	3086	1/1	0.97	0.10	76,76,76,76	0
55	MG	BQ	201	1/1	0.97	0.20	3,3,3,3	0
55	MG	BA	3183	1/1	0.97	0.21	12,12,12,12	0
55	MG	AA	1642	1/1	0.97	0.15	23,23,23,23	0
55	MG	BA	3072	1/1	0.97	0.08	3,3,3,3	0
55	MG	BA	3129	1/1	0.97	0.19	4,4,4,4	0
55	MG	BA	3010	1/1	0.97	0.11	0,0,0,0	0
55	MG	AA	1611	1/1	0.97	0.09	21,21,21,21	0
55	MG	BA	3128	1/1	0.98	0.10	0,0,0,0	0

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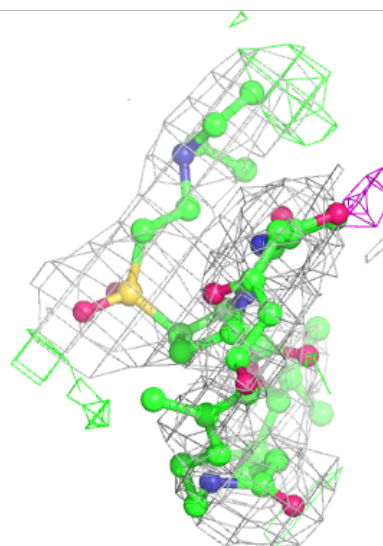
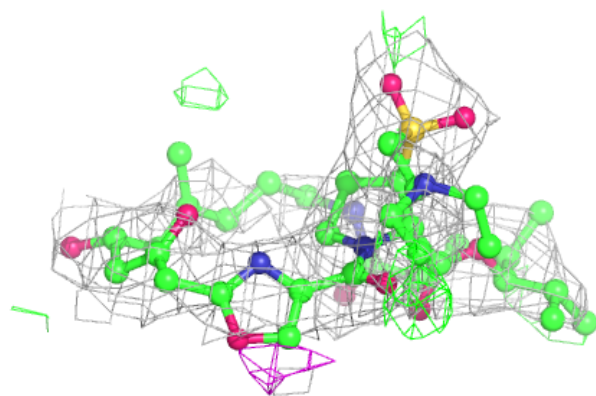
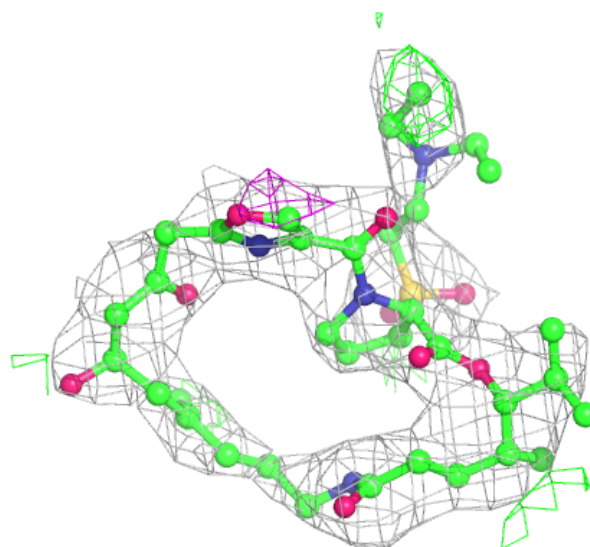
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	ZN	B4	101	1/1	0.98	0.10	33,33,33,33	0
55	MG	AA	1645	1/1	0.98	0.12	42,42,42,42	0
55	MG	BA	3162	1/1	0.98	0.07	36,36,36,36	0
55	MG	BA	3106	1/1	0.98	0.20	16,16,16,16	0
55	MG	BA	3144	1/1	0.98	0.26	15,15,15,15	0
55	MG	BA	3041	1/1	0.98	0.18	6,6,6,6	0
55	MG	BA	3105	1/1	0.98	0.10	4,4,4,4	0
55	MG	BA	3177	1/1	0.98	0.17	17,17,17,17	0
55	MG	BA	3109	1/1	0.98	0.19	12,12,12,12	0
55	MG	BA	3019	1/1	0.98	0.12	11,11,11,11	0
55	MG	DA	3162	1/1	0.98	0.21	38,38,38,38	0
55	MG	BA	3096	1/1	0.98	0.07	11,11,11,11	0
55	MG	BA	3107	1/1	0.98	0.19	0,0,0,0	0
55	MG	AA	1636	1/1	0.98	0.08	27,27,27,27	0
55	MG	BA	3139	1/1	0.98	0.37	0,0,0,0	0
55	MG	BA	3028	1/1	0.98	0.08	5,5,5,5	0
55	MG	BA	3097	1/1	0.98	0.07	4,4,4,4	0
55	MG	AA	1621	1/1	0.98	0.08	39,39,39,39	0
55	MG	BA	3194	1/1	0.98	0.07	8,8,8,8	0
55	MG	AA	1656	1/1	0.98	0.15	43,43,43,43	0
55	MG	BA	3099	1/1	0.98	0.12	4,4,4,4	0
57	ZN	D4	101	1/1	0.98	0.10	87,87,87,87	0
55	MG	AA	1622	1/1	0.98	0.20	16,16,16,16	0
55	MG	BA	3055	1/1	0.98	0.17	0,0,0,0	0
55	MG	DA	3139	1/1	0.99	0.33	30,30,30,30	0
55	MG	BA	3011	1/1	0.99	0.15	1,1,1,1	0
55	MG	BA	3048	1/1	0.99	0.15	8,8,8,8	0
55	MG	BA	3143	1/1	0.99	0.36	12,12,12,12	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.

