



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 04:48 am BST

PDB ID : 4WOI
Title : 4,5-linked aminoglycoside antibiotics regulate the bacterial ribosome by targeting dynamic conformational processes within intersubunit bridge B2
Authors : Pulk, A.; Cate, J.H.D.; Blanchard, S.; Wasserman, M.; Altman, R.; Zhou, Z.; Zinder, J.; Green, K.; Garneau-Tsodikova, S.
Deposited on : 2014-10-15
Resolution : 3.00 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

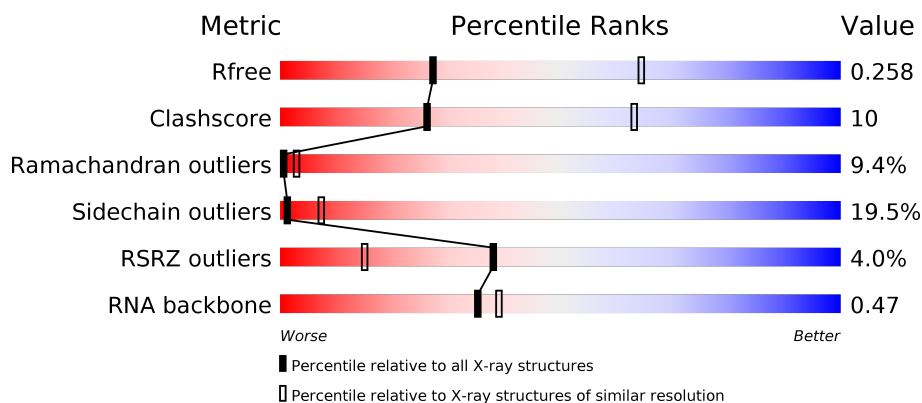
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



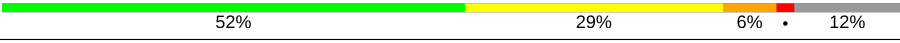

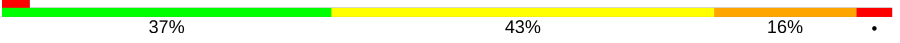
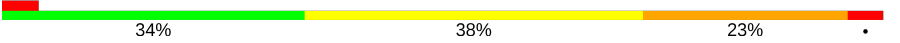


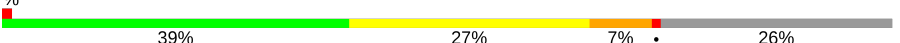
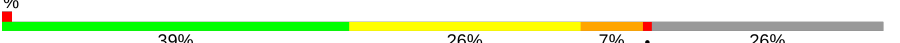
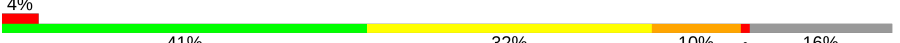




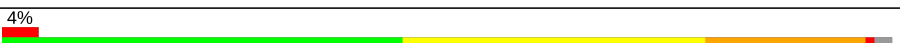
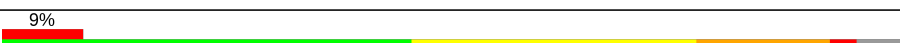

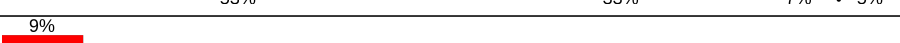
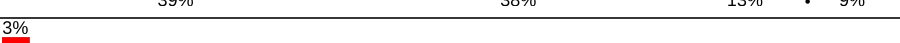
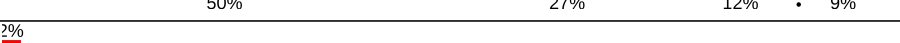

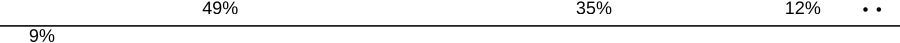
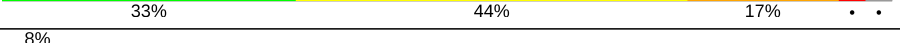

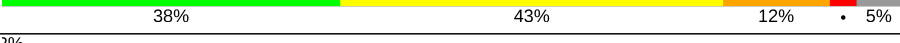

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	1542	
1	DA	1542	
2	AB	241	
2	DB	241	

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Mol	Chain	Length	Quality of chain
3	AC	233	
3	DC	233	
4	AD	206	
4	DD	206	
5	AE	167	
5	DE	167	
6	AF	135	
6	DF	135	
7	AG	179	
7	DG	179	
8	AH	130	
8	DH	130	
9	AI	130	
9	DI	130	
10	AJ	103	
10	DJ	103	
11	AK	129	
11	DK	129	
12	AL	124	
12	DL	124	
13	AM	118	
13	DM	118	
14	AN	101	
14	DN	101	
15	AO	89	






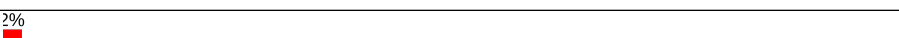
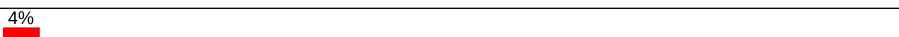
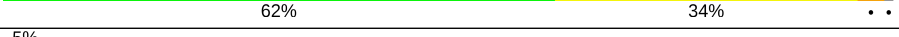
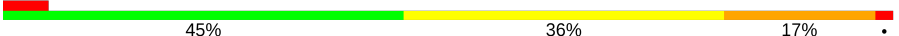














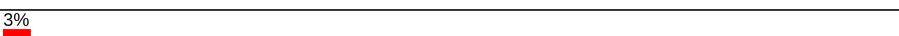

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Mol	Chain	Length	Quality of chain
15	DO	89	
16	AP	82	
16	DP	82	
17	AQ	84	
17	DQ	84	
18	AR	75	
18	DR	75	
19	AS	92	
19	DS	92	
20	AT	87	
20	DT	87	
21	AU	71	
21	DU	71	
22	AV	185	
23	AW	16	
23	DV	16	
24	AX	76	
24	DW	76	
25	BA	2904	
25	CA	2904	
26	BB	120	
26	CB	120	
27	BC	273	
27	CC	273	
28	BD	209	









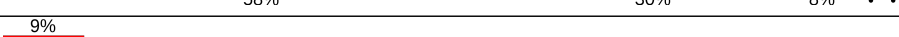








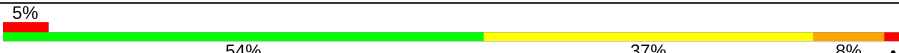

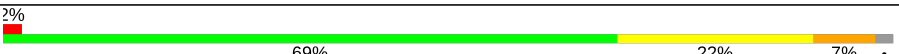


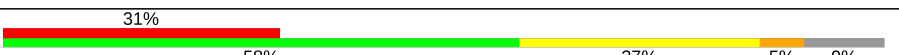
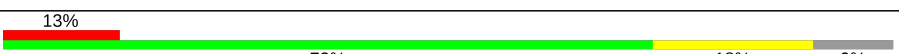

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Mol	Chain	Length	Quality of chain
28	CD	209	
29	BE	201	
29	CE	201	
30	BF	179	
30	CF	179	
31	BG	177	
31	CG	177	
32	BH	149	
32	CH	149	
33	BI	142	
33	CI	142	
34	BJ	142	
34	CJ	142	
35	BK	123	
35	CK	123	
36	BL	144	
36	CL	144	
37	BM	136	
37	CM	136	
38	BN	127	
38	CN	127	
39	BO	117	
39	CO	117	
40	BP	115	
40	CP	115	






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Mol	Chain	Length	Quality of chain
41	BQ	118	
41	CQ	118	
42	BR	103	
42	CR	103	
43	BS	110	
43	CS	110	
44	BT	100	
44	CT	100	
45	BU	104	
45	CU	104	
46	BV	94	
46	CV	94	
47	BW	85	
47	CW	85	
48	BX	78	
48	CX	78	
49	BY	63	
49	CY	63	
50	BZ	59	
50	CZ	59	
51	B0	57	
51	C0	57	
52	B1	55	
52	C1	55	
53	B2	46	

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Mol	Chain	Length	Quality of chain
53	C2	46	
54	B3	65	
54	C3	65	
55	B4	38	
55	C4	38	
56	B5	228	

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
57	MG	AA	1646	-	-	-	X
57	MG	AA	1658	-	-	-	X
57	MG	CA	3013	-	-	-	X
57	MG	CA	3095	-	-	-	X
58	PAR	BA	3005	-	-	X	-
58	PAR	CA	3168	-	-	-	X
58	PAR	CA	3169	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 294484 atoms, of which 450 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	DA	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
			1704	1081	305	311	7			
2	DB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	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
			1624	1028	305	288	3			
3	DC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	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	DD	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
			1105	687	211	201	6			
5	DE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
6	DF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
7	DG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	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	DH	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	DI	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
			786	493	150	142	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	DJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	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	DK	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	DL	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
			883	546	178	156	3			
13	DM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	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	DN	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
			716	440	146	129	1			
15	DO	88	Total	C	N	O	S	0	0	0
			716	440	146	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	DP	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
			648	411	121	113	3			
17	DQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	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
			455	288	86	81			
18	DR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- 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
			637	408	120	107	2			
19	DS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	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	DT	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
			425	265	86	73	1			
21	DU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a protein called Ribosome-recycling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	183	Total	C	N	O	S	0	0	0
			1419	871	260	283	5			

- Molecule 23 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	15	Total	C	N	O	P	0	0	0
			324	145	61	103	15			
23	DV	16	Total	C	N	O	P	0	0	0
			346	155	66	109	16			

- Molecule 24 is a RNA chain called Phenylalanine specific transfer RNA, tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
24	DW	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
27	CC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
30	CF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	149	Total	C	N	O	S	0	0	0
			1107	696	197	213	1			
32	CH	149	Total	C	N	O	S	0	0	0
			1107	696	197	213	1			

- Molecule 33 is a protein called 50S ribosomal protein L11.

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

- Molecule 34 is a protein called 50S ribosomal protein L13.

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

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
35	CK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 36 is a protein called 50S ribosomal protein L15.

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

- Molecule 37 is a protein called 50S ribosomal protein L16.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
38	CN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BO	116	Total	C	N	O	S	0	0	0
			892	552	178	162				
39	CO	116	Total	C	N	O	S	0	0	0
			892	552	178	162				

- Molecule 40 is a protein called 50S ribosomal protein L19.

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

- Molecule 41 is a protein called 50S ribosomal protein L20.

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

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

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

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
44	CT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BU	102	Total	C	N	O	0	0	0
			779	492	146	141			
45	CU	102	Total	C	N	O	0	0	0
			779	492	146	141			

- Molecule 46 is a protein called 50S ribosomal protein L25.

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

- Molecule 47 is a protein called 50S ribosomal protein L27.

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

- Molecule 48 is a protein called 50S ribosomal protein L28.

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

- Molecule 49 is a protein called 50S ribosomal protein L29.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
51	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	B1	50	Total	C	N	O	0	0	0
			409	263	75	71			
52	C1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
54	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
55	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 56 is a protein called 50S ribosomal protein L1.

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

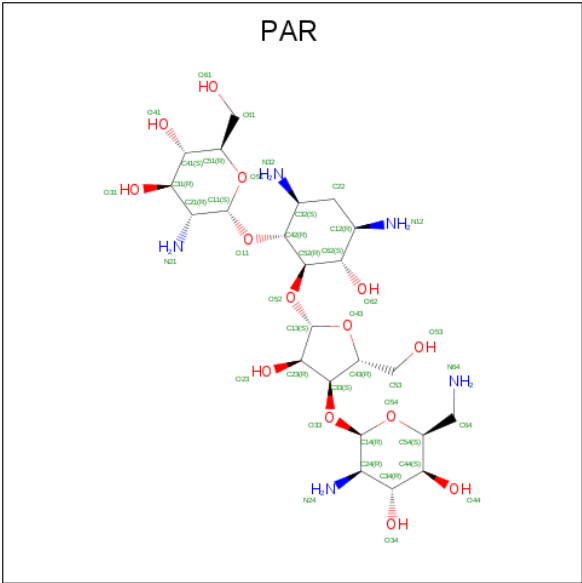
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BB	4	Total	Mg	0	0
			4	4		
57	BO	1	Total	Mg	0	0
			1	1		
57	BA	189	Total	Mg	0	0
			189	189		
57	CA	165	Total	Mg	0	0
			165	165		
57	CB	3	Total	Mg	0	0
			3	3		
57	BL	2	Total	Mg	0	0
			2	2		
57	DA	53	Total	Mg	0	0
			53	53		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CD	1	Total	Mg	0	0
			1	1		
57	AA	71	Total	Mg	0	0
			71	71		
57	BQ	1	Total	Mg	0	0
			1	1		
57	CQ	1	Total	Mg	0	0
			1	1		
57	AN	1	Total	Mg	0	0
			1	1		
57	DN	1	Total	Mg	0	0
			1	1		
57	DD	2	Total	Mg	0	0
			2	2		

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	AA	1	Total	C	H	N	O	0	0
			87	23	45	5	14		
58	BA	1	Total	C	H	N	O	0	0
			87	23	45	5	14		
58	BA	1	Total	C	H	N	O	0	0
			87	23	45	5	14		
58	BA	1	Total	C	H	N	O	0	0
			87	23	45	5	14		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	BA	1	Total C H N O 87 23 45 5 14	0	0
58	BA	1	Total C N O 42 23 5 14	0	0
58	CA	1	Total C N O 42 23 5 14	0	0
58	CA	1	Total C H N O 87 23 45 5 14	0	0
58	CA	1	Total C H N O 87 23 45 5 14	0	0
58	CA	1	Total C N O 42 23 5 14	0	0
58	CA	1	Total C H N O 87 23 45 5 14	0	0
58	DA	1	Total C H N O 87 23 45 5 14	0	0
58	DA	1	Total C H N O 87 23 45 5 14	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	B4	1	Total Zn 1 1	0	0
59	C4	1	Total Zn 1 1	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AA	192	Total O 192 192	0	0
60	AE	3	Total O 3 3	0	0
60	AL	1	Total O 1 1	0	0
60	AN	2	Total O 2 2	0	0
60	AT	5	Total O 5 5	0	0
60	BA	626	Total O 626 626	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BB	14	Total 14	O 14	0	0
60	BC	7	Total 7	O 7	0	0
60	BD	2	Total 2	O 2	0	0
60	BE	1	Total 1	O 1	0	0
60	BF	1	Total 1	O 1	0	0
60	BL	8	Total 8	O 8	0	0
60	BN	2	Total 2	O 2	0	0
60	BQ	1	Total 1	O 1	0	0
60	BS	1	Total 1	O 1	0	0
60	BT	3	Total 3	O 3	0	0
60	B3	1	Total 1	O 1	0	0
60	B4	1	Total 1	O 1	0	0
60	CA	608	Total 608	O 608	0	0
60	CB	14	Total 14	O 14	0	0
60	CC	10	Total 10	O 10	0	0
60	CD	5	Total 5	O 5	0	0
60	CE	3	Total 3	O 3	0	0
60	CJ	2	Total 2	O 2	0	0
60	CL	7	Total 7	O 7	0	0
60	CN	2	Total 2	O 2	0	0
60	CT	3	Total 3	O 3	0	0

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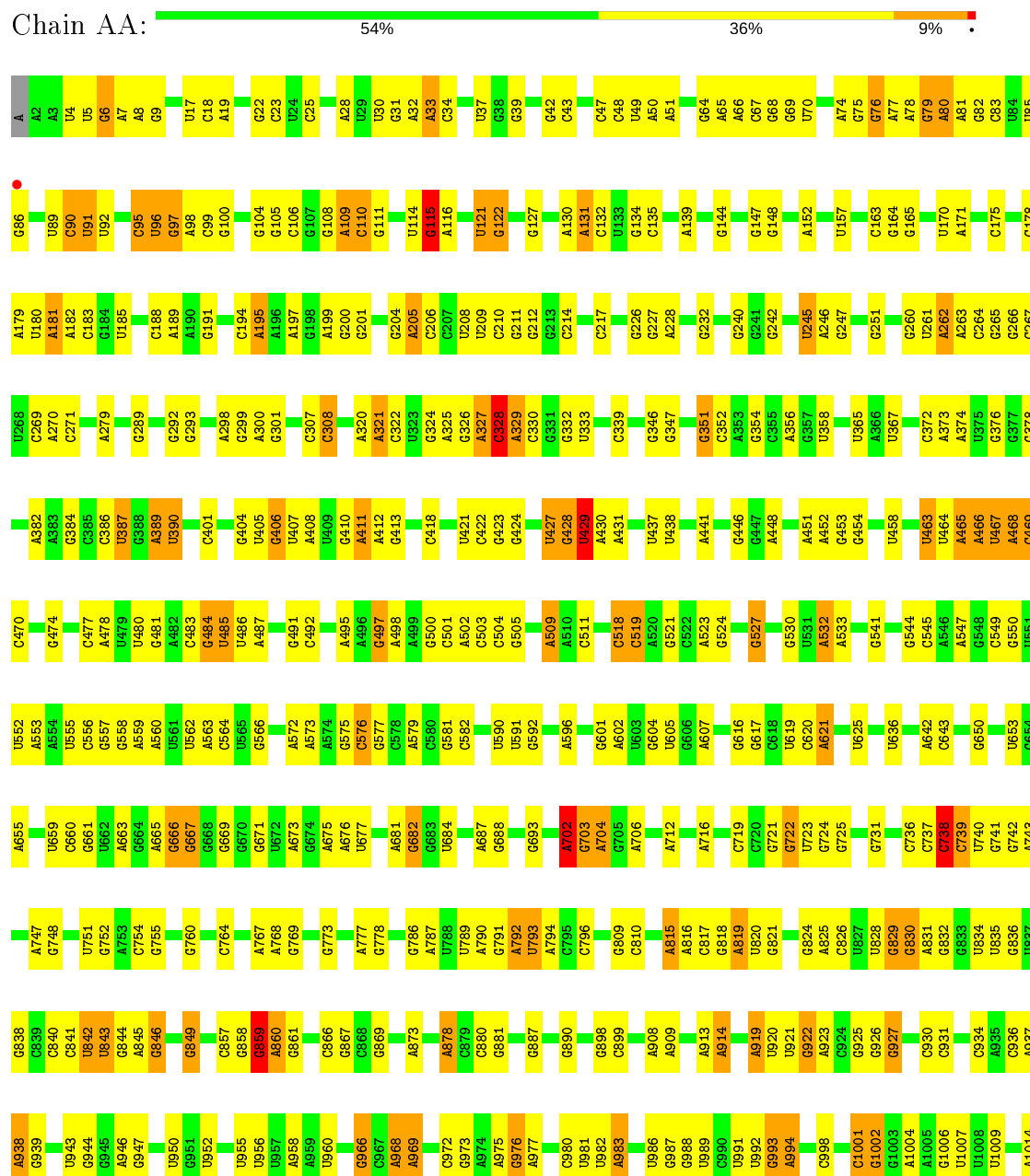
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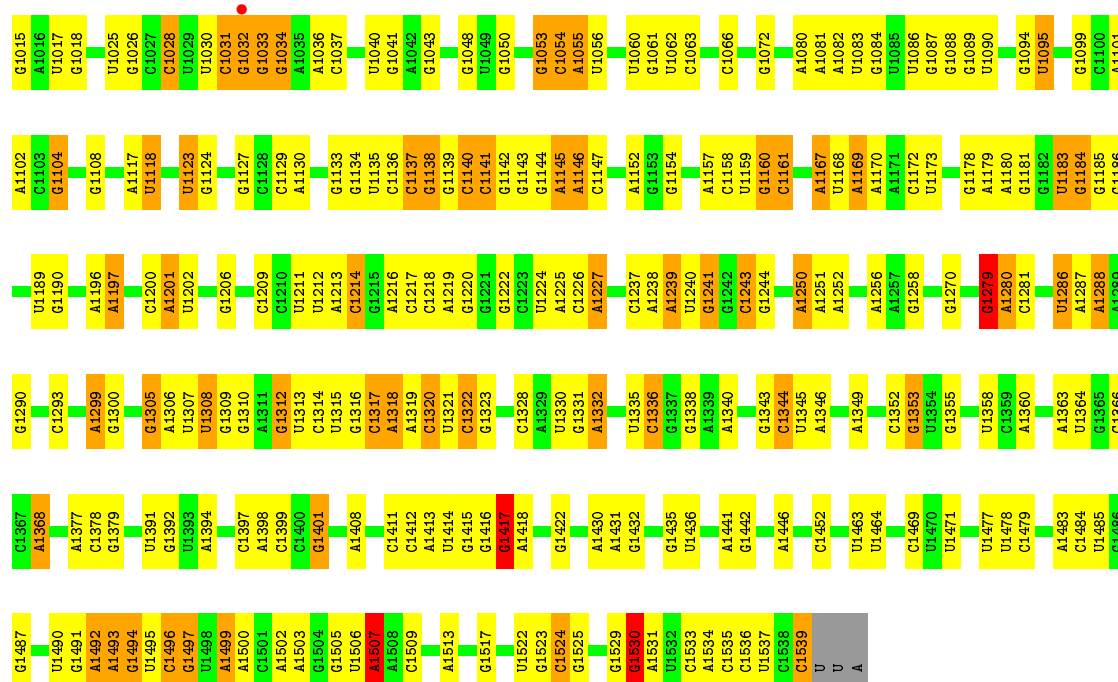
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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60	C3	1	Total 1	O 1	0	0
60	C4	2	Total 2	O 2	0	0
60	DA	184	Total 184	O 184	0	0
60	DD	2	Total 2	O 2	0	0
60	DK	2	Total 2	O 2	0	0
60	DL	2	Total 2	O 2	0	0
60	DN	4	Total 4	O 4	0	0
60	DT	3	Total 3	O 3	0	0
60	DU	1	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.