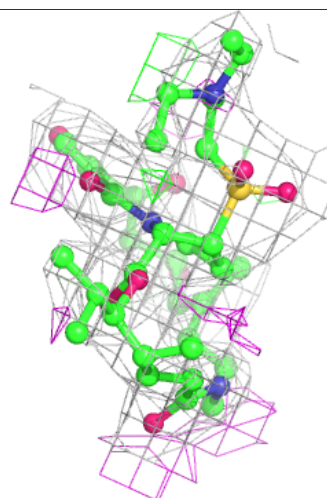
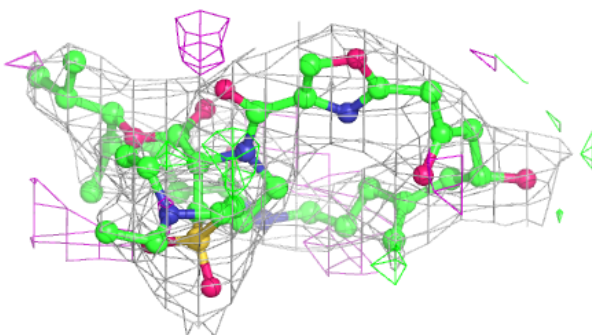
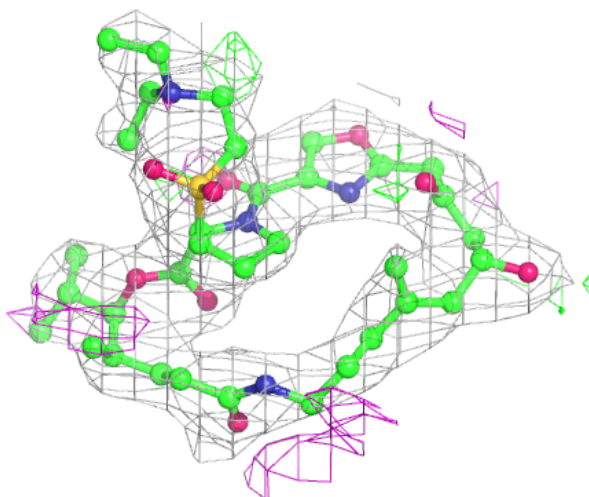
Electron density around DOL DA 3001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DOL BA 3001:

$2mF_o-DF_c$ (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.