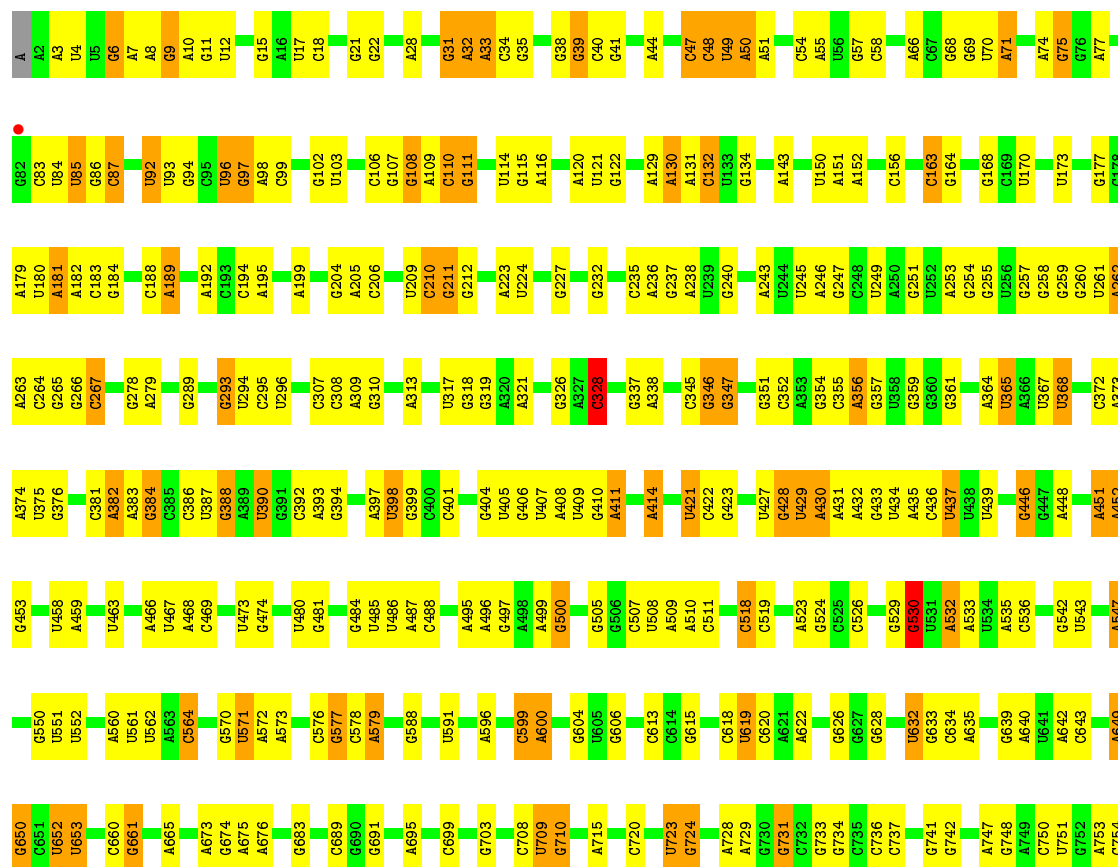
- Molecule 1: 16S ribosomal RNA

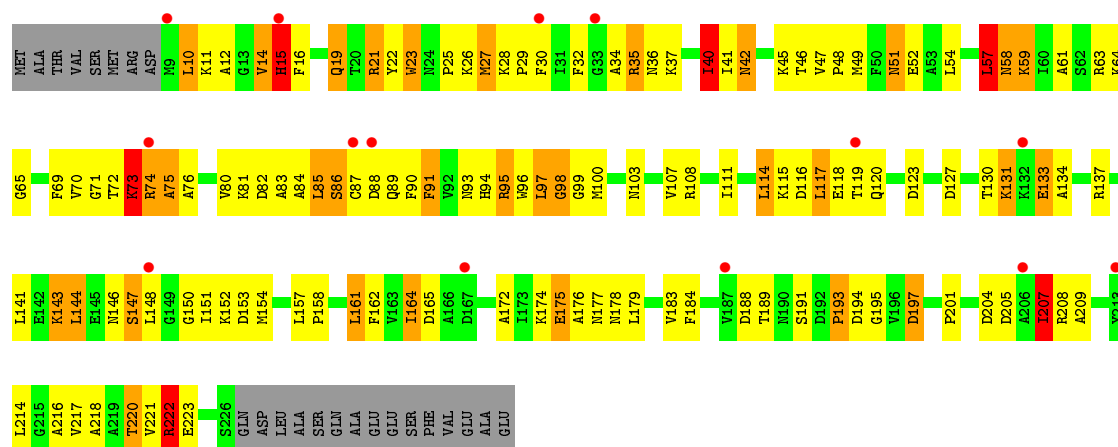




• Molecule 1: 16S ribosomal RNA

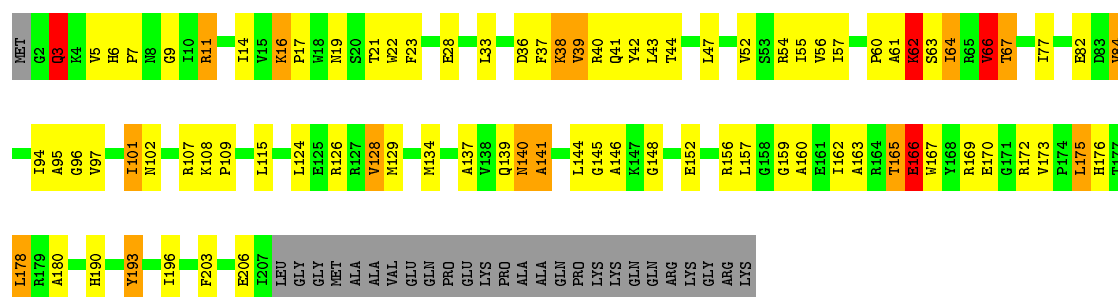
Chain DA: 56% 34% 10%





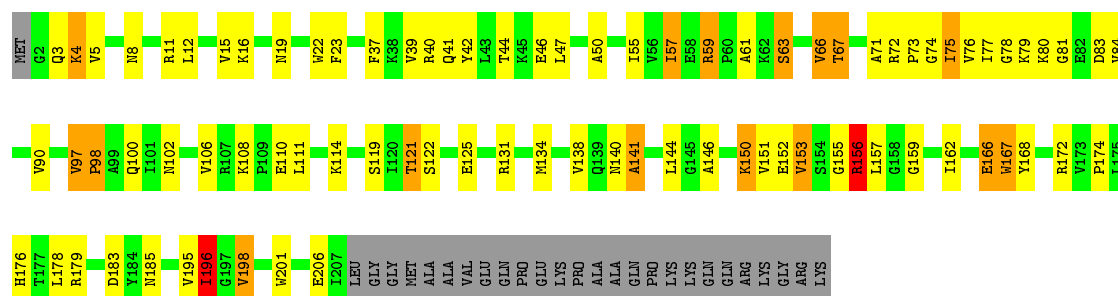
• Molecule 3: 30S ribosomal protein S3

Chain AC: 52% 29% 6% 12%



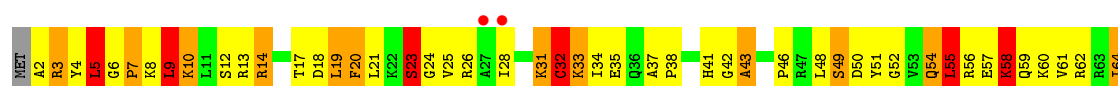
• Molecule 3: 30S ribosomal protein S3

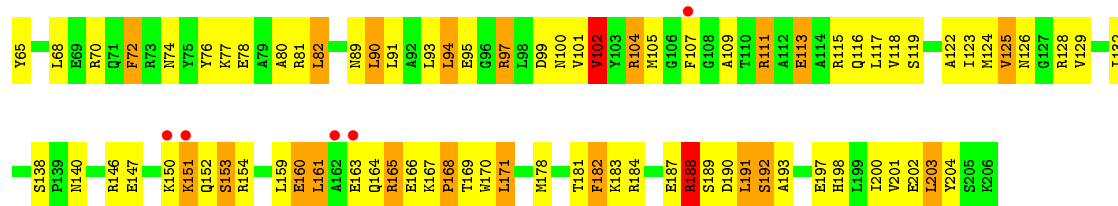
Chain DC: 52% 29% 7% 12%



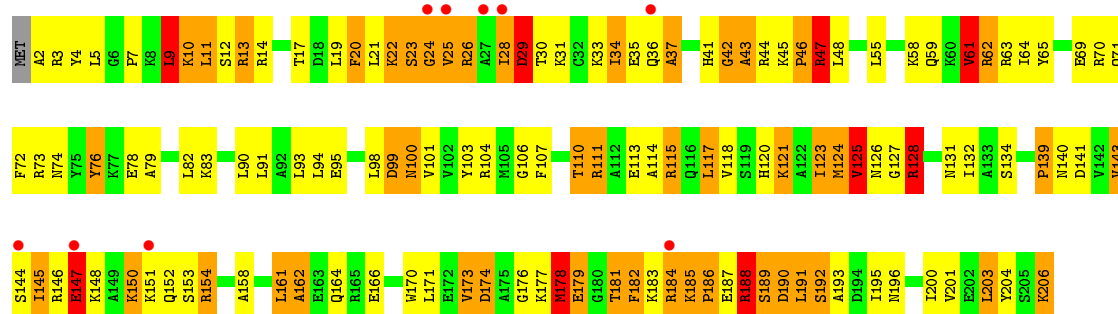
• Molecule 4: 30S ribosomal protein S4

Chain AD: 3% 37% 43% 16%

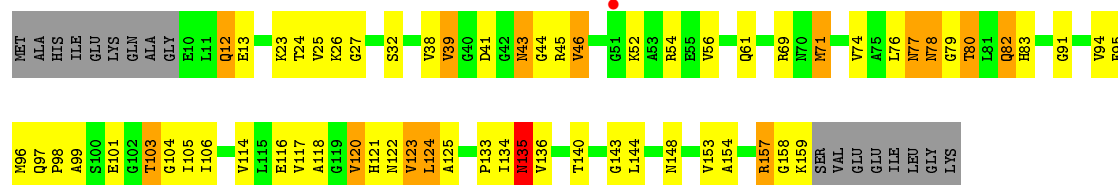




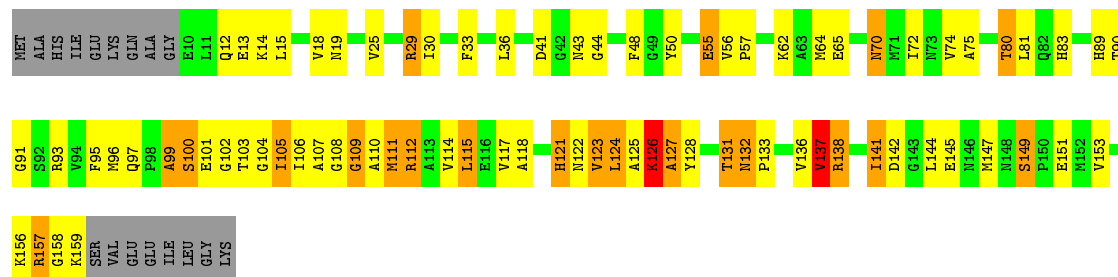
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

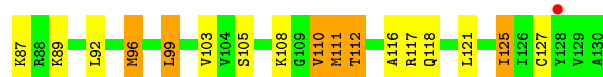


• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

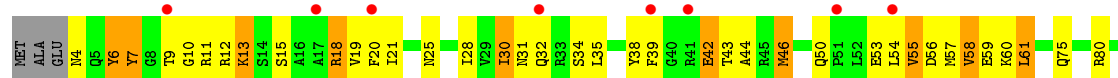




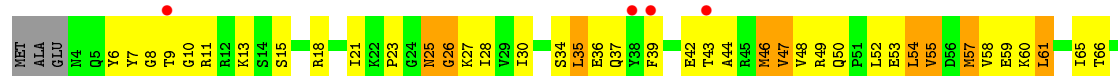
- Molecule 8: 30S ribosomal protein S8



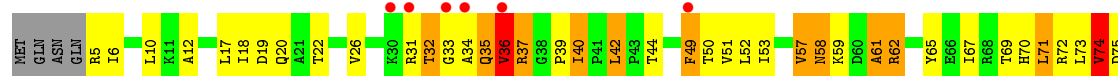
- Molecule 9: 30S ribosomal protein S9



- Molecule 9: 30S ribosomal protein S9

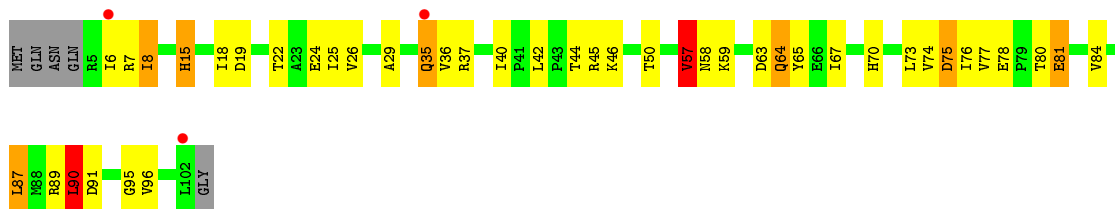


- Molecule 10: 30S ribosomal protein S10

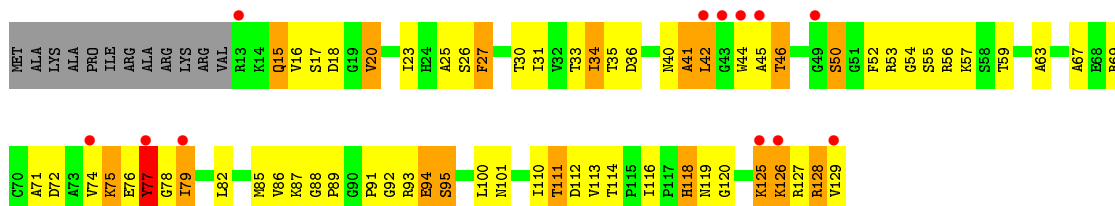


- Molecule 10: 30S ribosomal protein S10

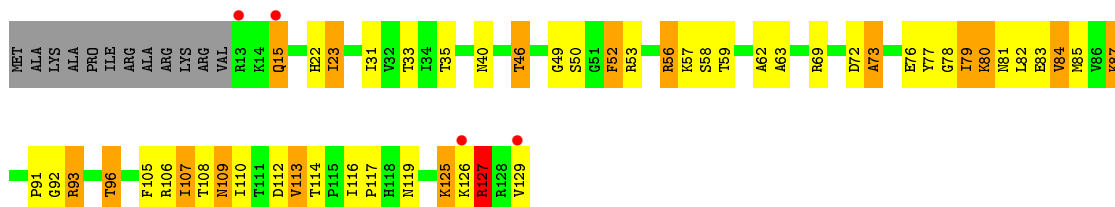




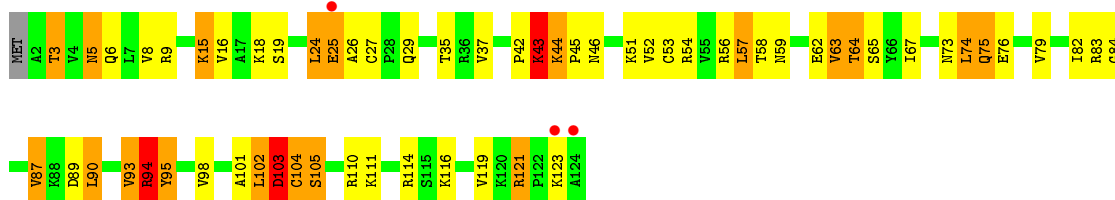
- Molecule 11: 30S ribosomal protein S11



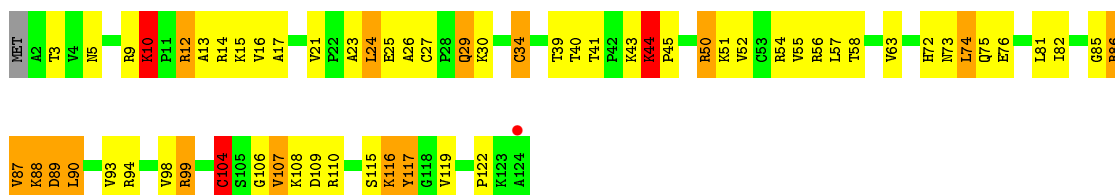
- Molecule 11: 30S ribosomal protein S11



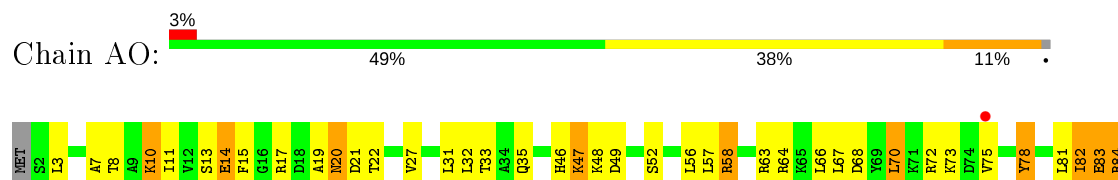
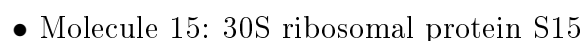
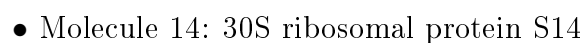
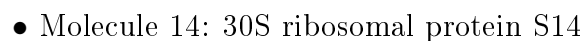
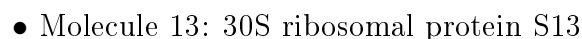
- Molecule 12: 30S ribosomal protein S12

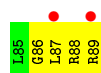


- Molecule 12: 30S ribosomal protein S12

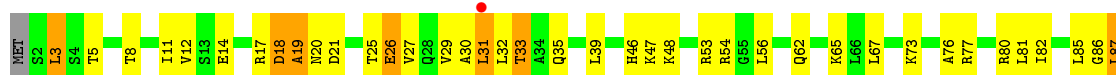


- Chain AM:

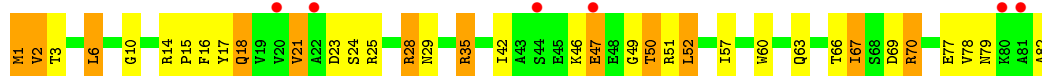




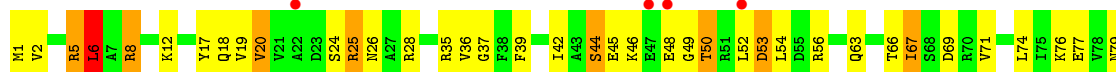
- Molecule 15: 30S ribosomal protein S15



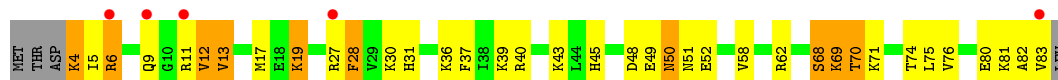
- Molecule 16: 30S ribosomal protein S16



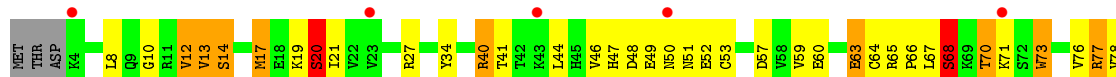
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

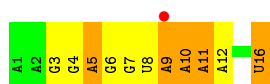


- Molecule 17: 30S ribosomal protein S17

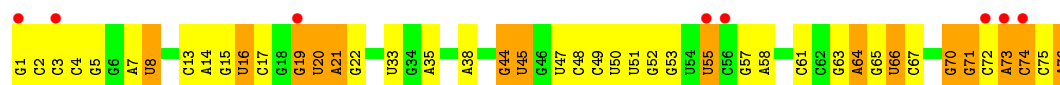
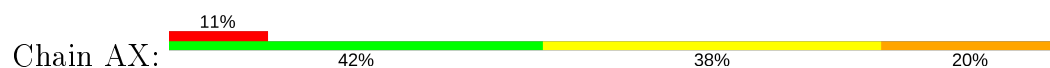


- Molecule 20: 30S ribosomal protein S20

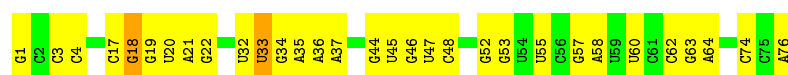




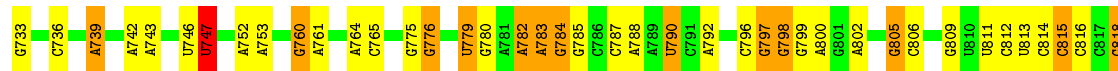
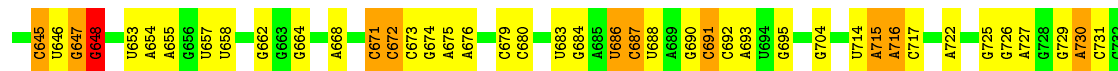
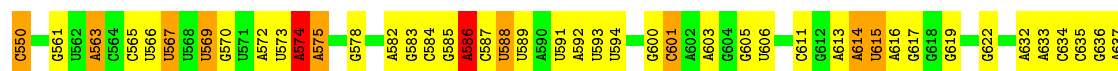
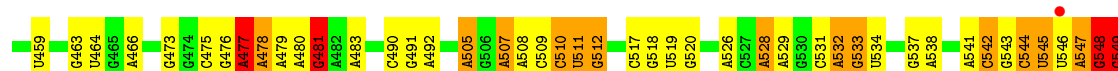
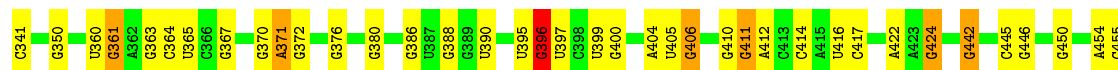
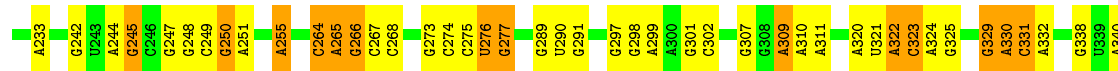
- Molecule 24: Phenylalanine specific transfer RNA, tRNA-Phe



- Molecule 24: Phenylalanine specific transfer RNA, tRNA-Phe



- Molecule 25: 23S ribosomal RNA





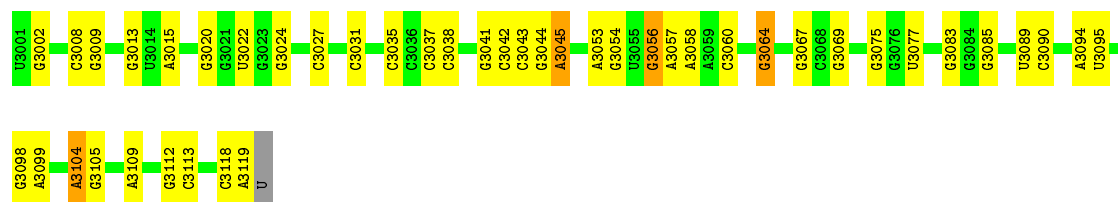




U2849	U2756	C2663	A2577	U2324	U2236	G2159	A2094	A2013	A1916	C1830
G2854	A2757	G2673	G2578	G2325	G2237	C2160	A2095	A2014	U1917	C1836
C2855	A2758	G2674	C2579	C2326	G2238	C2161	C2096	A2015	G1921	C1837
C2762	C2762	A2675	U2580	A2327	G2239	A2162	U2097	U2016	U1922	C1838
C2771	C2771	G2676	G2581	U2328	G2242	A2163	U2098	U2017	U1923	G1839
C2772	C2772	U2680	G2582	A2329	U2243	C2164	U2099	G2018		G1842
C2773	C2773	C2681	U2583	C2330	U2244	C2165	G2100	A2019		C1843
C2774	C2774	C2682	U2584	G2331	C2248	U2167	A2101	A2020	A1927	G1844
C2775	C2775	A2683	U2585	A2332	G2249	G2168	C2103	C2023	G1930	C1845
C2776	C2776	G2684	U2586	U2333	G2250	A2169	C2104	G2024	C1934	G1846
A2668	C2778	U2685	G2588	A2334	G2251	A2170	U2105	C2025	C1935	A1847
A2672	A2672	G2686	U2589	A2335	G2252	A2171	U2106	U2026	A1936	A1848
U2790	U2790		A2426	G2337	G2253	U2172		G2027	A1937	G1849
G2791	G2791	U2689	G2429	U2343	U2259	C2173	U2109	U2028	A1938	G1850
A2792	A2792	U2690	A2430	U2344	C2260	C2174	G2110	A2031	G1939	G1851
C2793	C2793		U2431	G2345	G2261	C2177	U2111	A2032	U1940	U1852
C2794	C2794	U2699	A2432	A2346	U2262	C2178	U2112	A2033		A1853
C2795	C2795		A2433	C2347	A2267	U2181	U2113	U2034	U1943	G1857
U2796	U2796	G2702	A2434		A2268	U2182	G2115	A2037	A1952	A1858
A2799	A2799	C2703	A2435	C2350	A2269	A2183	G2116	G2038	U1955	U1859
A2800	A2800	C2704	G2436	A2348	G2271	A2184	U2117	U2039		U1865
G2801	G2801	A2705	G2437	C2358	G2274	U2185	U2118		C1961	A1866
G2802	G2802	A2706	G2438	C2359	A2274		G2120	A2042	G1964	C1867
G2803	G2803	G2709	C2440		A2278	U2189	G2121	C2043	C1965	C1868
U2804	U2804	C2714	U2441	C2362	A2278	U2190	G2122	C2044	A1966	C1870
C2805	C2805	G2715	C2442	C2363	G2282	U2191	G2123	C2045	G1967	A1871
C2806	C2806	C2716	G2443	C2364	C2283	U2192	G2124	G2049	G1968	A1872
C2807	C2807	G2717	G2444	G2373	C2284	U2193	G2125	C2050	A1969	C1873
C2808	C2808	C2718	A2445	C2374	A2284	U2194	G2126	A2051	U1970	G1875
C2809	C2809	G2719	U2446	G2375	C2285	U2195	G2127	C2055	G1972	G1881
C2810	C2810	C2720	U2447	A2376	G2286	U2196	G2128	C2056	U1979	U1882
C2811	C2811	A2721	A2448	A2377	A2287	U2197	C2129	A2061	G1980	U1883
C2812	C2812	G2722	G2449	C2378	A2288	C2206	U2130	C2062	A1884	A1885
C2813	C2813	C2723	C2450	A2379	G2289	C2207	U2131	C2063		A1890
C2814	C2814		A2451	G2379	A2290	C2208	U2132	C2066	U1991	C1893
C2815	C2815		U2457	A2380	G2291	C2209	G2133	C2069	U1992	C1894
C2816	C2816	A2726	G2458	A2381	U2292	U2210	A2134	A2070	C1993	C1895
C2817	C2817	U2727	U2460	G2382	G2293	U2211	G2138	C2072	C1994	C1896
C2818	C2818	U2728	U2461	G2383		U2212	U2139	C2078	C1997	A1900
C2819	C2819	G2729	A2462	C2384	A2297	U2213	G2140	U2079	C1998	C1905
A2820	A2820		U2469	A2385	A2298	U2214	U2141	A2080	C2000	G1906
A2821	A2821		G2472	C2386	U2299	C2215	A2142	U2081	C2001	G1907
A2822	A2822		U2473	A2387	G2304	C2216	C2143	A2082	G2004	C1908
A2823	A2823		U2474	A2388	U2305	G2217	G2144	G2087	C2005	A1912
G2828	G2828		U2475	A2392	G2306	G2218	C2145		C2006	C1913
U2833	U2833		C2476	G2396	G2307		A2147			C1914
C2834	C2834		U2477	U2402	G2308		G2148			U1915
A2835	A2835		U2478	U2403	A2310		U2151			
U2836	U2836		U2479	U2404	U2311		G2152			
G2839	G2839		U2480	U2405	U2312		C2153			
C2840	C2840		C2483	A2406	U2320		G2156			
C2841	C2841		G2484	A2407	U2321		G2157			
G2842	G2842			U2408	A2322		A2158			
C2843	C2843			A2409	A2323					
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U2845	U2845									
G2846	G2846									
U2847	U2847									
G2848	G2848									

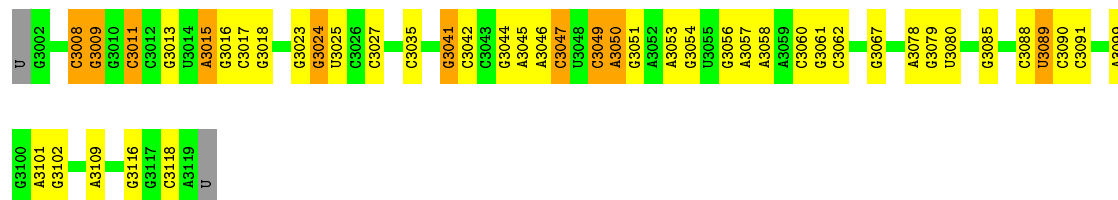
• Molecule 26: 5S ribosomal RNA

Chain BB: 63% 33%



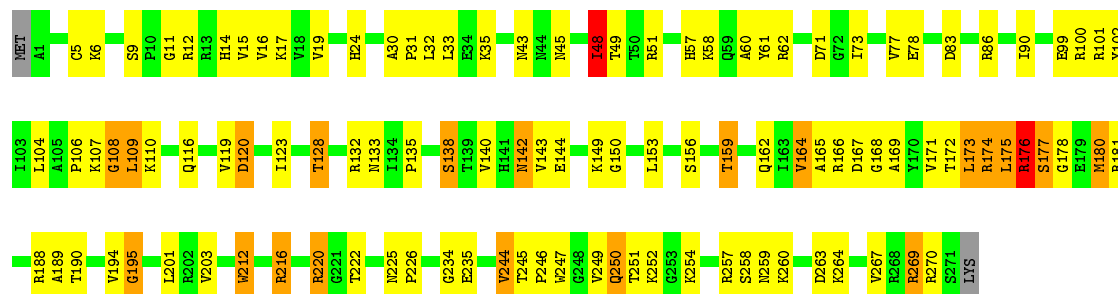
- Molecule 26: 5S ribosomal RNA

Chain CB: 61% 29% 8%



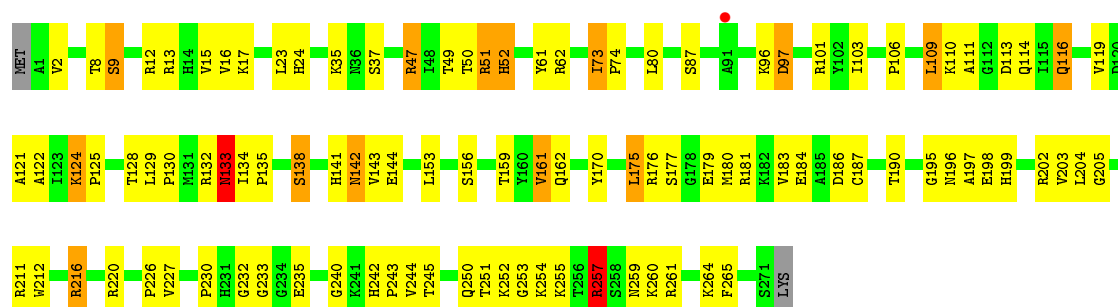
- Molecule 27: 50S ribosomal protein L2

Chain BC: 59% 33% 7%



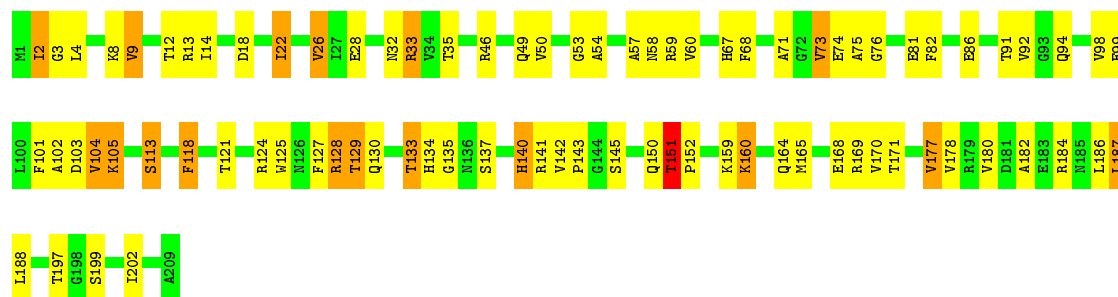
- Molecule 27: 50S ribosomal protein L2

Chain CC: 61% 32% 5%



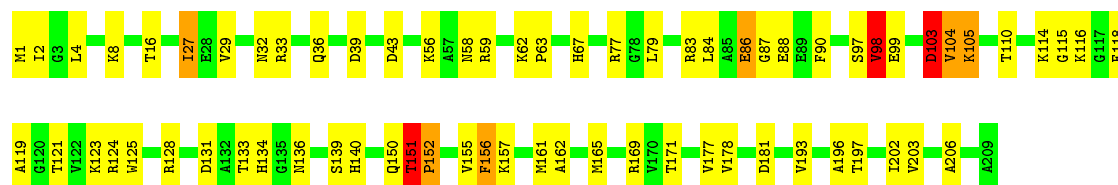
- Molecule 28: 50S ribosomal protein L3

Chain BD: 60% 32% 8%



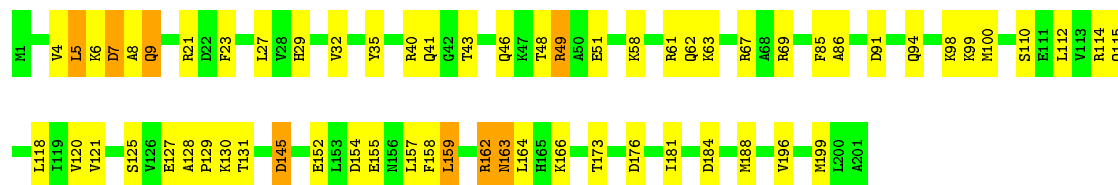
- Molecule 28: 50S ribosomal protein L3

Chain CD: 67% 29%



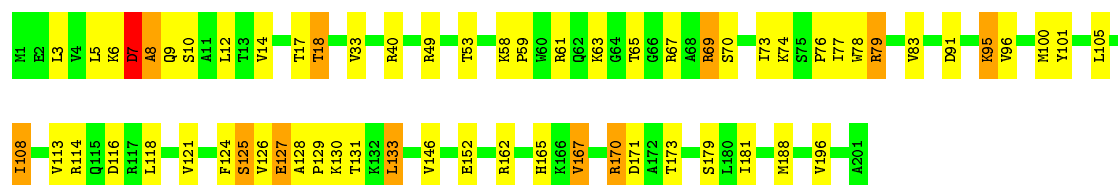
- Molecule 29: 50S ribosomal protein L4

Chain BE: 69% 27%



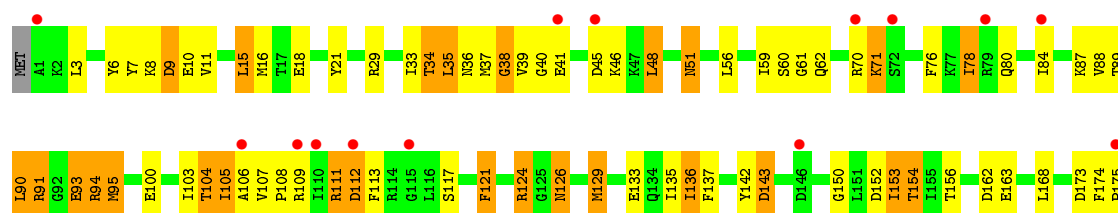
- Molecule 29: 50S ribosomal protein L4

Chain CE: 69% 25% 5%



- Molecule 30: 50S ribosomal protein L5

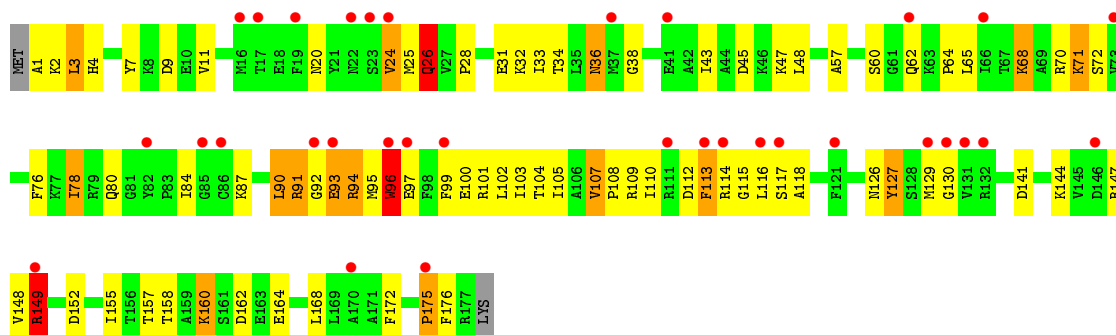
Chain BF: 8% 56% 28% 15%





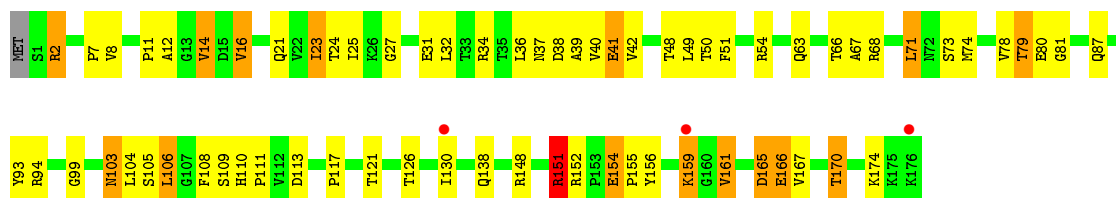
- Molecule 30: 50S ribosomal protein L5

Chain CF: 18% 53% 36% 8% ..



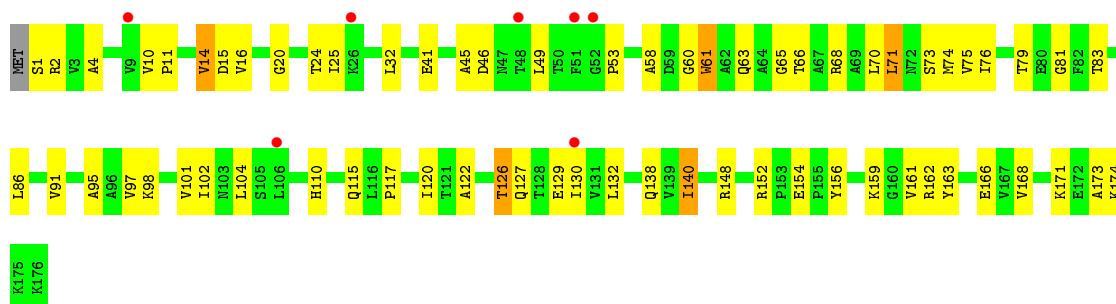
- Molecule 31: 50S ribosomal protein L6

Chain BG: 2% 60% 30% 8% ..



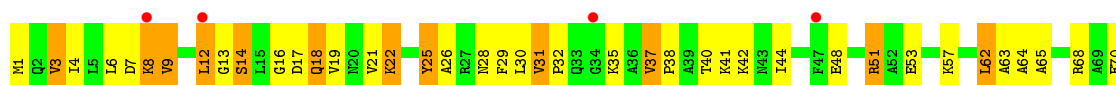
- Molecule 31: 50S ribosomal protein L6

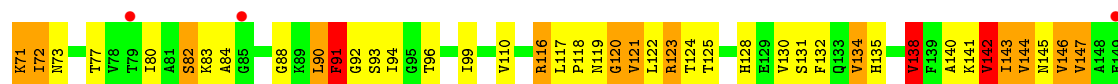
Chain CG: 4% 62% 34% ..



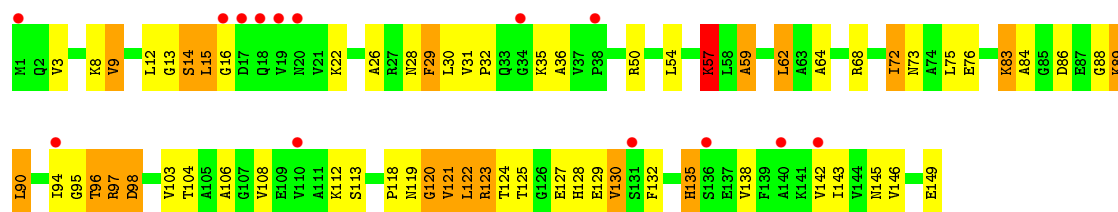
- Molecule 32: 50S ribosomal protein L9

Chain BH: 5% 45% 36% 17% ..

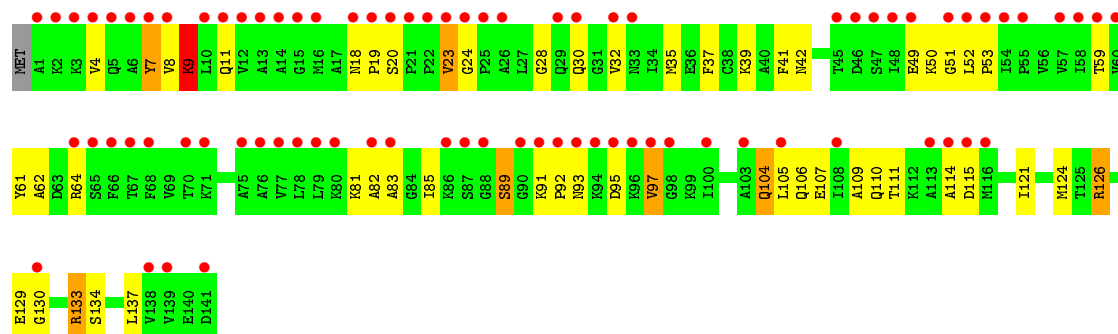




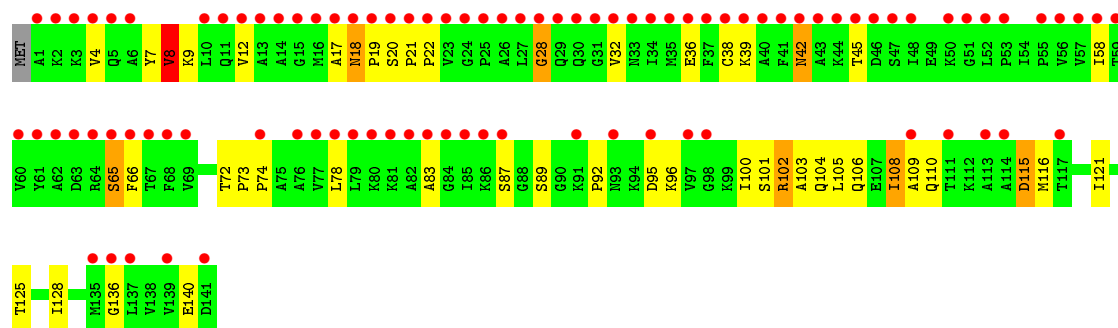
- Molecule 32: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L11

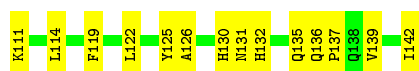


- Molecule 33: 50S ribosomal protein L11



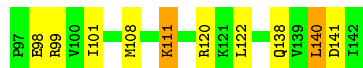
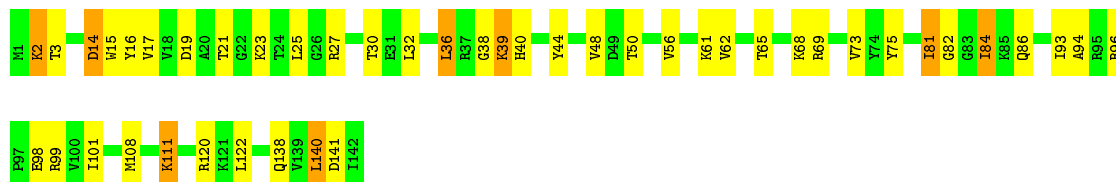
- Molecule 34: 50S ribosomal protein L13





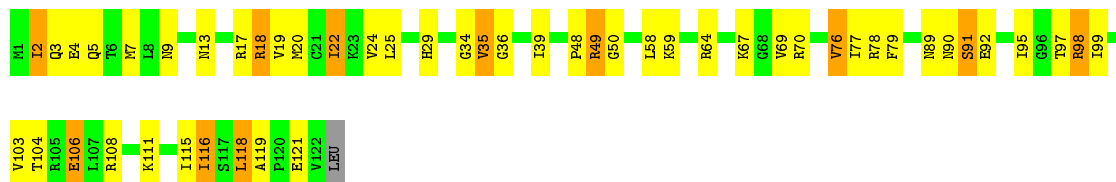
- Molecule 34: 50S ribosomal protein L13

Chain CJ: 68% 26% 6%



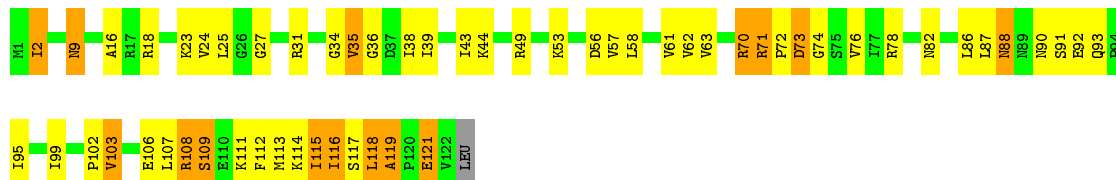
- Molecule 35: 50S ribosomal protein L14

Chain BK: 59% 32% 9%



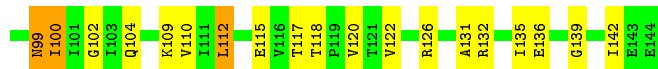
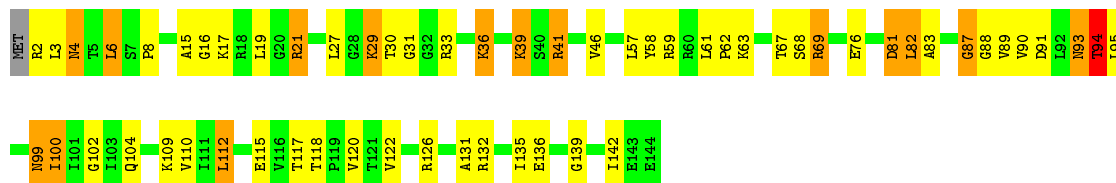
- Molecule 35: 50S ribosomal protein L14

Chain CK: 53% 34% 12%



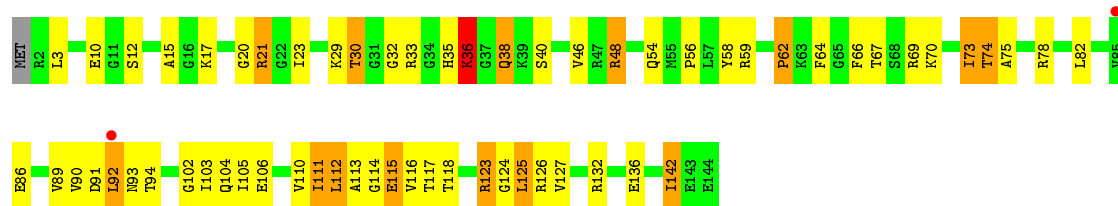
- Molecule 36: 50S ribosomal protein L15

Chain BL: 58% 30% 10%



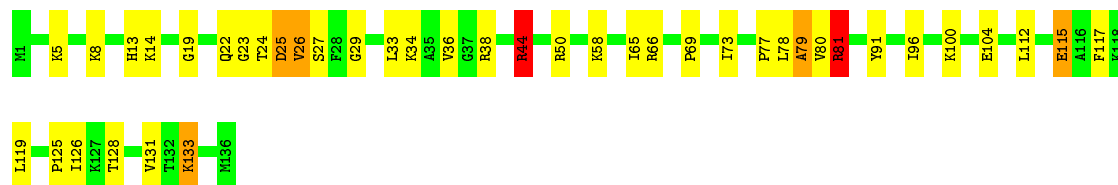
- Molecule 36: 50S ribosomal protein L15

Chain CL: 56% 33% 10%



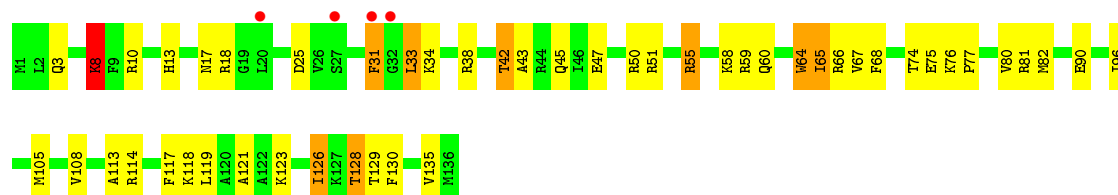
- Molecule 37: 50S ribosomal protein L16

Chain BM: 70% 25% • •



- Molecule 37: 50S ribosomal protein L16

Chain CM: 3% 64% 29% 6% •



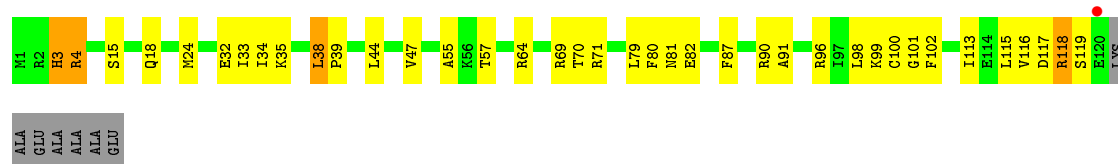
- Molecule 38: 50S ribosomal protein L17

Chain BN: 56% 30% 8% 6% •



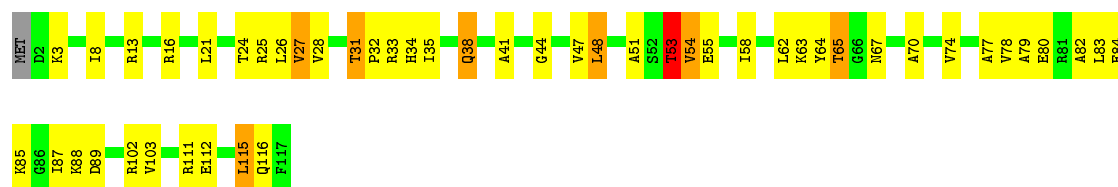
- Molecule 38: 50S ribosomal protein L17

Chain CN: % 65% 27% 6% •



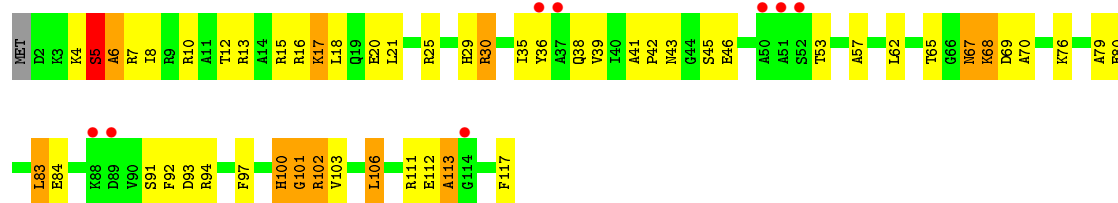
- Molecule 39: 50S ribosomal protein L18

Chain BO:  57% 35% 6% ..



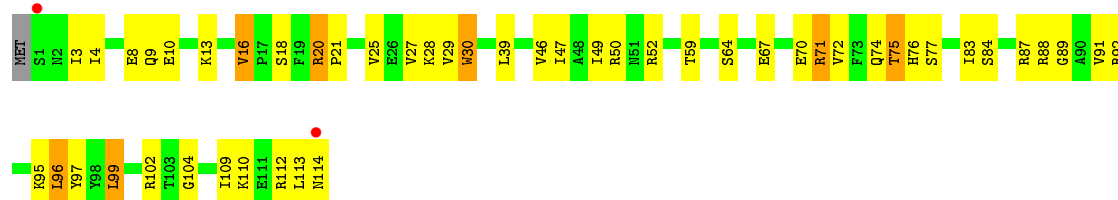
• Molecule 39: 50S ribosomal protein L18

Chain CO:  7% 54% 35% 9% ..



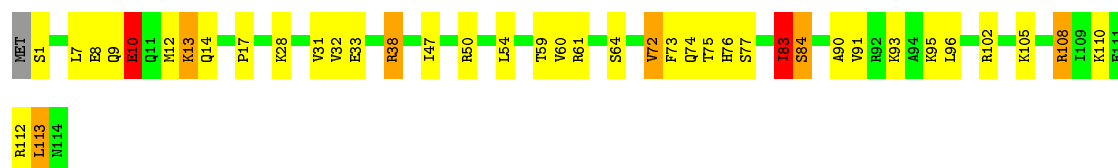
• Molecule 40: 50S ribosomal protein L19

Chain BP:  29% 57% 37% 6% ..



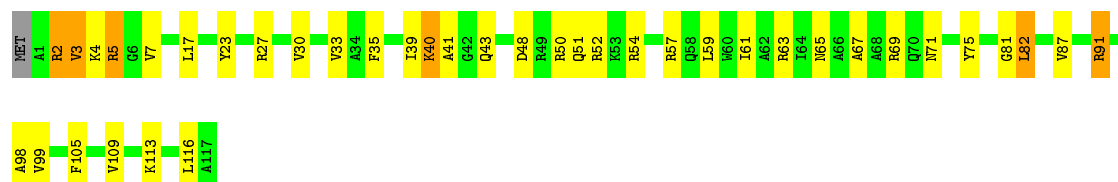
• Molecule 40: 50S ribosomal protein L19

Chain CP:  64% 28% 5% ..



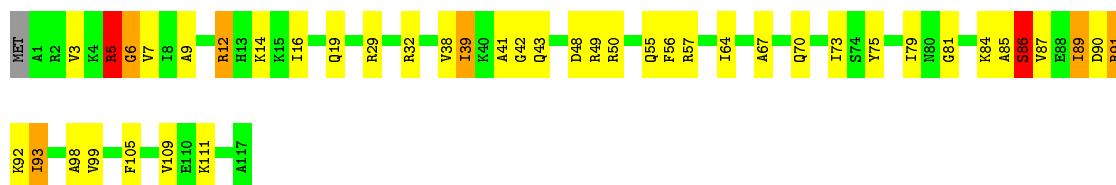
• Molecule 41: 50S ribosomal protein L20

Chain BQ:  66% 28% 5% ..



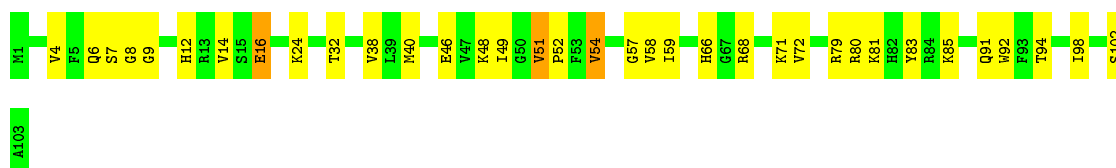
- Molecule 41: 50S ribosomal protein L20

Chain CQ:  63% 30% 5% ..



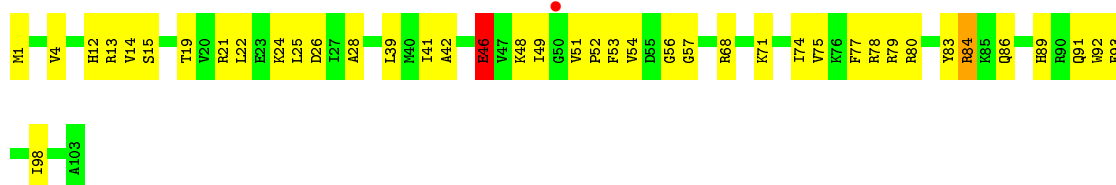
- Molecule 42: 50S ribosomal protein L21

Chain BR:  66% 31% ..



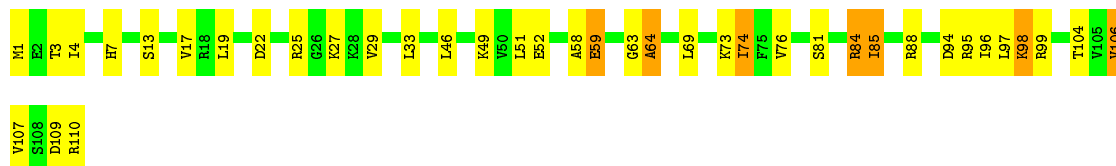
- Molecule 42: 50S ribosomal protein L21

Chain CR:  60% 38% ..



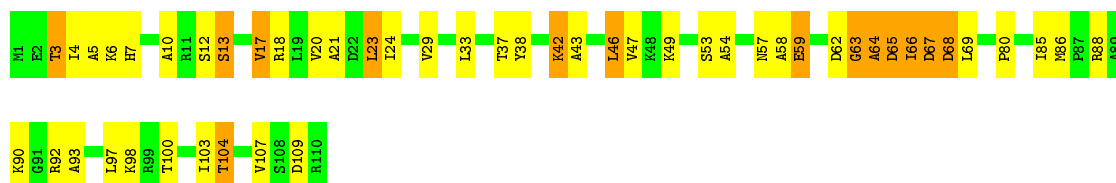
- Molecule 43: 50S ribosomal protein L22

Chain BS:  65% 29% 6% ..

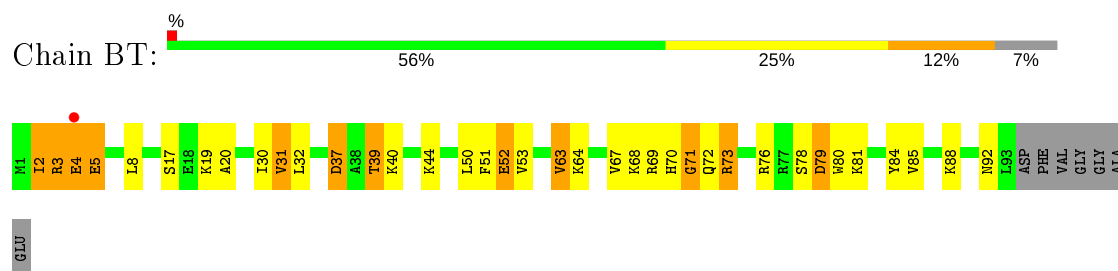


- Molecule 43: 50S ribosomal protein L22

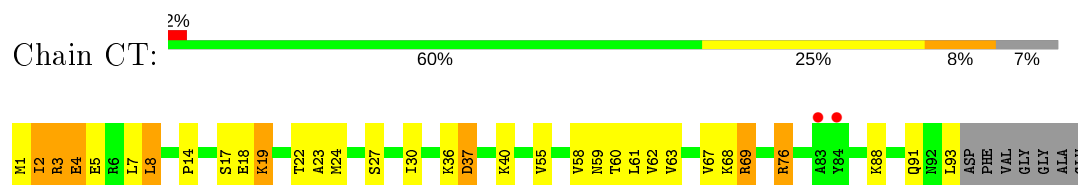
Chain CS:  55% 33% 13% ..



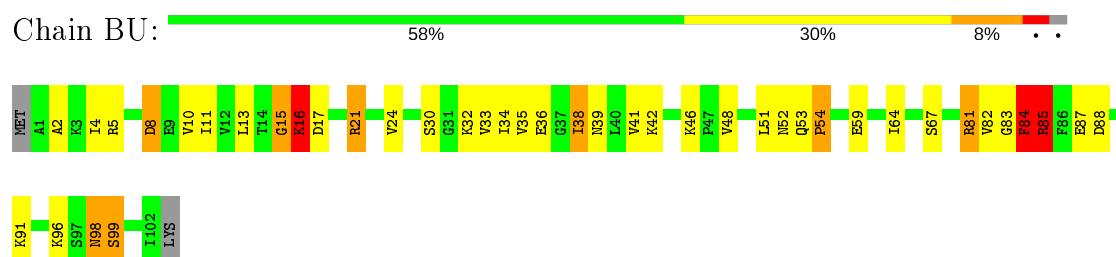
• Molecule 44: 50S ribosomal protein L23



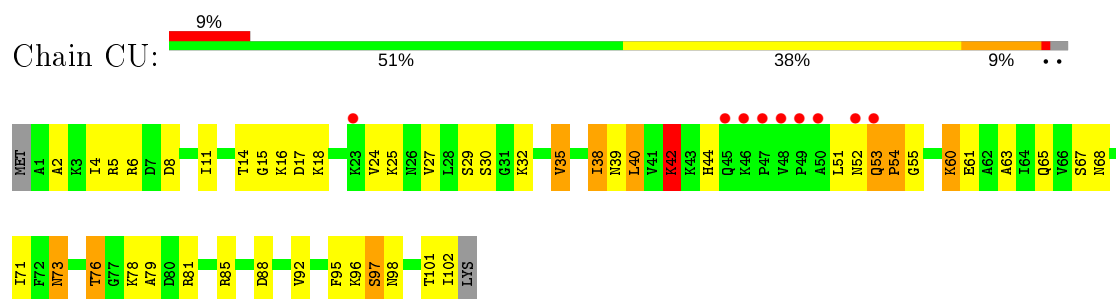
• Molecule 44: 50S ribosomal protein L23



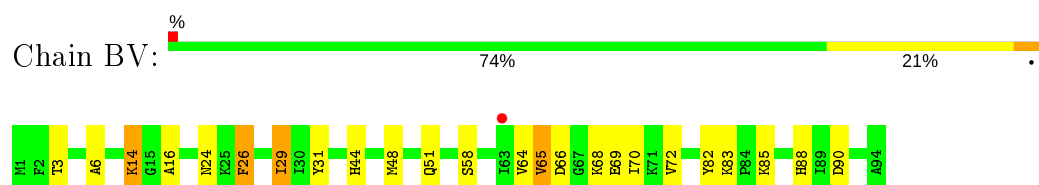
• Molecule 45: 50S ribosomal protein L24



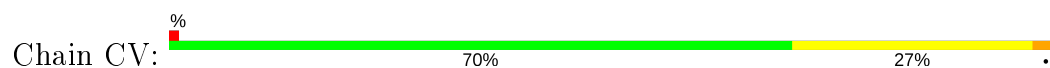
• Molecule 45: 50S ribosomal protein L24



• Molecule 46: 50S ribosomal protein L25



• Molecule 46: 50S ribosomal protein L25





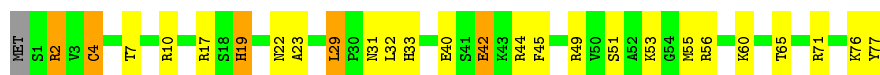
- Molecule 47: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L27



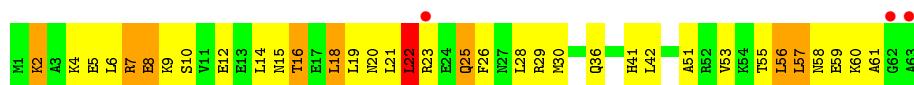
- Molecule 48: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L28




- Molecule 49: 50S ribosomal protein L29

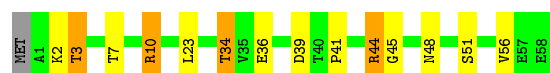


- Molecule 49: 50S ribosomal protein L29



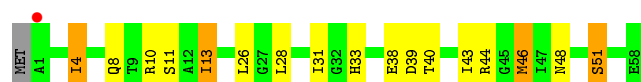
- Molecule 50: 50S ribosomal protein L30

Chain BZ: 



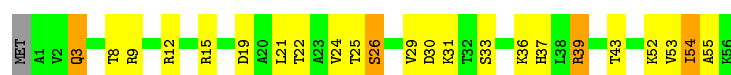
- Molecule 50: 50S ribosomal protein L30

Chain CZ: 



- Molecule 51: 50S ribosomal protein L32

Chain B0: 



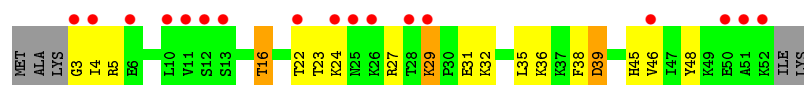
- Molecule 51: 50S ribosomal protein L32

Chain C0: 




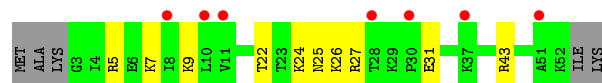
- Molecule 52: 50S ribosomal protein L33

Chain B1: 



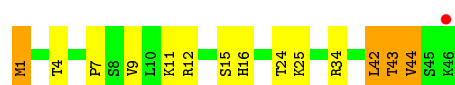
- Molecule 52: 50S ribosomal protein L33

Chain C1: 



- Molecule 53: 50S ribosomal protein L34

Chain B2: 



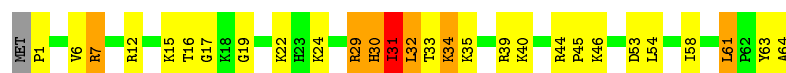
- Molecule 53: 50S ribosomal protein L34

Chain C2:  54% 43% .



- Molecule 54: 50S ribosomal protein L35

Chain B3:  55% 32% 9% ..



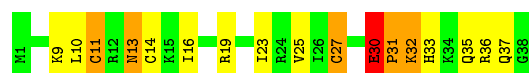
- Molecule 54: 50S ribosomal protein L35

Chain C3:  66% 26% 6% .



- Molecule 55: 50S ribosomal protein L36

Chain B4:  55% 29% 13% .



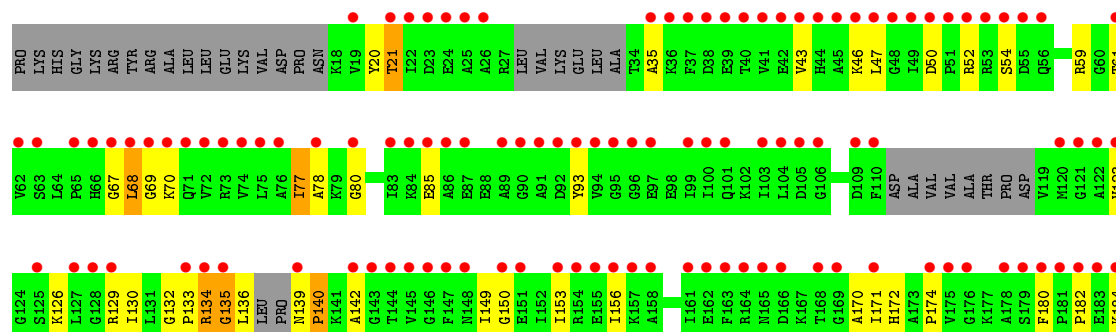
- Molecule 55: 50S ribosomal protein L36

Chain C4:  66% 32% .



- Molecule 56: 50S ribosomal protein L1

Chain B5:  68% 61% 20% 16%



I185	A186	D187	N188	I189	R190	A191	F192	I193	R194	A195	L196	E197	A198	H199	K200	P201	E202	G203	A204	K205	G206	T207	F208	L209	R210	S211	V212	Y213	V214	T215	T216	T217	M218	G219	P220	S221	V222	R223	I224	ASN	PRO	HIS	SER
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.10Å 435.24Å 614.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.00 69.34 – 2.93	Depositor EDS
% Data completeness (in resolution range)	81.1 (70.00-3.00) 76.0 (69.34-2.93)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.174 , 0.253 0.180 , 0.258	Depositor DCC
R_{free} test set	4548 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 95.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	294484	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.38% 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, MG, PAR

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	0.48	0/36944	0.99	30/57632 (0.1%)
1	DA	0.49	0/36966	1.00	37/57666 (0.1%)
2	AB	0.38	0/1735	0.64	0/2338
2	DB	0.41	0/1735	0.67	1/2338 (0.0%)
3	AC	0.45	0/1651	0.70	0/2225
3	DC	0.42	0/1651	0.66	0/2225
4	AD	0.46	0/1665	0.75	3/2227 (0.1%)
4	DD	0.51	0/1665	0.81	1/2227 (0.0%)
5	AE	0.40	0/1118	0.62	0/1504
5	DE	0.47	0/1118	0.73	0/1504
6	AF	0.42	0/835	0.69	0/1128
6	DF	0.43	0/835	0.71	0/1128
7	AG	2.14	8/1195 (0.7%)	0.81	4/1602 (0.2%)
7	DG	0.38	0/1195	0.57	0/1602
8	AH	0.41	0/989	0.66	0/1326
8	DH	0.45	0/989	0.77	1/1326 (0.1%)
9	AI	0.38	0/1034	0.65	0/1375
9	DI	0.42	0/1034	0.66	0/1375
10	AJ	0.42	0/796	0.69	1/1077 (0.1%)
10	DJ	0.38	0/796	0.64	0/1077
11	AK	0.43	0/893	0.69	0/1205
11	DK	0.43	0/893	0.67	0/1205
12	AL	0.52	0/969	0.77	0/1300
12	DL	0.52	0/969	0.81	1/1300 (0.1%)
13	AM	0.39	0/892	0.74	0/1193
13	DM	0.36	0/892	0.66	0/1193
14	AN	0.44	0/785	0.73	0/1043
14	DN	0.39	0/785	0.67	0/1043
15	AO	0.40	0/724	0.67	0/966
15	DO	0.38	0/724	0.63	0/966
16	AP	0.40	0/659	0.62	0/884
16	DP	0.44	0/659	0.72	1/884 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.40	0/657	0.72	0/881
17	DQ	0.45	0/657	0.69	0/881
18	AR	0.44	0/462	0.63	0/621
18	DR	0.44	0/462	0.71	1/621 (0.2%)
19	AS	0.37	0/652	0.71	0/877
19	DS	0.37	0/652	0.61	0/877
20	AT	0.41	0/671	0.64	0/888
20	DT	0.41	0/671	0.64	0/888
21	AU	0.50	0/430	0.91	1/570 (0.2%)
21	DU	0.58	0/430	0.89	0/570
22	AV	0.43	0/1430	0.63	0/1924
23	AW	0.58	0/363	1.12	0/564
23	DV	0.51	0/388	1.04	0/603
24	AX	0.49	1/1813 (0.1%)	0.95	0/2823
24	DW	0.52	1/1813 (0.1%)	0.95	0/2823
25	BA	0.67	8/69659 (0.0%)	1.20	303/108672 (0.3%)
25	CA	0.52	3/69659 (0.0%)	1.04	112/108672 (0.1%)
26	BB	0.54	0/2850	1.03	7/4444 (0.2%)
26	CB	0.40	0/2828	0.90	2/4410 (0.0%)
27	BC	0.47	0/2121	0.71	0/2852
27	CC	0.42	0/2121	0.68	0/2852
28	BD	0.53	0/1586	0.77	2/2134 (0.1%)
28	CD	0.44	0/1586	0.73	1/2134 (0.0%)
29	BE	0.49	0/1571	0.71	0/2113
29	CE	0.43	0/1571	0.65	0/2113
30	BF	0.40	0/1434	0.65	0/1926
30	CF	0.36	0/1434	0.61	0/1926
31	BG	0.43	0/1343	0.61	0/1816
31	CG	0.35	0/1343	0.56	0/1816
32	BH	0.43	0/1118	0.70	0/1511
32	CH	0.38	0/1118	0.60	1/1511 (0.1%)
33	BI	0.38	0/1046	0.60	0/1410
33	CI	0.33	0/1046	0.55	0/1410
34	BJ	0.53	0/1152	0.67	0/1551
34	CJ	0.43	0/1152	0.62	0/1551
35	BK	0.54	0/947	0.74	0/1268
35	CK	0.47	0/947	0.72	0/1268
36	BL	0.50	0/1054	0.80	0/1403
36	CL	0.45	0/1054	0.70	0/1403
37	BM	0.50	0/1093	0.75	1/1460 (0.1%)
37	CM	0.42	0/1093	0.59	0/1460
38	BN	0.49	0/973	0.69	0/1301
38	CN	0.50	0/973	0.66	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	BO	0.45	0/902	0.65	0/1209
39	CO	0.37	0/902	0.65	0/1209
40	BP	0.49	0/929	0.66	0/1242
40	CP	0.45	0/929	0.65	1/1242 (0.1%)
41	BQ	0.53	0/960	0.74	0/1278
41	CQ	0.49	0/960	0.72	1/1278 (0.1%)
42	BR	0.52	0/829	0.72	0/1107
42	CR	0.49	0/829	0.71	0/1107
43	BS	0.53	0/864	0.70	0/1156
43	CS	0.47	0/864	0.75	0/1156
44	BT	0.48	0/744	0.67	0/994
44	CT	0.40	0/744	0.56	0/994
45	BU	0.51	0/787	0.72	0/1051
45	CU	0.43	0/787	0.64	0/1051
46	BV	0.45	0/766	0.64	0/1025
46	CV	0.34	0/766	0.58	0/1025
47	BW	0.54	0/587	0.73	0/776
47	CW	0.41	0/576	0.65	0/762
48	BX	0.47	0/635	0.71	0/848
48	CX	0.38	0/635	0.64	0/848
49	BY	0.42	0/510	0.69	0/677
49	CY	0.40	0/510	0.72	0/677
50	BZ	0.51	0/453	0.78	0/605
50	CZ	0.41	0/453	0.62	0/605
51	B0	0.54	0/450	0.79	1/599 (0.2%)
51	C0	0.48	0/450	0.73	0/599
52	B1	0.39	0/416	0.61	0/554
52	C1	0.38	0/416	0.62	0/554
53	B2	0.50	0/380	0.74	0/498
53	C2	0.45	0/380	0.66	0/498
54	B3	0.55	0/513	0.78	0/676
54	C3	0.46	0/513	0.71	0/676
55	B4	0.53	0/303	0.77	0/397
55	C4	0.42	0/303	0.60	0/397
56	B5	0.33	0/1145	0.54	0/1556
All	All	0.54	21/316403 (0.0%)	0.99	515/473109 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	1
2	DB	0	1
4	AD	0	1
4	DD	0	1
5	DE	0	2
6	AF	0	1
7	AG	0	1
9	DI	0	1
10	AJ	0	2
11	AK	0	1
12	DL	0	1
14	AN	0	2
17	DQ	0	1
19	AS	0	1
20	AT	0	1
20	DT	0	2
21	AU	0	1
27	BC	0	3
28	BD	0	1
28	CD	0	2
30	BF	0	1
36	BL	0	1
36	CL	0	1
38	BN	0	1
38	CN	0	1
40	CP	0	1
42	CR	0	1
44	BT	0	1
48	CX	0	1
All	All	0	36

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	AG	103	TRP	CE3-CZ3	40.14	2.06	1.38
7	AG	100	ALA	CA-C	39.86	2.56	1.52
7	AG	103	TRP	CZ3-CH2	28.41	1.85	1.40
7	AG	103	TRP	CE2-CZ2	21.77	1.76	1.39
7	AG	103	TRP	CD2-CE2	18.20	1.63	1.41

The worst 5 of 515 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	984	A	C2-N3-C4	-15.53	102.84	110.60
25	BA	1936	A	C2-N3-C4	-12.94	104.13	110.60
28	CD	151	THR	C-N-CD	-11.23	95.90	120.60
25	BA	2623	G	O5'-P-OP1	-10.98	95.82	105.70
25	BA	1936	A	N1-C2-N3	10.97	134.79	129.30

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	148	LEU	Peptide
4	AD	18	ASP	Peptide
6	AF	79	ARG	Peptide
7	AG	126	ASP	Peptide
10	AJ	17	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	432	1
1	DA	33015	0	16617	426	0
2	AB	1704	0	1732	37	0
2	DB	1704	0	1732	80	0
3	AC	1624	0	1696	45	0
3	DC	1624	0	1696	39	0
4	AD	1643	0	1707	92	0
4	DD	1643	0	1707	117	0
5	AE	1105	0	1148	32	0
5	DE	1105	0	1148	53	0
6	AF	817	0	808	20	0
6	DF	817	0	808	22	0
7	AG	1181	0	1238	78	0
7	DG	1181	0	1238	25	0
8	AH	979	0	1031	34	0
8	DH	979	0	1031	49	0
9	AI	1022	0	1070	36	0
9	DI	1022	0	1070	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	786	0	828	36	0
10	DJ	786	0	828	16	0
11	AK	877	0	887	46	0
11	DK	877	0	887	35	0
12	AL	955	0	1016	47	0
12	DL	955	0	1016	42	0
13	AM	883	0	941	62	0
13	DM	883	0	941	42	0
14	AN	774	0	827	52	0
14	DN	774	0	827	25	0
15	AO	716	0	739	33	0
15	DO	716	0	739	18	0
16	AP	649	0	666	20	0
16	DP	649	0	666	36	0
17	AQ	648	0	691	17	0
17	DQ	648	0	691	15	0
18	AR	455	0	478	20	0
18	DR	455	0	478	15	0
19	AS	637	0	665	38	0
19	DS	637	0	665	26	0
20	AT	665	0	714	15	0
20	DT	665	0	714	20	0
21	AU	425	0	449	24	0
21	DU	425	0	449	35	0
22	AV	1419	0	1465	45	0
23	AW	324	0	162	4	0
23	DV	346	0	173	15	0
24	AX	1623	0	821	20	0
24	DW	1623	0	821	8	0
25	BA	62195	0	31279	791	0
25	CA	62195	0	31280	774	0
26	BB	2549	0	1291	25	0
26	CB	2529	0	1281	20	0
27	BC	2082	0	2157	64	0
27	CC	2082	0	2157	61	0
28	BD	1565	0	1616	46	0
28	CD	1565	0	1616	31	0
29	BE	1552	0	1619	39	0
29	CE	1552	0	1619	28	0
30	BF	1410	0	1447	53	0
30	CF	1410	0	1447	49	0
31	BG	1323	0	1374	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	CG	1323	0	1374	22	0
32	BH	1107	0	1139	90	0
32	CH	1107	0	1138	62	1
33	BI	1032	0	1088	17	0
33	CI	1032	0	1088	17	0
34	BJ	1129	0	1162	24	0
34	CJ	1129	0	1162	27	0
35	BK	938	0	1012	31	0
35	CK	938	0	1012	34	0
36	BL	1045	0	1117	35	0
36	CL	1045	0	1117	39	0
37	BM	1074	0	1157	23	0
37	CM	1074	0	1157	24	0
38	BN	960	0	1000	26	0
38	CN	960	0	1000	25	0
39	BO	892	0	922	24	0
39	CO	892	0	923	32	0
40	BP	917	0	965	30	0
40	CP	917	0	965	31	0
41	BQ	947	0	1022	36	0
41	CQ	947	0	1022	35	0
42	BR	816	0	839	25	0
42	CR	816	0	839	24	0
43	BS	857	0	922	25	0
43	CS	857	0	922	22	0
44	BT	738	0	807	37	0
44	CT	738	0	806	31	0
45	BU	779	0	834	25	0
45	CU	779	0	834	32	0
46	BV	753	0	780	18	0
46	CV	753	0	780	8	0
47	BW	580	0	594	17	0
47	CW	569	0	581	11	0
48	BX	625	0	655	15	0
48	CX	625	0	655	16	0
49	BY	509	0	543	22	0
49	CY	509	0	543	20	0
50	BZ	449	0	491	6	0
50	CZ	449	0	491	11	0
51	B0	444	0	461	15	0
51	C0	444	0	461	10	0
52	B1	409	0	440	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	C1	409	0	440	5	0
53	B2	377	0	418	9	0
53	C2	377	0	418	8	0
54	B3	504	0	574	38	0
54	C3	504	0	574	11	0
55	B4	302	0	340	13	0
55	C4	302	0	340	4	0
56	B5	1142	0	865	13	0
57	AA	71	0	0	0	0
57	AN	1	0	0	0	0
57	BA	189	0	0	0	0
57	BB	4	0	0	0	0
57	BL	2	0	0	0	0
57	BO	1	0	0	0	0
57	BQ	1	0	0	0	0
57	CA	165	0	0	0	0
57	CB	3	0	0	0	0
57	CD	1	0	0	0	0
57	CQ	1	0	0	0	0
57	DA	53	0	0	0	0
57	DD	2	0	0	0	0
57	DN	1	0	0	0	0
58	AA	42	45	45	9	0
58	BA	210	180	225	33	0
58	CA	210	135	224	51	0
58	DA	84	90	90	13	0
59	B4	1	0	0	0	0
59	C4	1	0	0	0	0
60	AA	192	0	0	17	0
60	AE	3	0	0	0	0
60	AL	1	0	0	0	0
60	AN	2	0	0	1	0
60	AT	5	0	0	0	0
60	B3	1	0	0	0	0
60	B4	1	0	0	0	0
60	BA	626	0	0	92	0
60	BB	14	0	0	3	0
60	BC	7	0	0	0	0
60	BD	2	0	0	1	0
60	BE	1	0	0	0	0
60	BF	1	0	0	0	0
60	BL	8	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BN	2	0	0	0	0
60	BQ	1	0	0	0	0
60	BS	1	0	0	0	0
60	BT	3	0	0	2	0
60	C3	1	0	0	0	0
60	C4	2	0	0	0	0
60	CA	608	0	0	82	0
60	CB	14	0	0	3	0
60	CC	10	0	0	1	0
60	CD	5	0	0	1	0
60	CE	3	0	0	0	0
60	CJ	2	0	0	2	0
60	CL	7	0	0	0	0
60	CN	2	0	0	0	0
60	CT	3	0	0	1	0
60	CU	1	0	0	0	0
60	DA	184	0	0	22	0
60	DD	2	0	0	1	0
60	DK	2	0	0	0	0
60	DL	2	0	0	0	0
60	DN	4	0	0	2	0
60	DT	3	0	0	0	0
60	DU	1	0	0	0	0
All	All	294034	450	196884	4955	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 10.

The worst 5 of 4955 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)
7:AG:103:TRP:CE2	7:AG:103:TRP:CZ2	1.76	1.63
7:AG:103:TRP:CH2	7:AG:103:TRP:CZ3	1.85	1.61
7:AG:100:ALA:HA	7:AG:103:TRP:CD2	1.52	1.44
7:AG:103:TRP:CZ3	7:AG:103:TRP:CE3	2.06	1.44
32:BH:124:THR:HG21	32:BH:128:HIS:NE2	1.32	1.44

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:AA:358:U:OP1	32:CH:123:ARG:NH2[4_455]	1.91	0.29

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	216/241 (90%)	120 (56%)	54 (25%)	42 (19%)	0	0
2	DB	216/241 (90%)	130 (60%)	50 (23%)	36 (17%)	0	0
3	AC	204/233 (88%)	148 (72%)	34 (17%)	22 (11%)	0	2
3	DC	204/233 (88%)	154 (76%)	33 (16%)	17 (8%)	1	4
4	AD	203/206 (98%)	115 (57%)	55 (27%)	33 (16%)	0	1
4	DD	203/206 (98%)	111 (55%)	41 (20%)	51 (25%)	0	0
5	AE	148/167 (89%)	116 (78%)	19 (13%)	13 (9%)	1	3
5	DE	148/167 (89%)	106 (72%)	25 (17%)	17 (12%)	0	2
6	AF	98/135 (73%)	62 (63%)	22 (22%)	14 (14%)	0	1
6	DF	98/135 (73%)	74 (76%)	11 (11%)	13 (13%)	0	1
7	AG	149/179 (83%)	88 (59%)	43 (29%)	18 (12%)	0	1
7	DG	149/179 (83%)	112 (75%)	24 (16%)	13 (9%)	1	3
8	AH	127/130 (98%)	92 (72%)	27 (21%)	8 (6%)	1	7
8	DH	127/130 (98%)	97 (76%)	14 (11%)	16 (13%)	0	1
9	AI	125/130 (96%)	84 (67%)	28 (22%)	13 (10%)	0	2
9	DI	125/130 (96%)	83 (66%)	23 (18%)	19 (15%)	0	1
10	AJ	96/103 (93%)	60 (62%)	22 (23%)	14 (15%)	0	1
10	DJ	96/103 (93%)	71 (74%)	17 (18%)	8 (8%)	1	4
11	AK	115/129 (89%)	67 (58%)	30 (26%)	18 (16%)	0	1
11	DK	115/129 (89%)	85 (74%)	17 (15%)	13 (11%)	0	2
12	AL	121/124 (98%)	94 (78%)	14 (12%)	13 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	DL	121/124 (98%)	72 (60%)	32 (26%)	17 (14%)	0	1
13	AM	112/118 (95%)	63 (56%)	29 (26%)	20 (18%)	0	0
13	DM	112/118 (95%)	71 (63%)	26 (23%)	15 (13%)	0	1
14	AN	92/101 (91%)	65 (71%)	18 (20%)	9 (10%)	0	2
14	DN	92/101 (91%)	63 (68%)	15 (16%)	14 (15%)	0	1
15	AO	86/89 (97%)	65 (76%)	17 (20%)	4 (5%)	2	14
15	DO	86/89 (97%)	66 (77%)	14 (16%)	6 (7%)	1	6
16	AP	80/82 (98%)	48 (60%)	26 (32%)	6 (8%)	1	5
16	DP	80/82 (98%)	48 (60%)	25 (31%)	7 (9%)	1	3
17	AQ	78/84 (93%)	55 (70%)	11 (14%)	12 (15%)	0	1
17	DQ	78/84 (93%)	47 (60%)	21 (27%)	10 (13%)	0	1
18	AR	53/75 (71%)	37 (70%)	9 (17%)	7 (13%)	0	1
18	DR	53/75 (71%)	38 (72%)	7 (13%)	8 (15%)	0	1
19	AS	77/92 (84%)	45 (58%)	17 (22%)	15 (20%)	0	0
19	DS	77/92 (84%)	53 (69%)	16 (21%)	8 (10%)	0	2
20	AT	83/87 (95%)	69 (83%)	6 (7%)	8 (10%)	0	3
20	DT	83/87 (95%)	62 (75%)	15 (18%)	6 (7%)	1	5
21	AU	49/71 (69%)	20 (41%)	16 (33%)	13 (26%)	0	0
21	DU	49/71 (69%)	25 (51%)	9 (18%)	15 (31%)	0	0
22	AV	181/185 (98%)	137 (76%)	30 (17%)	14 (8%)	1	5
27	BC	269/273 (98%)	216 (80%)	37 (14%)	16 (6%)	1	9
27	CC	269/273 (98%)	214 (80%)	41 (15%)	14 (5%)	2	12
28	BD	207/209 (99%)	176 (85%)	22 (11%)	9 (4%)	2	15
28	CD	207/209 (99%)	170 (82%)	25 (12%)	12 (6%)	1	10
29	BE	199/201 (99%)	160 (80%)	30 (15%)	9 (4%)	2	14
29	CE	199/201 (99%)	156 (78%)	31 (16%)	12 (6%)	1	9
30	BF	175/179 (98%)	127 (73%)	32 (18%)	16 (9%)	1	3
30	CF	175/179 (98%)	122 (70%)	37 (21%)	16 (9%)	1	3
31	BG	174/177 (98%)	133 (76%)	29 (17%)	12 (7%)	1	6
31	CG	174/177 (98%)	135 (78%)	27 (16%)	12 (7%)	1	6
32	BH	147/149 (99%)	84 (57%)	40 (27%)	23 (16%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	CH	147/149 (99%)	93 (63%)	36 (24%)	18 (12%)	0	1
33	BI	139/142 (98%)	77 (55%)	37 (27%)	25 (18%)	0	0
33	CI	139/142 (98%)	84 (60%)	39 (28%)	16 (12%)	0	2
34	BJ	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	2	15
34	CJ	140/142 (99%)	123 (88%)	13 (9%)	4 (3%)	4	24
35	BK	120/123 (98%)	99 (82%)	10 (8%)	11 (9%)	1	3
35	CK	120/123 (98%)	92 (77%)	22 (18%)	6 (5%)	2	12
36	BL	141/144 (98%)	114 (81%)	15 (11%)	12 (8%)	1	4
36	CL	141/144 (98%)	98 (70%)	29 (21%)	14 (10%)	0	2
37	BM	134/136 (98%)	110 (82%)	16 (12%)	8 (6%)	1	9
37	CM	134/136 (98%)	109 (81%)	17 (13%)	8 (6%)	1	9
38	BN	118/127 (93%)	98 (83%)	14 (12%)	6 (5%)	2	12
38	CN	118/127 (93%)	83 (70%)	32 (27%)	3 (2%)	5	28
39	BO	114/117 (97%)	90 (79%)	18 (16%)	6 (5%)	2	11
39	CO	114/117 (97%)	80 (70%)	23 (20%)	11 (10%)	0	3
40	BP	112/115 (97%)	94 (84%)	15 (13%)	3 (3%)	5	26
40	CP	112/115 (97%)	91 (81%)	16 (14%)	5 (4%)	2	14
41	BQ	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	17	55
41	CQ	115/118 (98%)	99 (86%)	13 (11%)	3 (3%)	5	27
42	BR	101/103 (98%)	89 (88%)	7 (7%)	5 (5%)	2	12
42	CR	101/103 (98%)	76 (75%)	18 (18%)	7 (7%)	1	6
43	BS	108/110 (98%)	96 (89%)	10 (9%)	2 (2%)	8	36
43	CS	108/110 (98%)	82 (76%)	16 (15%)	10 (9%)	0	3
44	BT	91/100 (91%)	72 (79%)	11 (12%)	8 (9%)	1	3
44	CT	91/100 (91%)	72 (79%)	11 (12%)	8 (9%)	1	3
45	BU	100/104 (96%)	79 (79%)	14 (14%)	7 (7%)	1	6
45	CU	100/104 (96%)	67 (67%)	23 (23%)	10 (10%)	0	2
46	BV	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
46	CV	92/94 (98%)	74 (80%)	14 (15%)	4 (4%)	2	15
47	BW	74/85 (87%)	60 (81%)	9 (12%)	5 (7%)	1	6
47	CW	73/85 (86%)	60 (82%)	10 (14%)	3 (4%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	BX	75/78 (96%)	62 (83%)	9 (12%)	4 (5%)	2	11
48	CX	75/78 (96%)	63 (84%)	10 (13%)	2 (3%)	5	26
49	BY	61/63 (97%)	46 (75%)	9 (15%)	6 (10%)	0	2
49	CY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	4
50	BZ	56/59 (95%)	45 (80%)	11 (20%)	0	100	100
50	CZ	56/59 (95%)	47 (84%)	9 (16%)	0	100	100
51	B0	54/57 (95%)	45 (83%)	4 (7%)	5 (9%)	0	3
51	C0	54/57 (95%)	42 (78%)	4 (7%)	8 (15%)	0	1
52	B1	48/55 (87%)	31 (65%)	12 (25%)	5 (10%)	0	2
52	C1	48/55 (87%)	37 (77%)	11 (23%)	0	100	100
53	B2	44/46 (96%)	37 (84%)	6 (14%)	1 (2%)	6	30
53	C2	44/46 (96%)	38 (86%)	4 (9%)	2 (4%)	2	14
54	B3	62/65 (95%)	51 (82%)	7 (11%)	4 (6%)	1	7
54	C3	62/65 (95%)	52 (84%)	8 (13%)	2 (3%)	4	22
55	B4	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	2	10
55	C4	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	5	25
56	B5	183/228 (80%)	80 (44%)	66 (36%)	37 (20%)	0	0
All	All	11599/12383 (94%)	8463 (73%)	2041 (18%)	1095 (9%)	0	3

5 of 1095 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	31	ILE
2	AB	34	ALA
2	AB	52	GLU
2	AB	73	LYS

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	180/199 (90%)	145 (81%)	35 (19%)	1	7
2	DB	180/199 (90%)	142 (79%)	38 (21%)	1	5
3	AC	170/190 (90%)	138 (81%)	32 (19%)	1	8
3	DC	170/190 (90%)	140 (82%)	30 (18%)	2	10
4	AD	172/173 (99%)	126 (73%)	46 (27%)	0	2
4	DD	172/173 (99%)	130 (76%)	42 (24%)	0	3
5	AE	113/126 (90%)	91 (80%)	22 (20%)	1	7
5	DE	113/126 (90%)	89 (79%)	24 (21%)	1	5
6	AF	87/116 (75%)	68 (78%)	19 (22%)	1	5
6	DF	87/116 (75%)	70 (80%)	17 (20%)	1	7
7	AG	124/147 (84%)	101 (82%)	23 (18%)	1	8
7	DG	124/147 (84%)	106 (86%)	18 (14%)	3	15
8	AH	104/105 (99%)	85 (82%)	19 (18%)	1	9
8	DH	104/105 (99%)	87 (84%)	17 (16%)	2	11
9	AI	105/107 (98%)	78 (74%)	27 (26%)	0	3
9	DI	105/107 (98%)	82 (78%)	23 (22%)	1	5
10	AJ	86/90 (96%)	66 (77%)	20 (23%)	1	4
10	DJ	86/90 (96%)	67 (78%)	19 (22%)	1	4
11	AK	90/99 (91%)	72 (80%)	18 (20%)	1	7
11	DK	90/99 (91%)	75 (83%)	15 (17%)	2	11
12	AL	103/104 (99%)	74 (72%)	29 (28%)	0	2
12	DL	103/104 (99%)	82 (80%)	21 (20%)	1	6
13	AM	92/96 (96%)	68 (74%)	24 (26%)	0	2
13	DM	92/96 (96%)	74 (80%)	18 (20%)	1	7
14	AN	79/84 (94%)	60 (76%)	19 (24%)	0	3
14	DN	79/84 (94%)	59 (75%)	20 (25%)	0	3
15	AO	76/77 (99%)	59 (78%)	17 (22%)	1	4
15	DO	76/77 (99%)	60 (79%)	16 (21%)	1	5
16	AP	65/65 (100%)	47 (72%)	18 (28%)	0	2
16	DP	65/65 (100%)	51 (78%)	14 (22%)	1	5
17	AQ	74/78 (95%)	61 (82%)	13 (18%)	2	10
17	DQ	74/78 (95%)	54 (73%)	20 (27%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	48/65 (74%)	33 (69%)	15 (31%)	0	1
18	DR	48/65 (74%)	36 (75%)	12 (25%)	0	3
19	AS	70/79 (89%)	47 (67%)	23 (33%)	0	1
19	DS	70/79 (89%)	56 (80%)	14 (20%)	1	7
20	AT	65/66 (98%)	48 (74%)	17 (26%)	0	2
20	DT	65/66 (98%)	51 (78%)	14 (22%)	1	5
21	AU	44/61 (72%)	31 (70%)	13 (30%)	0	1
21	DU	44/61 (72%)	30 (68%)	14 (32%)	0	1
22	AV	157/160 (98%)	128 (82%)	29 (18%)	1	8
27	BC	216/218 (99%)	173 (80%)	43 (20%)	1	7
27	CC	216/218 (99%)	176 (82%)	40 (18%)	1	8
28	BD	164/164 (100%)	131 (80%)	33 (20%)	1	6
28	CD	164/164 (100%)	135 (82%)	29 (18%)	2	9
29	BE	165/165 (100%)	142 (86%)	23 (14%)	3	16
29	CE	165/165 (100%)	137 (83%)	28 (17%)	2	10
30	BF	148/150 (99%)	118 (80%)	30 (20%)	1	6
30	CF	148/150 (99%)	125 (84%)	23 (16%)	2	13
31	BG	137/138 (99%)	109 (80%)	28 (20%)	1	6
31	CG	137/138 (99%)	112 (82%)	25 (18%)	1	9
32	BH	113/114 (99%)	90 (80%)	23 (20%)	1	6
32	CH	113/114 (99%)	85 (75%)	28 (25%)	0	3
33	BI	109/110 (99%)	94 (86%)	15 (14%)	3	17
33	CI	109/110 (99%)	96 (88%)	13 (12%)	5	22
34	BJ	116/116 (100%)	98 (84%)	18 (16%)	2	13
34	CJ	116/116 (100%)	97 (84%)	19 (16%)	2	11
35	BK	103/104 (99%)	86 (84%)	17 (16%)	2	11
35	CK	103/104 (99%)	79 (77%)	24 (23%)	1	4
36	BL	102/103 (99%)	78 (76%)	24 (24%)	1	3
36	CL	102/103 (99%)	82 (80%)	20 (20%)	1	7
37	BM	109/109 (100%)	96 (88%)	13 (12%)	5	22
37	CM	109/109 (100%)	90 (83%)	19 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BN	100/103 (97%)	80 (80%)	20 (20%)	1	7
38	CN	100/103 (97%)	91 (91%)	9 (9%)	9	35
39	BO	86/87 (99%)	65 (76%)	21 (24%)	0	3
39	CO	86/87 (99%)	63 (73%)	23 (27%)	0	2
40	BP	99/100 (99%)	78 (79%)	21 (21%)	1	5
40	CP	99/100 (99%)	86 (87%)	13 (13%)	4	18
41	BQ	89/90 (99%)	77 (86%)	12 (14%)	4	17
41	CQ	89/90 (99%)	74 (83%)	15 (17%)	2	11
42	BR	84/84 (100%)	74 (88%)	10 (12%)	5	22
42	CR	84/84 (100%)	73 (87%)	11 (13%)	4	18
43	BS	93/93 (100%)	77 (83%)	16 (17%)	2	10
43	CS	93/93 (100%)	72 (77%)	21 (23%)	1	4
44	BT	80/84 (95%)	65 (81%)	15 (19%)	1	8
44	CT	80/84 (95%)	66 (82%)	14 (18%)	2	10
45	BU	83/85 (98%)	63 (76%)	20 (24%)	0	3
45	CU	83/85 (98%)	67 (81%)	16 (19%)	1	8
46	BV	78/78 (100%)	68 (87%)	10 (13%)	4	19
46	CV	78/78 (100%)	63 (81%)	15 (19%)	1	8
47	BW	57/63 (90%)	46 (81%)	11 (19%)	1	8
47	CW	56/63 (89%)	48 (86%)	8 (14%)	3	15
48	BX	67/68 (98%)	55 (82%)	12 (18%)	2	9
48	CX	67/68 (98%)	55 (82%)	12 (18%)	2	9
49	BY	55/55 (100%)	43 (78%)	12 (22%)	1	5
49	CY	55/55 (100%)	45 (82%)	10 (18%)	1	9
50	BZ	48/49 (98%)	40 (83%)	8 (17%)	2	11
50	CZ	48/49 (98%)	40 (83%)	8 (17%)	2	11
51	B0	47/48 (98%)	44 (94%)	3 (6%)	17	51
51	C0	47/48 (98%)	41 (87%)	6 (13%)	4	19
52	B1	45/49 (92%)	39 (87%)	6 (13%)	4	17
52	C1	45/49 (92%)	38 (84%)	7 (16%)	2	13
53	B2	38/38 (100%)	31 (82%)	7 (18%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	C2	38/38 (100%)	31 (82%)	7 (18%)	1	9
54	B3	51/52 (98%)	43 (84%)	8 (16%)	2	13
54	C3	51/52 (98%)	42 (82%)	9 (18%)	2	10
55	B4	34/34 (100%)	26 (76%)	8 (24%)	1	3
55	C4	34/34 (100%)	27 (79%)	7 (21%)	1	6
56	B5	61/180 (34%)	52 (85%)	9 (15%)	3	14
All	All	9543/10096 (94%)	7684 (80%)	1859 (20%)	1	7

5 of 1859 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	BS	97	LEU
28	CD	177	VAL
13	DM	14	HIS
45	BU	34	ILE
53	B2	15	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
34	BJ	47	HIS
56	B5	66	HIS
12	DL	77	HIS
45	BU	44	HIS
27	CC	116	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1542 (99%)	349 (22%)	15 (0%)
1	DA	1538/1542 (99%)	330 (21%)	17 (1%)
23	AW	14/16 (87%)	5 (35%)	0
23	DV	15/16 (93%)	6 (40%)	0
24	AX	75/76 (98%)	27 (36%)	6 (8%)
24	DW	75/76 (98%)	20 (26%)	0
25	BA	2896/2904 (99%)	590 (20%)	35 (1%)
25	CA	2895/2904 (99%)	618 (21%)	34 (1%)
26	BB	118/120 (98%)	16 (13%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	CB	117/120 (97%)	27 (23%)	0
All	All	9280/9316 (99%)	1988 (21%)	107 (1%)

5 of 1988 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	28	A
1	AA	30	U

5 of 107 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2324	U
25	CA	479	A
1	DA	723	U
25	BA	2326	C
25	BA	2756	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 510 ligands modelled in this entry, 497 are monoatomic - leaving 13 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
58	PAR	CA	3169	-	45,45,45	0.49	0	64,67,67	0.95	4 (6%)
58	PAR	BA	3002	-	45,45,45	0.79	1 (2%)	64,67,67	0.99	3 (4%)
58	PAR	CA	3168	-	45,45,45	0.54	0	64,67,67	1.33	5 (7%)
58	PAR	CA	3166	-	45,45,45	0.49	0	64,67,67	0.95	4 (6%)
58	PAR	BA	3001	-	45,45,45	0.71	0	64,67,67	1.04	5 (7%)
58	PAR	BA	3005	-	45,45,45	0.54	0	64,67,67	1.10	4 (6%)
58	PAR	BA	3004	-	45,45,45	0.71	0	64,67,67	1.05	5 (7%)
58	PAR	AA	1672	-	45,45,45	0.77	0	64,67,67	1.14	4 (6%)
58	PAR	BA	3003	-	45,45,45	0.74	0	64,67,67	1.08	5 (7%)
58	PAR	CA	3167	-	45,45,45	0.57	0	64,67,67	0.89	3 (4%)
58	PAR	DA	1654	-	45,45,45	0.53	0	64,67,67	0.83	2 (3%)
58	PAR	CA	3170	-	45,45,45	0.50	0	64,67,67	0.94	4 (6%)
58	PAR	DA	1655	-	45,45,45	0.50	0	64,67,67	0.92	3 (4%)

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
58	PAR	CA	3169	-	-	4/18/94/94	0/4/4/4
58	PAR	BA	3002	-	-	6/18/94/94	0/4/4/4
58	PAR	CA	3168	-	-	1/18/94/94	0/4/4/4
58	PAR	CA	3166	-	-	2/18/94/94	0/4/4/4
58	PAR	BA	3001	-	-	6/18/94/94	0/4/4/4
58	PAR	BA	3005	-	-	7/18/94/94	0/4/4/4
58	PAR	BA	3004	-	-	7/18/94/94	0/4/4/4
58	PAR	AA	1672	-	-	8/18/94/94	0/4/4/4
58	PAR	BA	3003	-	-	8/18/94/94	0/4/4/4
58	PAR	CA	3167	-	-	3/18/94/94	0/4/4/4
58	PAR	DA	1654	-	-	1/18/94/94	0/4/4/4
58	PAR	CA	3170	-	-	3/18/94/94	0/4/4/4
58	PAR	DA	1655	-	-	3/18/94/94	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BA	3002	PAR	C13-C23	-2.04	1.50	1.52

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	CA	3168	PAR	C14-O33-C33	-4.52	106.77	117.96
58	CA	3168	PAR	C11-O11-C42	-4.50	106.83	117.96
58	CA	3168	PAR	C13-O52-C52	-4.48	106.88	117.96
58	BA	3004	PAR	O52-C13-O43	-3.78	107.33	111.43
58	BA	3005	PAR	C13-O52-C52	-3.61	109.03	117.96

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BA	3003	PAR	C23-C13-O52-C52
58	BA	3003	PAR	O43-C13-O52-C52
58	BA	3003	PAR	C24-C14-O33-C33
58	BA	3003	PAR	C44-C54-C64-N64
58	BA	3003	PAR	O54-C54-C64-N64

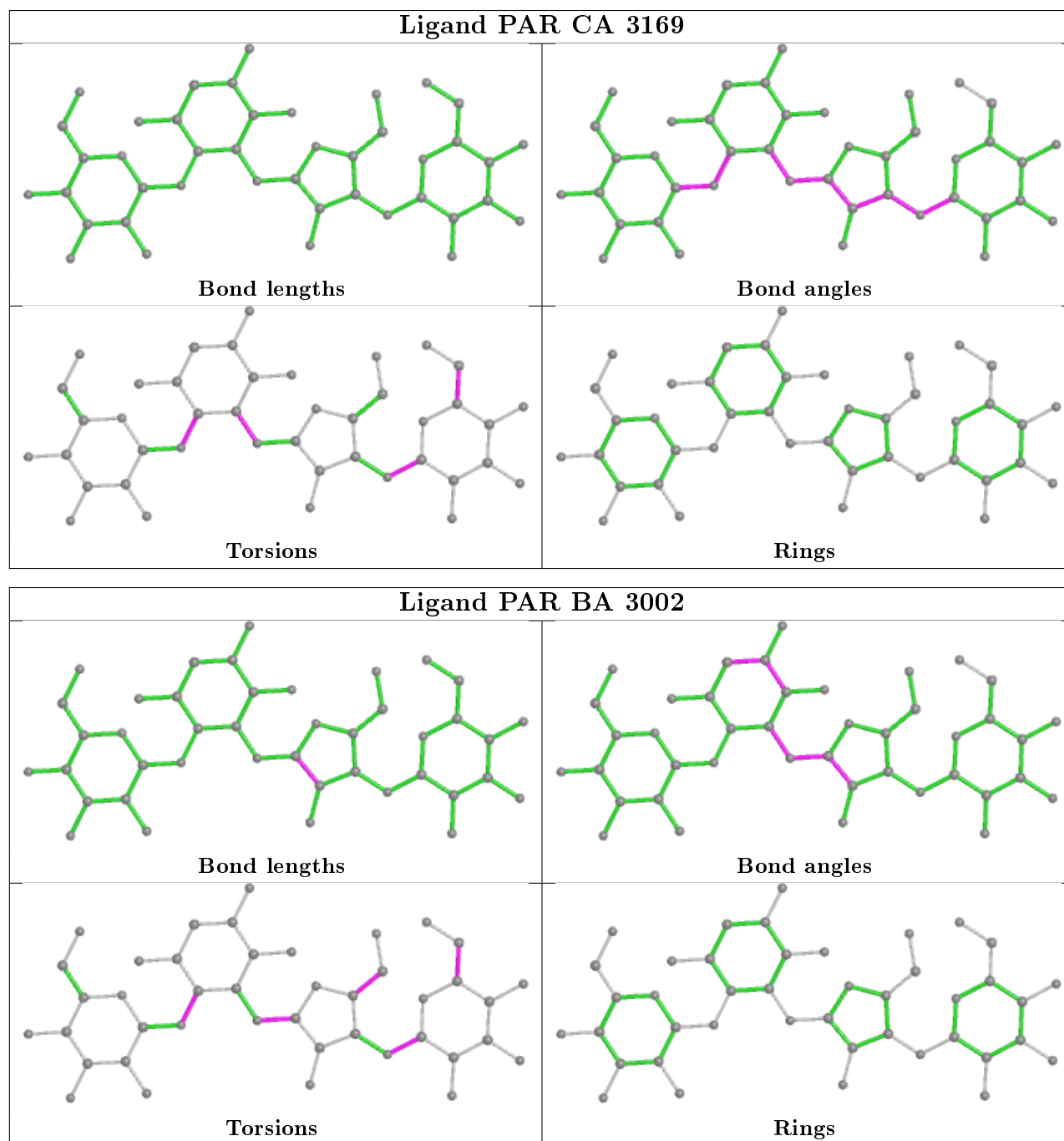
There are no ring outliers.

13 monomers are involved in 106 short contacts:

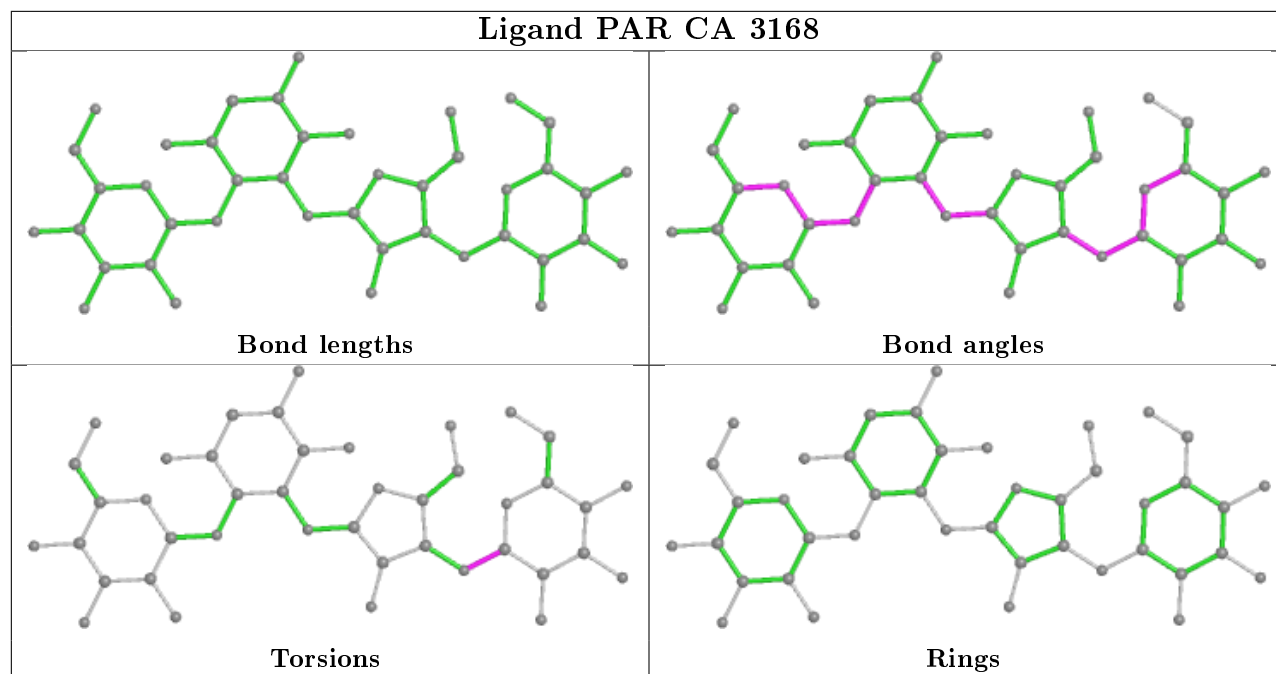
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	CA	3169	PAR	20	0
58	BA	3002	PAR	2	0
58	CA	3168	PAR	5	0
58	CA	3166	PAR	14	0
58	BA	3001	PAR	3	0
58	BA	3005	PAR	21	0
58	BA	3004	PAR	3	0
58	AA	1672	PAR	9	0
58	BA	3003	PAR	4	0
58	CA	3167	PAR	7	0
58	DA	1654	PAR	5	0
58	CA	3170	PAR	5	0
58	DA	1655	PAR	8	0

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

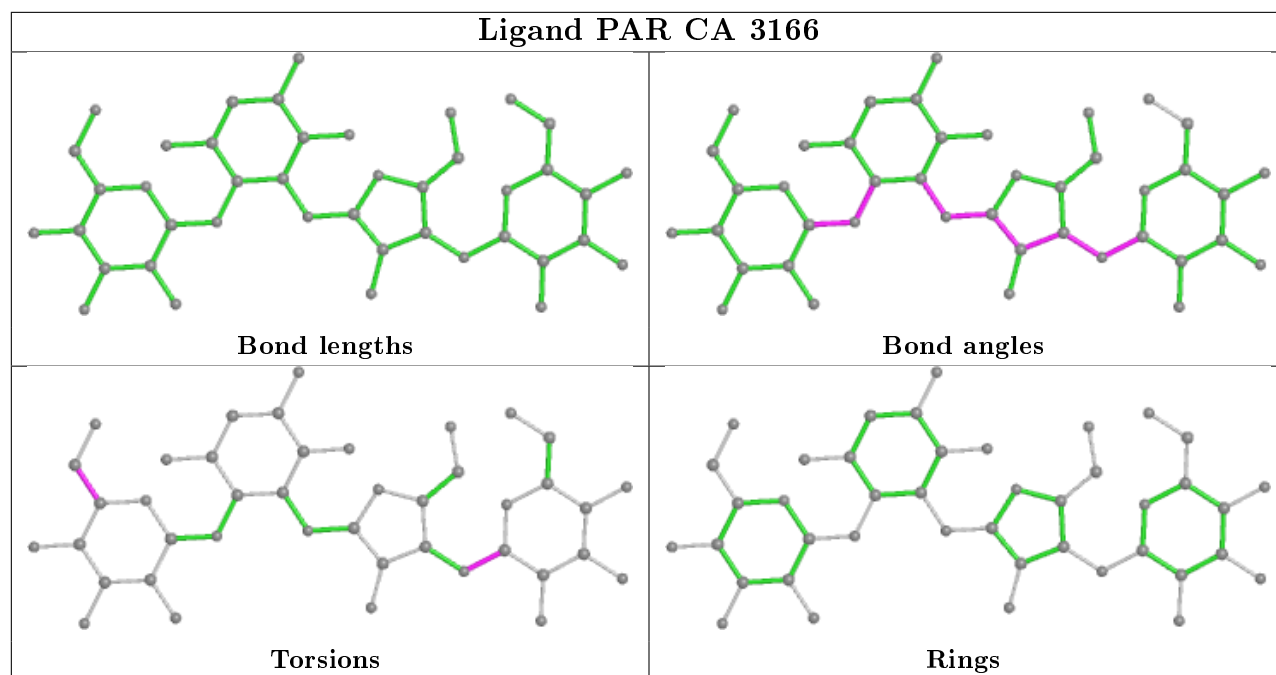
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



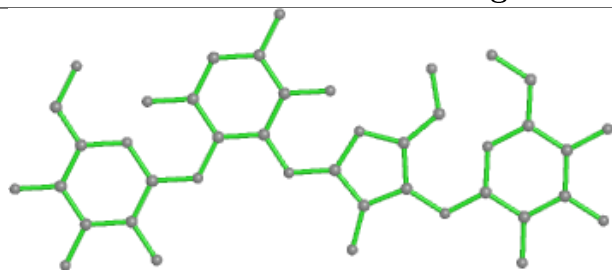
Ligand PAR CA 3168



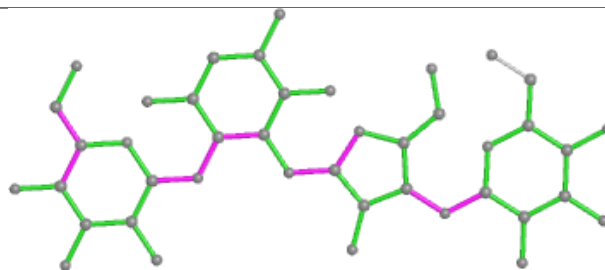
Ligand PAR CA 3166



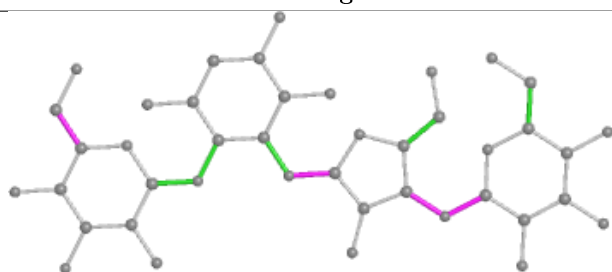
Ligand PAR BA 3001



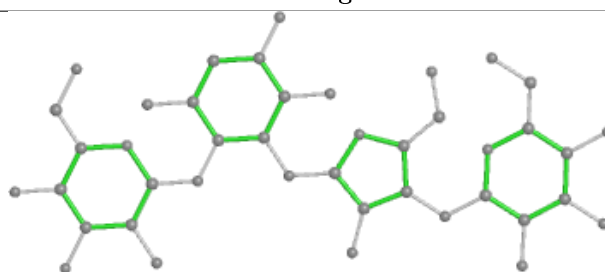
Bond lengths



Bond angles

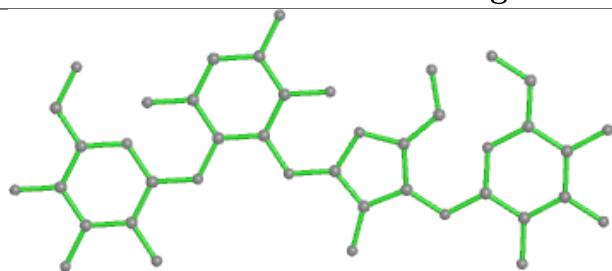


Torsions

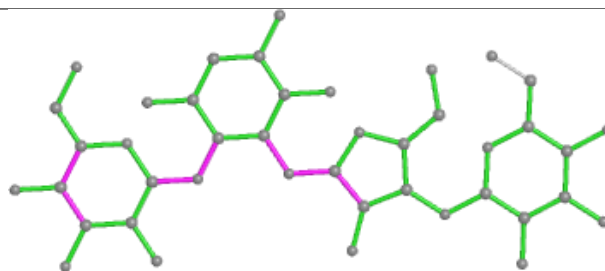


Rings

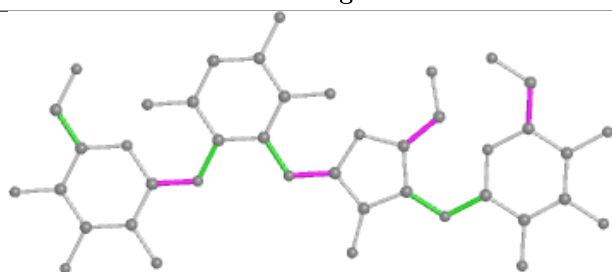
Ligand PAR BA 3005



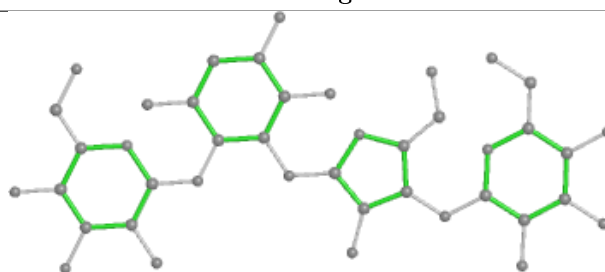
Bond lengths



Bond angles

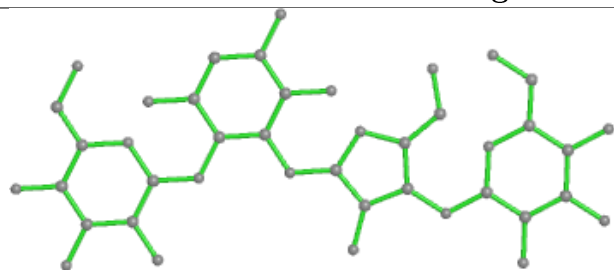


Torsions

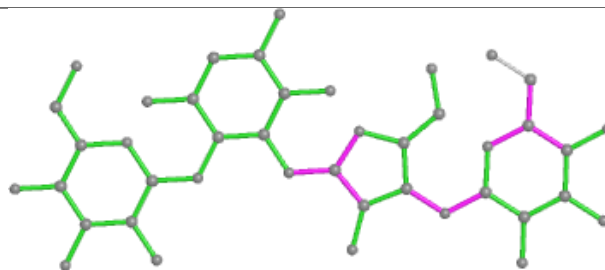


Rings

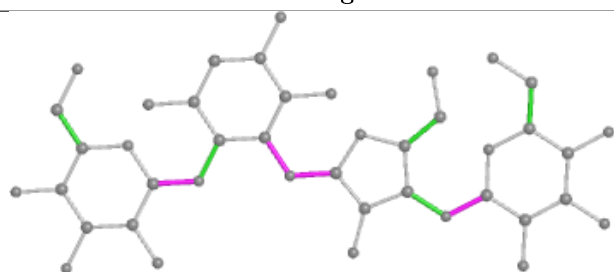
Ligand PAR BA 3004



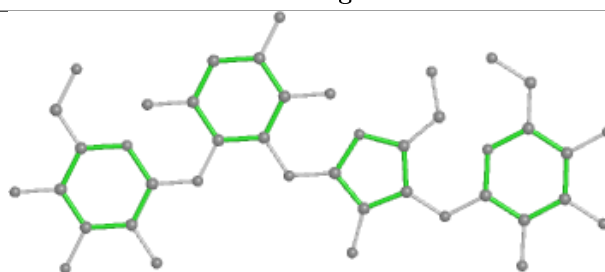
Bond lengths



Bond angles

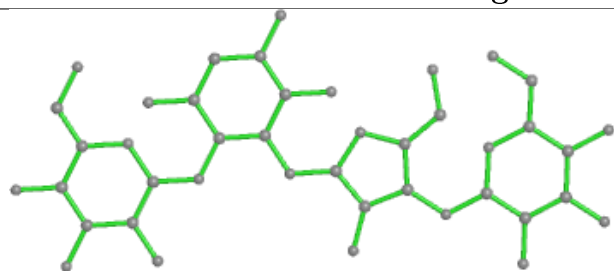


Torsions

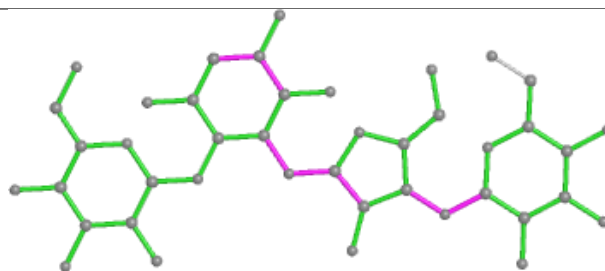


Rings

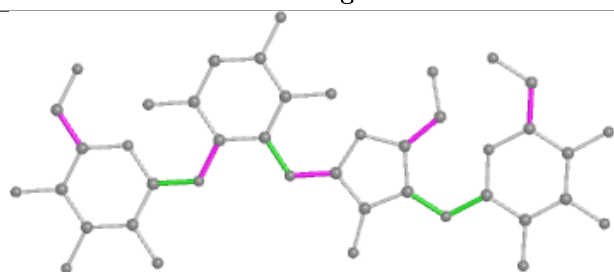
Ligand PAR AA 1672



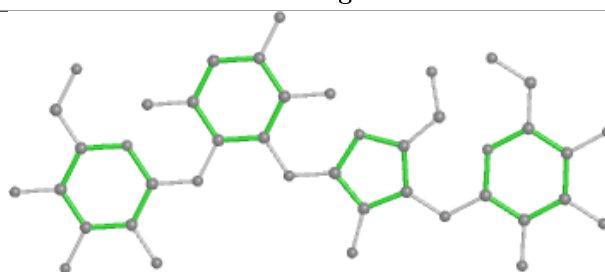
Bond lengths



Bond angles

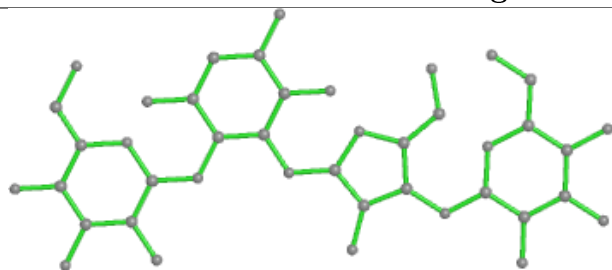


Torsions

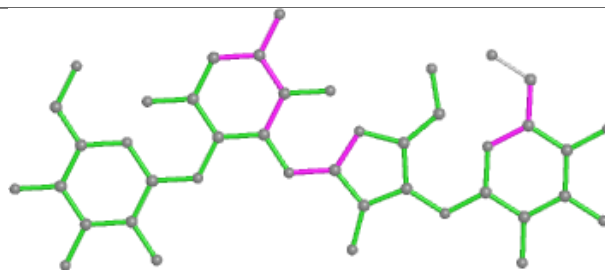


Rings

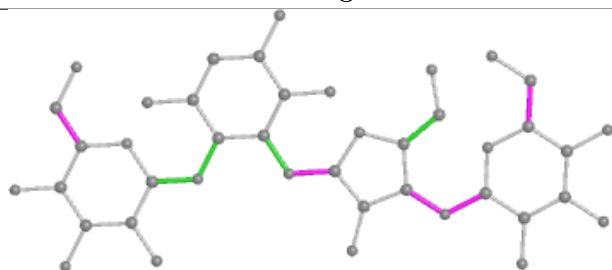
Ligand PAR BA 3003



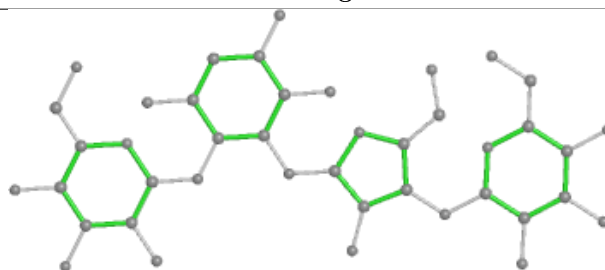
Bond lengths



Bond angles

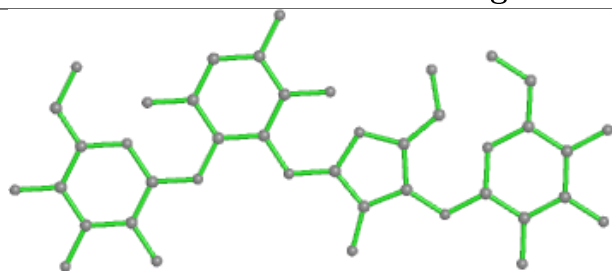


Torsions

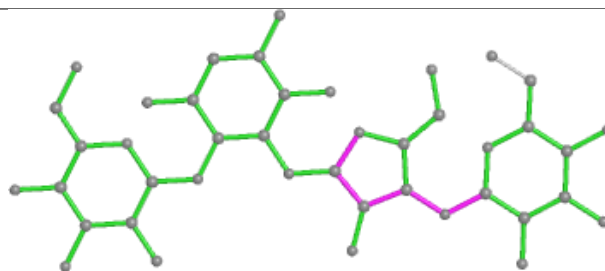


Rings

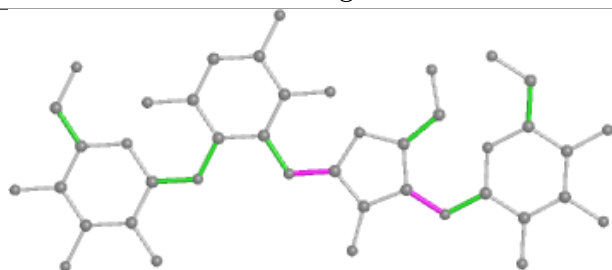
Ligand PAR CA 3167



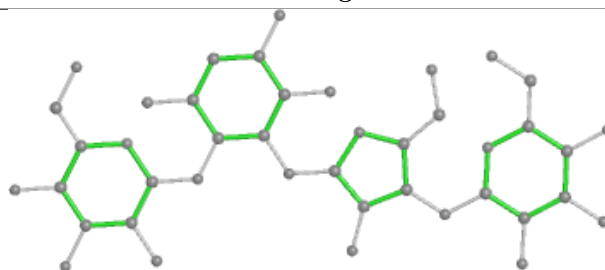
Bond lengths



Bond angles

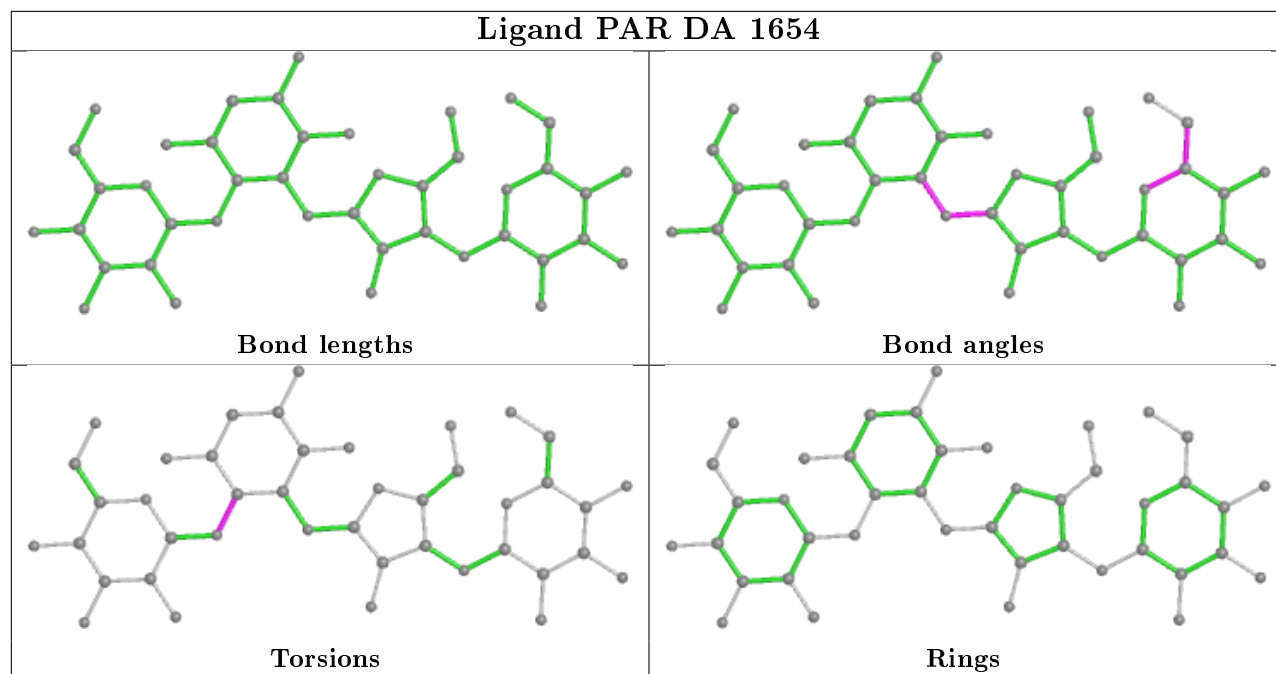


Torsions

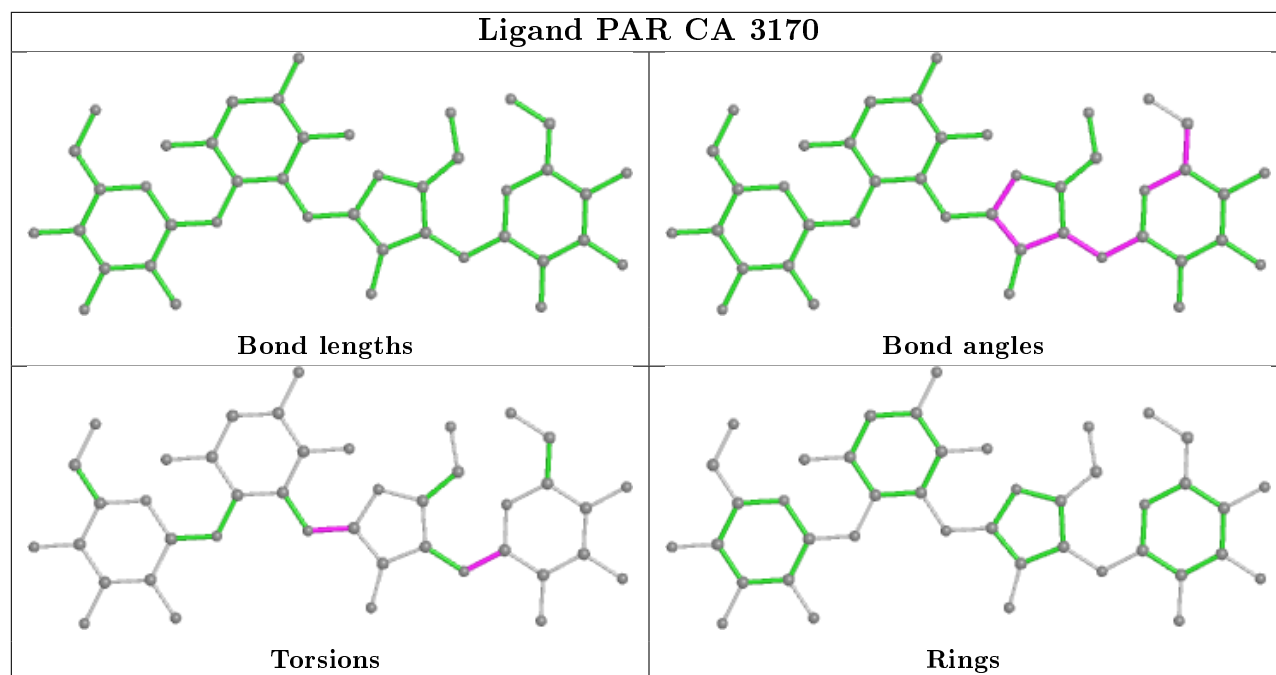


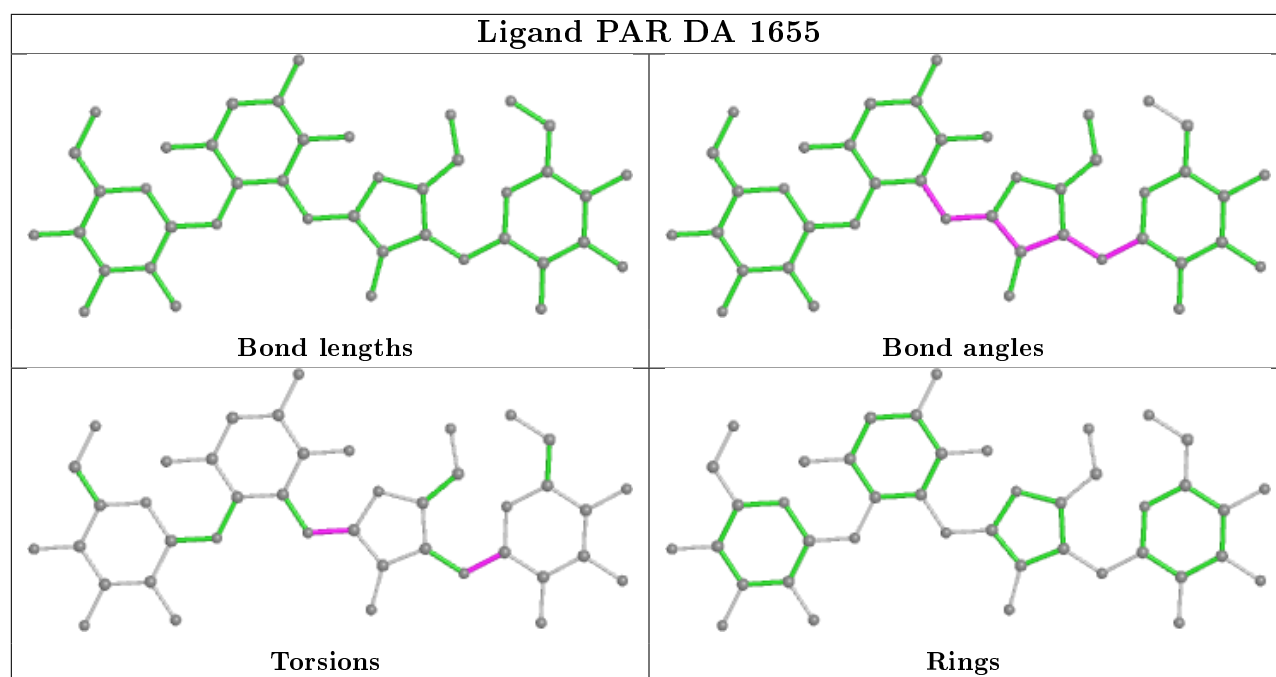
Rings

Ligand PAR DA 1654



Ligand PAR CA 3170





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	1538/1542 (99%)	-0.65	2 (0%) 95 89	44, 86, 166, 303	0
1	DA	1539/1542 (99%)	-0.63	1 (0%) 95 89	47, 85, 145, 285	0
2	AB	218/241 (90%)	0.80	28 (12%) 3 1	64, 133, 196, 238	0
2	DB	218/241 (90%)	0.48	14 (6%) 19 6	68, 115, 176, 210	0
3	AC	206/233 (88%)	-0.44	0 100 100	44, 77, 114, 170	0
3	DC	206/233 (88%)	-0.17	0 100 100	49, 90, 145, 213	0
4	AD	205/206 (99%)	0.03	7 (3%) 45 19	62, 104, 170, 243	0
4	DD	205/206 (99%)	0.01	9 (4%) 34 13	47, 92, 166, 215	0
5	AE	150/167 (89%)	-0.16	1 (0%) 87 69	53, 81, 124, 222	0
5	DE	150/167 (89%)	-0.39	0 100 100	44, 79, 132, 171	0
6	AF	100/135 (74%)	-0.11	1 (1%) 82 59	67, 122, 177, 211	0
6	DF	100/135 (74%)	-0.27	2 (2%) 65 36	50, 94, 135, 153	0
7	AG	151/179 (84%)	0.18	8 (5%) 26 10	62, 119, 169, 239	0
7	DG	151/179 (84%)	-0.05	4 (2%) 56 27	61, 104, 150, 211	0
8	AH	129/130 (99%)	-0.05	3 (2%) 60 31	59, 92, 136, 159	0
8	DH	129/130 (99%)	-0.20	2 (1%) 72 44	49, 84, 119, 174	0
9	AI	127/130 (97%)	0.34	9 (7%) 16 5	57, 108, 158, 215	0
9	DI	127/130 (97%)	0.23	5 (3%) 39 15	70, 116, 174, 197	0
10	AJ	98/103 (95%)	0.47	9 (9%) 9 3	57, 111, 175, 216	0
10	DJ	98/103 (95%)	-0.03	3 (3%) 49 21	65, 111, 168, 200	0
11	AK	117/129 (90%)	0.36	12 (10%) 6 2	58, 108, 177, 232	0
11	DK	117/129 (90%)	-0.20	4 (3%) 45 19	47, 75, 131, 186	0
12	AL	123/124 (99%)	-0.23	3 (2%) 59 30	33, 65, 115, 216	0
12	DL	123/124 (99%)	0.05	1 (0%) 86 65	33, 71, 115, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/118 (96%)	0.70	11 (9%) 8 2	73, 132, 191, 263	0
13	DM	114/118 (96%)	0.35	9 (7%) 12 4	92, 135, 174, 254	0
14	AN	96/101 (95%)	0.05	4 (4%) 36 14	59, 95, 188, 237	0
14	DN	96/101 (95%)	0.05	2 (2%) 63 34	62, 104, 164, 215	0
15	AO	88/89 (98%)	0.10	3 (3%) 45 19	60, 102, 166, 216	0
15	DO	88/89 (98%)	-0.10	2 (2%) 60 31	55, 85, 131, 156	0
16	AP	82/82 (100%)	0.40	6 (7%) 15 4	61, 86, 144, 198	0
16	DP	82/82 (100%)	0.43	6 (7%) 15 4	53, 79, 141, 227	0
17	AQ	80/84 (95%)	0.29	5 (6%) 20 6	52, 97, 152, 198	0
17	DQ	80/84 (95%)	0.51	6 (7%) 14 4	58, 96, 161, 233	0
18	AR	55/75 (73%)	0.02	2 (3%) 42 17	57, 97, 151, 178	0
18	DR	55/75 (73%)	-0.25	2 (3%) 42 17	57, 83, 134, 176	0
19	AS	79/92 (85%)	0.77	9 (11%) 5 1	91, 129, 184, 223	0
19	DS	79/92 (85%)	0.80	9 (11%) 5 1	83, 129, 181, 234	0
20	AT	85/87 (97%)	0.25	3 (3%) 44 18	54, 92, 134, 194	0
20	DT	85/87 (97%)	0.16	2 (2%) 59 30	64, 96, 132, 179	0
21	AU	51/71 (71%)	0.09	0 100 100	67, 117, 167, 203	0
21	DU	51/71 (71%)	-0.17	2 (3%) 39 15	54, 105, 159, 224	0
22	AV	183/185 (98%)	-0.13	3 (1%) 72 44	20, 86, 171, 232	0
23	AW	15/16 (93%)	-0.19	0 100 100	57, 128, 176, 205	0
23	DV	16/16 (100%)	-0.30	1 (6%) 20 6	44, 99, 143, 191	0
24	AX	76/76 (100%)	0.38	8 (10%) 6 2	44, 167, 277, 328	0
24	DW	76/76 (100%)	-0.48	0 100 100	51, 93, 135, 164	0
25	BA	2897/2904 (99%)	-0.44	94 (3%) 47 20	22, 52, 194, 368	0
25	CA	2897/2904 (99%)	-0.51	46 (1%) 72 44	37, 75, 205, 328	0
26	BB	119/120 (99%)	-0.82	0 100 100	41, 71, 101, 165	0
26	CB	118/120 (98%)	-0.81	0 100 100	63, 118, 153, 186	0
27	BC	271/273 (99%)	-0.46	0 100 100	32, 60, 94, 149	0
27	CC	271/273 (99%)	-0.34	1 (0%) 92 79	38, 73, 106, 185	0
28	BD	209/209 (100%)	-0.53	0 100 100	21, 45, 77, 170	0
28	CD	209/209 (100%)	-0.37	0 100 100	41, 68, 109, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	BE	201/201 (100%)	-0.34	0 100 100	23, 56, 105, 161	0
29	CE	201/201 (100%)	-0.18	0 100 100	32, 79, 125, 175	0
30	BF	177/179 (98%)	0.48	15 (8%) 10 3	44, 104, 177, 231	0
30	CF	177/179 (98%)	0.90	33 (18%) 1 0	87, 140, 202, 243	0
31	BG	176/177 (99%)	-0.15	3 (1%) 70 41	32, 72, 114, 158	0
31	CG	176/177 (99%)	0.40	7 (3%) 38 15	72, 112, 153, 195	0
32	BH	149/149 (100%)	0.25	7 (4%) 31 11	28, 118, 177, 265	0
32	CH	149/149 (100%)	0.57	14 (9%) 8 3	28, 133, 188, 220	0
33	BI	141/142 (99%)	2.88	81 (57%) 0 0	118, 197, 266, 320	0
33	CI	141/142 (99%)	3.46	92 (65%) 0 0	137, 210, 253, 292	0
34	BJ	142/142 (100%)	-0.57	0 100 100	21, 44, 79, 102	0
34	CJ	142/142 (100%)	-0.31	0 100 100	37, 65, 99, 167	0
35	BK	122/123 (99%)	-0.59	0 100 100	23, 49, 77, 104	0
35	CK	122/123 (99%)	-0.25	0 100 100	42, 69, 112, 148	0
36	BL	143/144 (99%)	-0.51	0 100 100	24, 54, 83, 118	0
36	CL	143/144 (99%)	-0.15	2 (1%) 75 49	39, 82, 125, 180	0
37	BM	136/136 (100%)	-0.48	0 100 100	27, 51, 89, 121	0
37	CM	136/136 (100%)	0.19	4 (2%) 51 23	44, 78, 106, 141	0
38	BN	120/127 (94%)	-0.58	0 100 100	22, 47, 71, 156	0
38	CN	120/127 (94%)	-0.20	1 (0%) 86 65	46, 76, 103, 191	0
39	BO	116/117 (99%)	-0.17	0 100 100	37, 67, 99, 123	0
39	CO	116/117 (99%)	0.48	8 (6%) 16 5	70, 122, 164, 201	0
40	BP	114/115 (99%)	-0.52	2 (1%) 68 40	30, 56, 99, 206	0
40	CP	114/115 (99%)	-0.32	0 100 100	45, 77, 116, 140	0
41	BQ	117/118 (99%)	-0.63	0 100 100	15, 39, 71, 91	0
41	CQ	117/118 (99%)	-0.42	0 100 100	32, 61, 85, 114	0
42	BR	103/103 (100%)	-0.48	0 100 100	21, 52, 87, 118	0
42	CR	103/103 (100%)	-0.36	1 (0%) 82 59	32, 73, 108, 171	0
43	BS	110/110 (100%)	-0.47	0 100 100	20, 44, 76, 117	0
43	CS	110/110 (100%)	-0.37	0 100 100	31, 65, 103, 140	0
44	BT	93/100 (93%)	-0.10	1 (1%) 80 56	43, 60, 126, 213	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	CT	93/100 (93%)	0.06	2 (2%) 62 33	56, 94, 142, 202	0
45	BU	102/104 (98%)	-0.41	0 100 100	33, 61, 118, 185	0
45	CU	102/104 (98%)	0.42	9 (8%) 10 3	56, 90, 177, 215	0
46	BV	94/94 (100%)	-0.29	1 (1%) 80 56	41, 71, 109, 127	0
46	CV	94/94 (100%)	0.10	1 (1%) 80 56	66, 110, 151, 196	0
47	BW	76/85 (89%)	-0.41	1 (1%) 77 51	32, 54, 92, 126	0
47	CW	75/85 (88%)	0.14	1 (1%) 77 51	46, 82, 120, 146	0
48	BX	77/78 (98%)	-0.31	0 100 100	39, 59, 101, 111	0
48	CX	77/78 (98%)	-0.08	2 (2%) 56 27	38, 82, 121, 150	0
49	BY	63/63 (100%)	-0.17	3 (4%) 30 11	39, 69, 114, 179	0
49	CY	63/63 (100%)	0.29	3 (4%) 30 11	66, 103, 165, 221	0
50	BZ	58/59 (98%)	-0.33	0 100 100	30, 47, 75, 106	0
50	CZ	58/59 (98%)	-0.21	1 (1%) 70 41	45, 73, 112, 188	0
51	B0	56/57 (98%)	-0.62	0 100 100	22, 46, 94, 143	0
51	C0	56/57 (98%)	-0.33	1 (1%) 68 40	37, 73, 117, 194	0
52	B1	50/55 (90%)	2.19	17 (34%) 0 0	76, 105, 185, 196	0
52	C1	50/55 (90%)	1.02	7 (14%) 2 1	79, 109, 138, 164	0
53	B2	46/46 (100%)	-0.38	1 (2%) 62 33	27, 45, 76, 155	0
53	C2	46/46 (100%)	-0.23	0 100 100	39, 68, 92, 151	0
54	B3	64/65 (98%)	-0.42	0 100 100	27, 48, 74, 122	0
54	C3	64/65 (98%)	-0.29	0 100 100	38, 69, 96, 109	0
55	B4	38/38 (100%)	-0.33	0 100 100	29, 52, 91, 122	0
55	C4	38/38 (100%)	0.01	0 100 100	47, 83, 109, 119	0
56	B5	191/228 (83%)	5.27	155 (81%) 0 0	28, 219, 264, 311	0
All	All	21100/21699 (97%)	-0.17	840 (3%) 38 15	15, 80, 183, 368	0

The worst 5 of 840 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
56	B5	222	VAL	25.3
33	CI	1	ALA	21.4
56	B5	38	ASP	20.9
56	B5	223	ARG	19.9
56	B5	105	ASP	19.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1646	1/1	0.41	0.46	99,99,99,99	0
57	MG	CA	3084	1/1	0.57	0.20	193,193,193,193	0
57	MG	DA	1650	1/1	0.58	0.17	81,81,81,81	0
57	MG	CA	3015	1/1	0.59	0.11	126,126,126,126	0
58	PAR	CA	3169	42/42	0.64	0.44	21,68,103,144	42
57	MG	CA	3055	1/1	0.72	0.12	114,114,114,114	0
57	MG	AA	1604	1/1	0.72	0.09	173,173,173,173	0
57	MG	AA	1658	1/1	0.73	0.71	97,97,97,97	0
58	PAR	CA	3168	42/42	0.73	0.61	10,10,10,10	0
57	MG	BA	3109	1/1	0.75	0.37	189,189,189,189	0
57	MG	BA	3021	1/1	0.77	0.39	276,276,276,276	0
57	MG	DA	1608	1/1	0.77	0.16	218,218,218,218	0
57	MG	BA	3179	1/1	0.79	0.39	88,88,88,88	0
57	MG	CA	3095	1/1	0.79	0.77	270,270,270,270	0
57	MG	DA	1634	1/1	0.79	0.06	128,128,128,128	0
57	MG	CA	3013	1/1	0.79	0.85	362,362,362,362	0
57	MG	DA	1606	1/1	0.79	0.08	144,144,144,144	0
57	MG	CA	3049	1/1	0.82	0.12	76,76,76,76	0
57	MG	BA	3095	1/1	0.82	0.16	187,187,187,187	0
57	MG	CA	3110	1/1	0.82	0.09	61,61,61,61	0
57	MG	CA	3053	1/1	0.82	0.16	46,46,46,46	0
57	MG	AA	1648	1/1	0.83	0.23	77,77,77,77	0
58	PAR	DA	1655	42/42	0.83	0.51	10,10,10,10	0
58	PAR	CA	3166	42/42	0.83	0.32	38,86,109,128	42
57	MG	CA	3030	1/1	0.83	0.17	154,154,154,154	0
57	MG	BA	3178	1/1	0.84	0.28	63,63,63,63	0
57	MG	BA	3173	1/1	0.84	0.38	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3141	1/1	0.85	0.51	68,68,68,68	0
57	MG	CA	3119	1/1	0.85	0.18	215,215,215,215	0
57	MG	AA	1608	1/1	0.85	0.15	159,159,159,159	0
57	MG	AA	1621	1/1	0.85	0.08	157,157,157,157	0
57	MG	AA	1667	1/1	0.85	0.27	81,81,81,81	0
57	MG	DA	1614	1/1	0.85	0.07	96,96,96,96	0
58	PAR	BA	3005	42/42	0.85	0.28	41,100,141,152	42
57	MG	CA	3103	1/1	0.86	0.04	116,116,116,116	0
57	MG	BA	3102	1/1	0.86	1.00	293,293,293,293	0
57	MG	BA	3019	1/1	0.86	0.25	169,169,169,169	0
57	MG	AA	1636	1/1	0.86	1.03	313,313,313,313	0
57	MG	BQ	201	1/1	0.86	1.38	108,108,108,108	0
57	MG	BA	3092	1/1	0.86	0.16	173,173,173,173	0
57	MG	CA	3092	1/1	0.87	0.20	134,134,134,134	0
57	MG	BA	3162	1/1	0.88	0.29	44,44,44,44	0
57	MG	BA	3138	1/1	0.88	0.44	227,227,227,227	0
57	MG	DA	1622	1/1	0.88	0.87	331,331,331,331	0
57	MG	AA	1628	1/1	0.88	0.14	106,106,106,106	0
57	MG	BA	3181	1/1	0.88	0.25	106,106,106,106	0
57	MG	AA	1645	1/1	0.89	0.33	75,75,75,75	0
57	MG	DA	1604	1/1	0.89	0.38	166,166,166,166	0
57	MG	BA	3010	1/1	0.89	0.11	56,56,56,56	0
57	MG	AA	1651	1/1	0.89	0.27	60,60,60,60	0
57	MG	AA	1656	1/1	0.89	0.17	73,73,73,73	0
57	MG	AA	1611	1/1	0.89	0.08	125,125,125,125	0
57	MG	AA	1644	1/1	0.89	0.26	86,86,86,86	0
57	MG	BA	3060	1/1	0.89	0.15	146,146,146,146	0
57	MG	AA	1637	1/1	0.89	0.23	138,138,138,138	0
57	MG	AA	1609	1/1	0.89	0.18	227,227,227,227	0
57	MG	DA	1619	1/1	0.89	0.04	155,155,155,155	0
57	MG	CA	3131	1/1	0.89	0.14	75,75,75,75	0
57	MG	CA	3078	1/1	0.89	0.05	113,113,113,113	0
57	MG	AA	1665	1/1	0.89	0.70	106,106,106,106	0
58	PAR	CA	3167	42/42	0.89	0.36	10,10,10,10	0
57	MG	BA	3190	1/1	0.89	0.23	68,68,68,68	0
57	MG	CA	3061	1/1	0.89	0.26	102,102,102,102	0
58	PAR	BA	3003	42/42	0.89	0.39	10,10,10,10	0
57	MG	BA	3009	1/1	0.89	0.14	63,63,63,63	0
57	MG	BA	3074	1/1	0.89	0.20	105,105,105,105	0
57	MG	BA	3159	1/1	0.89	0.40	38,38,38,38	0
57	MG	BA	3119	1/1	0.90	0.24	262,262,262,262	0
57	MG	CA	3160	1/1	0.90	0.21	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3160	1/1	0.90	0.35	74,74,74,74	0
57	MG	AA	1616	1/1	0.90	0.10	118,118,118,118	0
57	MG	CA	3147	1/1	0.90	0.38	77,77,77,77	0
57	MG	DA	1636	1/1	0.90	0.09	82,82,82,82	0
57	MG	BA	3012	1/1	0.90	0.07	100,100,100,100	0
57	MG	AA	1618	1/1	0.90	0.20	43,43,43,43	0
57	MG	AA	1652	1/1	0.90	0.10	50,50,50,50	0
57	MG	CA	3162	1/1	0.91	0.29	71,71,71,71	0
57	MG	AA	1642	1/1	0.91	0.30	60,60,60,60	0
57	MG	CA	3074	1/1	0.91	0.15	53,53,53,53	0
57	MG	CA	3083	1/1	0.91	0.14	79,79,79,79	0
57	MG	DA	1645	1/1	0.91	0.23	57,57,57,57	0
57	MG	CA	3054	1/1	0.91	0.12	41,41,41,41	0
57	MG	BA	3044	1/1	0.91	0.25	62,62,62,62	0
58	PAR	CA	3170	42/42	0.91	0.35	10,10,10,10	0
57	MG	DN	201	1/1	0.91	0.48	317,317,317,317	0
57	MG	AA	1643	1/1	0.91	0.70	162,162,162,162	0
57	MG	AA	1627	1/1	0.91	0.21	111,111,111,111	0
57	MG	CA	3086	1/1	0.91	0.23	83,83,83,83	0
57	MG	AA	1619	1/1	0.91	0.19	70,70,70,70	0
57	MG	CA	3087	1/1	0.91	0.20	75,75,75,75	0
57	MG	AA	1671	1/1	0.91	0.25	47,47,47,47	0
57	MG	DA	1638	1/1	0.91	0.30	93,93,93,93	0
57	MG	CA	3065	1/1	0.92	0.09	76,76,76,76	0
57	MG	CA	3071	1/1	0.92	0.51	218,218,218,218	0
57	MG	BA	3182	1/1	0.92	0.28	59,59,59,59	0
57	MG	CA	3068	1/1	0.92	0.19	58,58,58,58	0
57	MG	BA	3172	1/1	0.92	0.27	57,57,57,57	0
57	MG	BA	3075	1/1	0.92	0.17	88,88,88,88	0
57	MG	DA	1641	1/1	0.92	0.21	69,69,69,69	0
57	MG	CD	301	1/1	0.92	0.54	234,234,234,234	0
57	MG	CA	3153	1/1	0.92	0.32	47,47,47,47	0
57	MG	CA	3165	1/1	0.92	0.38	83,83,83,83	0
57	MG	CA	3048	1/1	0.92	0.19	157,157,157,157	0
57	MG	DA	1616	1/1	0.92	0.12	98,98,98,98	0
57	MG	AA	1630	1/1	0.92	0.10	113,113,113,113	0
57	MG	CA	3080	1/1	0.92	0.13	102,102,102,102	0
57	MG	CA	3126	1/1	0.92	0.15	146,146,146,146	0
57	MG	CA	3011	1/1	0.92	0.07	54,54,54,54	0
57	MG	AA	1663	1/1	0.92	0.32	52,52,52,52	0
57	MG	BA	3091	1/1	0.93	0.12	94,94,94,94	0
57	MG	BA	3017	1/1	0.93	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3042	1/1	0.93	0.10	67,67,67,67	0
57	MG	CA	3014	1/1	0.93	0.12	82,82,82,82	0
57	MG	DA	1632	1/1	0.93	0.14	71,71,71,71	0
58	PAR	DA	1654	42/42	0.93	0.31	10,10,10,10	0
57	MG	BB	3201	1/1	0.93	0.10	107,107,107,107	0
57	MG	AA	1661	1/1	0.93	0.14	53,53,53,53	0
57	MG	BA	3167	1/1	0.93	0.35	53,53,53,53	0
57	MG	BA	3093	1/1	0.93	0.11	72,72,72,72	0
57	MG	CA	3109	1/1	0.93	0.20	74,74,74,74	0
57	MG	CA	3085	1/1	0.93	0.33	260,260,260,260	0
58	PAR	BA	3001	42/42	0.93	0.30	10,10,10,10	0
57	MG	CA	3123	1/1	0.93	0.25	177,177,177,177	0
58	PAR	BA	3004	42/42	0.93	0.27	10,10,10,10	0
57	MG	CA	3151	1/1	0.93	0.30	44,44,44,44	0
57	MG	CA	3038	1/1	0.93	0.10	71,71,71,71	0
57	MG	CA	3097	1/1	0.93	0.07	63,63,63,63	0
57	MG	DA	1647	1/1	0.94	0.14	59,59,59,59	0
57	MG	BA	3194	1/1	0.94	0.25	46,46,46,46	0
57	MG	BA	3137	1/1	0.94	0.10	95,95,95,95	0
57	MG	BA	3168	1/1	0.94	0.32	39,39,39,39	0
57	MG	AA	1668	1/1	0.94	0.39	70,70,70,70	0
57	MG	BA	3183	1/1	0.94	0.17	37,37,37,37	0
57	MG	CA	3102	1/1	0.94	0.11	123,123,123,123	0
57	MG	CA	3008	1/1	0.94	0.17	74,74,74,74	0
57	MG	BL	202	1/1	0.94	0.43	259,259,259,259	0
57	MG	CB	3201	1/1	0.94	0.11	216,216,216,216	0
57	MG	BA	3165	1/1	0.94	0.26	60,60,60,60	0
57	MG	BA	3170	1/1	0.94	0.10	51,51,51,51	0
57	MG	DA	1617	1/1	0.94	0.24	65,65,65,65	0
57	MG	BA	3056	1/1	0.94	0.11	59,59,59,59	0
57	MG	CA	3047	1/1	0.94	0.20	211,211,211,211	0
57	MG	CA	3135	1/1	0.94	0.14	121,121,121,121	0
57	MG	BA	3145	1/1	0.94	1.48	164,164,164,164	0
57	MG	BA	3164	1/1	0.94	0.31	54,54,54,54	0
57	MG	BA	3083	1/1	0.94	0.14	84,84,84,84	0
57	MG	CA	3156	1/1	0.94	0.17	45,45,45,45	0
57	MG	AA	1607	1/1	0.94	0.74	327,327,327,327	0
57	MG	BA	3082	1/1	0.94	0.24	139,139,139,139	0
57	MG	CA	3138	1/1	0.94	0.36	39,39,39,39	0
57	MG	CA	3006	1/1	0.94	0.06	83,83,83,83	0
57	MG	CA	3043	1/1	0.94	0.07	57,57,57,57	0
57	MG	CA	3146	1/1	0.94	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3125	1/1	0.94	0.08	38,38,38,38	0
57	MG	BA	3154	1/1	0.94	0.76	56,56,56,56	0
58	PAR	AA	1672	42/42	0.94	0.24	10,10,10,10	0
57	MG	CA	3064	1/1	0.94	0.24	118,118,118,118	0
57	MG	BA	3080	1/1	0.95	0.19	75,75,75,75	0
57	MG	CA	3136	1/1	0.95	0.05	107,107,107,107	0
57	MG	CA	3091	1/1	0.95	0.07	93,93,93,93	0
57	MG	CA	3124	1/1	0.95	0.15	125,125,125,125	0
57	MG	CA	3019	1/1	0.95	0.98	252,252,252,252	0
57	MG	AA	1664	1/1	0.95	0.07	67,67,67,67	0
57	MG	CA	3034	1/1	0.95	0.29	157,157,157,157	0
57	MG	BA	3023	1/1	0.95	0.25	38,38,38,38	0
57	MG	DA	1633	1/1	0.95	0.85	264,264,264,264	0
57	MG	CA	3026	1/1	0.95	0.14	202,202,202,202	0
57	MG	BA	3061	1/1	0.95	0.04	70,70,70,70	0
57	MG	AA	1655	1/1	0.95	0.47	77,77,77,77	0
57	MG	DA	1648	1/1	0.95	0.50	41,41,41,41	0
57	MG	BA	3055	1/1	0.95	0.09	34,34,34,34	0
57	MG	BA	3034	1/1	0.95	0.15	41,41,41,41	0
57	MG	AA	1602	1/1	0.95	0.07	107,107,107,107	0
57	MG	BA	3110	1/1	0.95	0.44	89,89,89,89	0
57	MG	DA	1602	1/1	0.95	0.12	83,83,83,83	0
57	MG	BA	3064	1/1	0.95	0.17	80,80,80,80	0
57	MG	BA	3013	1/1	0.95	0.10	40,40,40,40	0
58	PAR	BA	3002	42/42	0.95	0.23	10,10,10,10	0
57	MG	DA	1620	1/1	0.95	0.11	78,78,78,78	0
57	MG	CA	3157	1/1	0.95	0.16	54,54,54,54	0
57	MG	CA	3164	1/1	0.95	0.33	44,44,44,44	0
57	MG	BA	3123	1/1	0.95	0.06	115,115,115,115	0
57	MG	BA	3029	1/1	0.95	0.48	240,240,240,240	0
57	MG	AA	1659	1/1	0.95	0.09	84,84,84,84	0
57	MG	AA	1660	1/1	0.95	0.09	67,67,67,67	0
57	MG	DA	1609	1/1	0.95	0.08	97,97,97,97	0
57	MG	AA	1662	1/1	0.95	0.18	69,69,69,69	0
57	MG	CA	3094	1/1	0.95	0.20	94,94,94,94	0
57	MG	BA	3018	1/1	0.95	0.13	59,59,59,59	0
57	MG	BA	3025	1/1	0.95	0.30	134,134,134,134	0
57	MG	AA	1632	1/1	0.95	0.18	149,149,149,149	0
57	MG	BA	3054	1/1	0.95	0.07	46,46,46,46	0
57	MG	AA	1633	1/1	0.95	0.10	86,86,86,86	0
57	MG	AA	1654	1/1	0.96	0.15	82,82,82,82	0
57	MG	CA	3132	1/1	0.96	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	1651	1/1	0.96	0.21	51,51,51,51	0
57	MG	BA	3106	1/1	0.96	0.08	71,71,71,71	0
57	MG	BA	3039	1/1	0.96	0.18	48,48,48,48	0
57	MG	BA	3059	1/1	0.96	0.10	60,60,60,60	0
57	MG	DA	1640	1/1	0.96	0.30	66,66,66,66	0
57	MG	CA	3099	1/1	0.96	0.16	58,58,58,58	0
57	MG	BA	3180	1/1	0.96	0.32	48,48,48,48	0
57	MG	CA	3117	1/1	0.96	0.08	45,45,45,45	0
57	MG	BA	3105	1/1	0.96	0.26	80,80,80,80	0
57	MG	BA	3031	1/1	0.96	0.08	60,60,60,60	0
57	MG	AA	1669	1/1	0.96	0.43	58,58,58,58	0
57	MG	DA	1612	1/1	0.96	0.12	123,123,123,123	0
57	MG	CA	3037	1/1	0.96	0.14	90,90,90,90	0
57	MG	BA	3144	1/1	0.96	0.25	34,34,34,34	0
57	MG	BA	3104	1/1	0.96	0.10	37,37,37,37	0
57	MG	DA	1627	1/1	0.96	0.09	80,80,80,80	0
57	MG	BA	3169	1/1	0.96	0.34	88,88,88,88	0
57	MG	BA	3115	1/1	0.96	0.25	133,133,133,133	0
57	MG	DA	1628	1/1	0.96	0.25	177,177,177,177	0
57	MG	CA	3009	1/1	0.96	0.15	88,88,88,88	0
57	MG	BA	3108	1/1	0.96	0.18	81,81,81,81	0
57	MG	CA	3158	1/1	0.96	0.45	57,57,57,57	0
57	MG	CA	3005	1/1	0.96	0.05	90,90,90,90	0
57	MG	DA	1613	1/1	0.96	0.12	89,89,89,89	0
57	MG	BA	3032	1/1	0.96	0.11	33,33,33,33	0
57	MG	CA	3052	1/1	0.96	0.09	54,54,54,54	0
57	MG	DD	302	1/1	0.96	0.30	53,53,53,53	0
57	MG	BA	3112	1/1	0.96	0.21	29,29,29,29	0
57	MG	BA	3036	1/1	0.96	0.13	38,38,38,38	0
57	MG	BA	3089	1/1	0.96	0.15	44,44,44,44	0
57	MG	CA	3012	1/1	0.96	0.10	30,30,30,30	0
57	MG	BA	3142	1/1	0.96	0.18	63,63,63,63	0
57	MG	BA	3081	1/1	0.96	0.07	57,57,57,57	0
57	MG	AA	1605	1/1	0.96	0.03	122,122,122,122	0
57	MG	DA	1601	1/1	0.96	0.13	47,47,47,47	0
57	MG	CA	3133	1/1	0.96	0.17	182,182,182,182	0
57	MG	CA	3100	1/1	0.96	0.10	155,155,155,155	0
57	MG	CA	3113	1/1	0.96	0.23	85,85,85,85	0
57	MG	BA	3149	1/1	0.96	0.14	33,33,33,33	0
57	MG	CA	3090	1/1	0.96	0.09	69,69,69,69	0
57	MG	CA	3072	1/1	0.96	0.11	99,99,99,99	0
57	MG	BA	3107	1/1	0.96	0.07	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3086	1/1	0.96	0.12	74,74,74,74	0
57	MG	BA	3186	1/1	0.96	0.37	37,37,37,37	0
57	MG	AA	1653	1/1	0.96	0.22	82,82,82,82	0
57	MG	BA	3175	1/1	0.96	0.17	44,44,44,44	0
57	MG	BA	3174	1/1	0.96	0.24	45,45,45,45	0
57	MG	DA	1639	1/1	0.96	0.24	161,161,161,161	0
57	MG	BA	3045	1/1	0.96	0.40	217,217,217,217	0
57	MG	CA	3145	1/1	0.96	0.26	59,59,59,59	0
57	MG	AA	1666	1/1	0.96	0.24	44,44,44,44	0
57	MG	BA	3014	1/1	0.96	0.20	101,101,101,101	0
57	MG	CA	3161	1/1	0.96	0.36	39,39,39,39	0
57	MG	BA	3087	1/1	0.96	0.06	139,139,139,139	0
57	MG	CA	3134	1/1	0.96	0.14	55,55,55,55	0
57	MG	BA	3052	1/1	0.96	0.16	50,50,50,50	0
57	MG	BA	3090	1/1	0.96	0.21	71,71,71,71	0
57	MG	AA	1620	1/1	0.96	0.13	133,133,133,133	0
57	MG	BA	3103	1/1	0.96	0.08	41,41,41,41	0
57	MG	CA	3045	1/1	0.96	0.17	46,46,46,46	0
57	MG	BA	3122	1/1	0.96	0.06	60,60,60,60	0
57	MG	CA	3149	1/1	0.96	0.24	69,69,69,69	0
57	MG	CB	3202	1/1	0.96	0.08	114,114,114,114	0
57	MG	BA	3015	1/1	0.96	0.10	58,58,58,58	0
57	MG	CB	3203	1/1	0.97	0.07	115,115,115,115	0
57	MG	AA	1670	1/1	0.97	0.55	50,50,50,50	0
57	MG	CA	3163	1/1	0.97	0.26	44,44,44,44	0
57	MG	CA	3137	1/1	0.97	0.31	22,22,22,22	0
57	MG	DA	1653	1/1	0.97	0.20	51,51,51,51	0
57	MG	AA	1657	1/1	0.97	0.21	78,78,78,78	0
57	MG	BA	3114	1/1	0.97	0.15	65,65,65,65	0
57	MG	BA	3128	1/1	0.97	0.21	99,99,99,99	0
57	MG	BA	3079	1/1	0.97	0.13	42,42,42,42	0
57	MG	BA	3135	1/1	0.97	0.07	79,79,79,79	0
57	MG	DA	1611	1/1	0.97	0.05	60,60,60,60	0
57	MG	CA	3063	1/1	0.97	0.09	50,50,50,50	0
57	MG	BA	3037	1/1	0.97	0.17	52,52,52,52	0
57	MG	BA	3027	1/1	0.97	0.16	57,57,57,57	0
57	MG	DA	1642	1/1	0.97	0.29	60,60,60,60	0
57	MG	CA	3028	1/1	0.97	0.41	312,312,312,312	0
57	MG	CA	3024	1/1	0.97	0.14	65,65,65,65	0
57	MG	DA	1618	1/1	0.97	0.14	51,51,51,51	0
57	MG	BA	3094	1/1	0.97	0.14	153,153,153,153	0
57	MG	AN	201	1/1	0.97	0.08	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3096	1/1	0.97	0.07	100,100,100,100	0
57	MG	BA	3077	1/1	0.97	0.22	63,63,63,63	0
57	MG	CA	3106	1/1	0.97	0.20	33,33,33,33	0
57	MG	AA	1634	1/1	0.97	0.08	87,87,87,87	0
57	MG	AA	1614	1/1	0.97	0.21	146,146,146,146	0
57	MG	BA	3065	1/1	0.97	0.16	98,98,98,98	0
57	MG	CA	3056	1/1	0.97	0.23	155,155,155,155	0
57	MG	BA	3088	1/1	0.97	0.09	147,147,147,147	0
57	MG	CA	3101	1/1	0.97	0.15	58,58,58,58	0
57	MG	CA	3077	1/1	0.97	0.15	131,131,131,131	0
57	MG	BA	3152	1/1	0.97	0.15	56,56,56,56	0
57	MG	BA	3068	1/1	0.97	0.09	27,27,27,27	0
57	MG	BA	3117	1/1	0.97	0.19	65,65,65,65	0
57	MG	AA	1631	1/1	0.97	0.23	115,115,115,115	0
57	MG	DA	1629	1/1	0.97	0.09	86,86,86,86	0
57	MG	AA	1641	1/1	0.97	0.11	124,124,124,124	0
57	MG	CA	3143	1/1	0.97	0.24	69,69,69,69	0
57	MG	CA	3115	1/1	0.97	0.12	235,235,235,235	0
57	MG	DA	1635	1/1	0.97	0.24	126,126,126,126	0
57	MG	BA	3067	1/1	0.97	0.30	218,218,218,218	0
57	MG	BA	3153	1/1	0.97	0.35	34,34,34,34	0
57	MG	DA	1626	1/1	0.97	0.07	98,98,98,98	0
57	MG	CA	3059	1/1	0.97	0.10	88,88,88,88	0
57	MG	AA	1623	1/1	0.97	0.16	67,67,67,67	0
57	MG	CA	3089	1/1	0.97	0.17	215,215,215,215	0
57	MG	BA	3040	1/1	0.97	0.09	66,66,66,66	0
57	MG	AA	1601	1/1	0.97	0.15	50,50,50,50	0
57	MG	AA	1624	1/1	0.97	0.07	99,99,99,99	0
57	MG	CA	3108	1/1	0.97	0.18	101,101,101,101	0
57	MG	CA	3154	1/1	0.97	0.28	42,42,42,42	0
57	MG	DA	1646	1/1	0.97	0.29	31,31,31,31	0
57	MG	DA	1643	1/1	0.97	0.16	73,73,73,73	0
57	MG	DA	1623	1/1	0.97	0.07	64,64,64,64	0
57	MG	AA	1617	1/1	0.97	0.10	104,104,104,104	0
57	MG	DD	301	1/1	0.97	0.26	314,314,314,314	0
57	MG	BA	3071	1/1	0.97	0.11	43,43,43,43	0
57	MG	CA	3032	1/1	0.97	0.18	97,97,97,97	0
57	MG	BA	3130	1/1	0.97	0.32	270,270,270,270	0
57	MG	BO	201	1/1	0.97	0.10	67,67,67,67	0
57	MG	CA	3140	1/1	0.97	0.27	29,29,29,29	0
57	MG	BA	3129	1/1	0.97	0.19	78,78,78,78	0
57	MG	CA	3098	1/1	0.97	0.64	242,242,242,242	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3003	1/1	0.97	0.07	95,95,95,95	0
57	MG	DA	1631	1/1	0.97	0.16	196,196,196,196	0
57	MG	CA	3107	1/1	0.97	0.13	95,95,95,95	0
57	MG	CA	3033	1/1	0.97	0.13	56,56,56,56	0
57	MG	CA	3148	1/1	0.97	0.18	37,37,37,37	0
57	MG	BA	3035	1/1	0.97	0.12	43,43,43,43	0
57	MG	AA	1650	1/1	0.97	0.40	55,55,55,55	0
57	MG	CA	3070	1/1	0.97	0.14	251,251,251,251	0
57	MG	BA	3048	1/1	0.97	0.16	69,69,69,69	0
57	MG	BA	3140	1/1	0.97	0.06	73,73,73,73	0
57	MG	AA	1615	1/1	0.97	0.09	123,123,123,123	0
57	MG	BA	3016	1/1	0.97	0.10	56,56,56,56	0
57	MG	BA	3176	1/1	0.97	0.30	51,51,51,51	0
57	MG	CA	3073	1/1	0.97	0.12	64,64,64,64	0
57	MG	DA	1649	1/1	0.97	0.09	63,63,63,63	0
57	MG	AA	1622	1/1	0.97	0.06	76,76,76,76	0
57	MG	DA	1630	1/1	0.97	0.14	72,72,72,72	0
57	MG	BA	3006	1/1	0.97	0.12	40,40,40,40	0
57	MG	CA	3001	1/1	0.97	0.09	54,54,54,54	0
57	MG	BA	3101	1/1	0.97	0.16	70,70,70,70	0
57	MG	DA	1624	1/1	0.97	0.11	30,30,30,30	0
57	MG	BA	3118	1/1	0.97	0.37	164,164,164,164	0
57	MG	CA	3069	1/1	0.97	0.17	63,63,63,63	0
57	MG	AA	1638	1/1	0.97	0.08	58,58,58,58	0
57	MG	AA	1649	1/1	0.97	0.27	51,51,51,51	0
57	MG	CA	3007	1/1	0.97	0.28	204,204,204,204	0
57	MG	CA	3060	1/1	0.97	0.08	67,67,67,67	0
57	MG	BA	3024	1/1	0.97	0.08	68,68,68,68	0
57	MG	CA	3159	1/1	0.97	0.17	52,52,52,52	0
57	MG	CA	3150	1/1	0.97	0.24	54,54,54,54	0
57	MG	CA	3031	1/1	0.98	0.17	30,30,30,30	0
57	MG	BA	3020	1/1	0.98	0.08	41,41,41,41	0
57	MG	BA	3139	1/1	0.98	0.12	47,47,47,47	0
57	MG	CA	3027	1/1	0.98	0.04	47,47,47,47	0
57	MG	CA	3128	1/1	0.98	0.10	66,66,66,66	0
57	MG	AA	1626	1/1	0.98	0.09	66,66,66,66	0
57	MG	CA	3021	1/1	0.98	0.05	57,57,57,57	0
57	MG	BA	3148	1/1	0.98	0.32	34,34,34,34	0
57	MG	BA	3070	1/1	0.98	0.12	50,50,50,50	0
57	MG	CA	3062	1/1	0.98	0.11	97,97,97,97	0
57	MG	BA	3072	1/1	0.98	0.08	41,41,41,41	0
57	MG	CA	3039	1/1	0.98	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	1621	1/1	0.98	0.09	47,47,47,47	0
57	MG	BB	3202	1/1	0.98	0.08	34,34,34,34	0
57	MG	DA	1652	1/1	0.98	0.17	67,67,67,67	0
57	MG	CA	3076	1/1	0.98	0.18	77,77,77,77	0
57	MG	BA	3150	1/1	0.98	0.71	38,38,38,38	0
57	MG	CA	3127	1/1	0.98	0.06	47,47,47,47	0
57	MG	BA	3163	1/1	0.98	0.18	27,27,27,27	0
57	MG	BA	3157	1/1	0.98	0.30	44,44,44,44	0
57	MG	BA	3147	1/1	0.98	0.15	54,54,54,54	0
57	MG	BA	3097	1/1	0.98	0.06	91,91,91,91	0
57	MG	BA	3057	1/1	0.98	0.12	26,26,26,26	0
57	MG	CA	3104	1/1	0.98	0.26	57,57,57,57	0
57	MG	CA	3118	1/1	0.98	0.05	53,53,53,53	0
57	MG	BA	3030	1/1	0.98	0.08	43,43,43,43	0
57	MG	CQ	201	1/1	0.98	0.39	32,32,32,32	0
57	MG	DA	1615	1/1	0.98	0.20	213,213,213,213	0
57	MG	AA	1613	1/1	0.98	0.10	97,97,97,97	0
57	MG	CA	3081	1/1	0.98	0.05	48,48,48,48	0
57	MG	CA	3152	1/1	0.98	0.09	44,44,44,44	0
57	MG	DA	1607	1/1	0.98	0.15	63,63,63,63	0
57	MG	CA	3093	1/1	0.98	0.08	127,127,127,127	0
57	MG	BA	3098	1/1	0.98	0.46	157,157,157,157	0
57	MG	BA	3100	1/1	0.98	0.15	66,66,66,66	0
57	MG	BA	3026	1/1	0.98	0.15	47,47,47,47	0
57	MG	DA	1605	1/1	0.98	0.14	96,96,96,96	0
57	MG	BA	3125	1/1	0.98	0.11	36,36,36,36	0
57	MG	DA	1644	1/1	0.98	0.29	62,62,62,62	0
57	MG	BA	3046	1/1	0.98	0.06	58,58,58,58	0
57	MG	CA	3046	1/1	0.98	0.27	130,130,130,130	0
57	MG	BA	3066	1/1	0.98	0.17	77,77,77,77	0
57	MG	BA	3151	1/1	0.98	0.22	44,44,44,44	0
57	MG	CA	3116	1/1	0.98	0.18	94,94,94,94	0
57	MG	BA	3076	1/1	0.98	0.10	32,32,32,32	0
57	MG	BA	3121	1/1	0.98	0.10	34,34,34,34	0
57	MG	AA	1606	1/1	0.98	0.04	102,102,102,102	0
57	MG	CA	3004	1/1	0.98	0.12	130,130,130,130	0
57	MG	BA	3099	1/1	0.98	0.06	96,96,96,96	0
57	MG	BA	3028	1/1	0.98	0.14	35,35,35,35	0
57	MG	AA	1635	1/1	0.98	0.15	234,234,234,234	0
57	MG	CA	3155	1/1	0.98	0.30	39,39,39,39	0
57	MG	CA	3044	1/1	0.98	0.05	53,53,53,53	0
57	MG	BA	3062	1/1	0.98	0.10	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3136	1/1	0.98	0.10	61,61,61,61	0
57	MG	DA	1603	1/1	0.98	0.12	37,37,37,37	0
57	MG	CA	3022	1/1	0.98	0.09	59,59,59,59	0
57	MG	CA	3111	1/1	0.98	0.44	164,164,164,164	0
59	ZN	B4	9501	1/1	0.98	0.54	386,386,386,386	0
57	MG	AA	1629	1/1	0.98	0.06	54,54,54,54	0
57	MG	BA	3063	1/1	0.98	0.24	93,93,93,93	0
57	MG	CA	3035	1/1	0.98	0.11	35,35,35,35	0
57	MG	DA	1625	1/1	0.98	0.11	42,42,42,42	0
57	MG	CA	3122	1/1	0.98	0.20	88,88,88,88	0
57	MG	BA	3184	1/1	0.98	0.22	40,40,40,40	0
57	MG	BA	3111	1/1	0.98	0.14	52,52,52,52	0
57	MG	CA	3016	1/1	0.98	0.06	40,40,40,40	0
57	MG	CA	3029	1/1	0.98	0.37	168,168,168,168	0
57	MG	BA	3078	1/1	0.98	0.11	86,86,86,86	0
57	MG	BA	3143	1/1	0.98	0.35	25,25,25,25	0
57	MG	CA	3066	1/1	0.98	0.06	45,45,45,45	0
57	MG	BA	3051	1/1	0.98	0.10	70,70,70,70	0
57	MG	AA	1603	1/1	0.98	0.16	45,45,45,45	0
57	MG	BA	3126	1/1	0.99	0.17	39,39,39,39	0
57	MG	CA	3082	1/1	0.99	0.12	50,50,50,50	0
57	MG	CA	3088	1/1	0.99	0.07	98,98,98,98	0
57	MG	BA	3189	1/1	0.99	0.15	47,47,47,47	0
57	MG	CA	3017	1/1	0.99	0.10	36,36,36,36	0
57	MG	BA	3008	1/1	0.99	0.09	62,62,62,62	0
57	MG	CA	3036	1/1	0.99	0.12	53,53,53,53	0
57	MG	BA	3156	1/1	0.99	0.41	35,35,35,35	0
57	MG	BA	3191	1/1	0.99	0.13	43,43,43,43	0
57	MG	BA	3069	1/1	0.99	0.09	20,20,20,20	0
57	MG	CA	3129	1/1	0.99	0.09	33,33,33,33	0
57	MG	BA	3155	1/1	0.99	0.26	23,23,23,23	0
57	MG	BA	3127	1/1	0.99	0.11	88,88,88,88	0
57	MG	CA	3144	1/1	0.99	0.07	56,56,56,56	0
57	MG	CA	3105	1/1	0.99	0.13	44,44,44,44	0
57	MG	BA	3022	1/1	0.99	0.09	28,28,28,28	0
57	MG	AA	1639	1/1	0.99	0.18	59,59,59,59	0
57	MG	BA	3042	1/1	0.99	0.14	32,32,32,32	0
57	MG	BA	3132	1/1	0.99	0.18	30,30,30,30	0
57	MG	CA	3023	1/1	0.99	0.10	37,37,37,37	0
57	MG	BA	3085	1/1	0.99	0.11	57,57,57,57	0
57	MG	BA	3049	1/1	0.99	0.10	57,57,57,57	0
57	MG	CA	3057	1/1	0.99	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3047	1/1	0.99	0.08	42,42,42,42	0
57	MG	BA	3158	1/1	0.99	0.39	30,30,30,30	0
57	MG	CA	3121	1/1	0.99	0.06	27,27,27,27	0
57	MG	CA	3020	1/1	0.99	0.14	37,37,37,37	0
57	MG	AA	1640	1/1	0.99	0.17	21,21,21,21	0
57	MG	BA	3185	1/1	0.99	0.39	32,32,32,32	0
57	MG	BA	3011	1/1	0.99	0.07	34,34,34,34	0
57	MG	BA	3096	1/1	0.99	0.03	66,66,66,66	0
57	MG	BB	3204	1/1	0.99	0.19	24,24,24,24	0
57	MG	BA	3193	1/1	0.99	0.34	28,28,28,28	0
57	MG	BA	3007	1/1	0.99	0.07	61,61,61,61	0
57	MG	BA	3043	1/1	0.99	0.13	66,66,66,66	0
57	MG	BA	3166	1/1	0.99	0.23	34,34,34,34	0
57	MG	CA	3067	1/1	0.99	0.11	64,64,64,64	0
57	MG	CA	3114	1/1	0.99	0.12	169,169,169,169	0
57	MG	CA	3010	1/1	0.99	0.10	34,34,34,34	0
57	MG	BA	3041	1/1	0.99	0.13	32,32,32,32	0
57	MG	CA	3002	1/1	0.99	0.04	49,49,49,49	0
57	MG	CA	3139	1/1	0.99	0.29	52,52,52,52	0
57	MG	CA	3050	1/1	0.99	0.09	42,42,42,42	0
57	MG	AA	1647	1/1	0.99	0.20	44,44,44,44	0
57	MG	DA	1637	1/1	0.99	0.17	158,158,158,158	0
57	MG	CA	3120	1/1	0.99	0.12	62,62,62,62	0
57	MG	CA	3130	1/1	0.99	0.08	44,44,44,44	0
57	MG	BA	3053	1/1	0.99	0.14	29,29,29,29	0
57	MG	BA	3192	1/1	0.99	0.18	46,46,46,46	0
57	MG	BA	3133	1/1	0.99	0.12	39,39,39,39	0
57	MG	BA	3161	1/1	0.99	0.18	45,45,45,45	0
57	MG	CA	3142	1/1	0.99	0.21	33,33,33,33	0
57	MG	AA	1610	1/1	0.99	0.04	66,66,66,66	0
57	MG	CA	3075	1/1	0.99	0.10	107,107,107,107	0
57	MG	BA	3073	1/1	0.99	0.09	141,141,141,141	0
57	MG	AA	1612	1/1	0.99	0.13	94,94,94,94	0
57	MG	CA	3025	1/1	0.99	0.14	121,121,121,121	0
57	MG	BA	3134	1/1	0.99	0.28	143,143,143,143	0
57	MG	BA	3038	1/1	0.99	0.25	73,73,73,73	0
57	MG	CA	3058	1/1	0.99	0.13	55,55,55,55	0
57	MG	BA	3146	1/1	0.99	0.31	48,48,48,48	0
57	MG	BA	3177	1/1	0.99	0.06	86,86,86,86	0
57	MG	BA	3116	1/1	0.99	0.22	133,133,133,133	0
57	MG	BA	3120	1/1	0.99	0.25	91,91,91,91	0
57	MG	BB	3203	1/1	0.99	0.05	52,52,52,52	0

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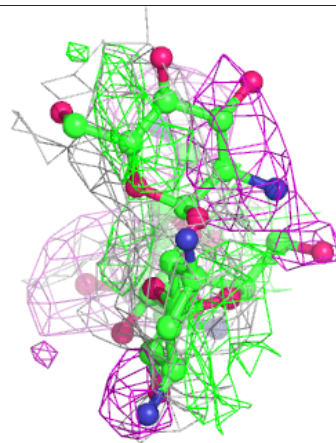
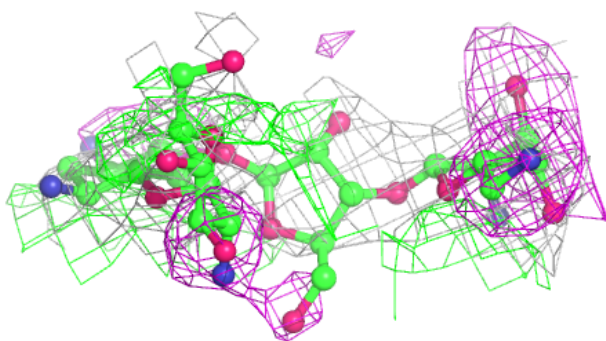
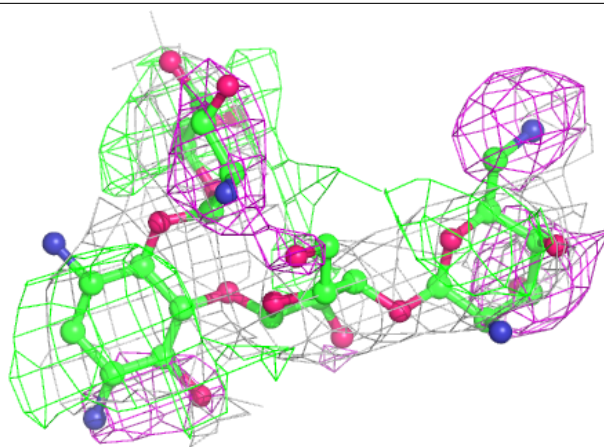
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3084	1/1	0.99	0.11	36,36,36,36	0
57	MG	BA	3141	1/1	0.99	0.19	31,31,31,31	0
57	MG	CA	3041	1/1	0.99	0.19	36,36,36,36	0
57	MG	DA	1610	1/1	0.99	0.10	67,67,67,67	0
57	MG	BA	3050	1/1	0.99	0.10	27,27,27,27	0
57	MG	BA	3187	1/1	0.99	0.23	29,29,29,29	0
57	MG	BA	3058	1/1	0.99	0.12	25,25,25,25	0
57	MG	CA	3112	1/1	0.99	0.20	137,137,137,137	0
57	MG	CA	3018	1/1	0.99	0.05	41,41,41,41	0
57	MG	BA	3188	1/1	0.99	0.15	39,39,39,39	0
57	MG	BA	3124	1/1	0.99	0.13	45,45,45,45	0
57	MG	BA	3131	1/1	0.99	0.08	39,39,39,39	0
59	ZN	C4	9501	1/1	0.99	0.15	109,109,109,109	0
57	MG	CA	3079	1/1	0.99	0.12	195,195,195,195	0
57	MG	BA	3033	1/1	0.99	0.09	48,48,48,48	0
57	MG	BA	3113	1/1	0.99	0.15	96,96,96,96	0
57	MG	BL	201	1/1	0.99	0.12	21,21,21,21	0
57	MG	CA	3051	1/1	1.00	0.07	24,24,24,24	0
57	MG	AA	1625	1/1	1.00	0.13	50,50,50,50	0
57	MG	CA	3040	1/1	1.00	0.14	98,98,98,98	0
57	MG	BA	3171	1/1	1.00	0.19	47,47,47,47	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.

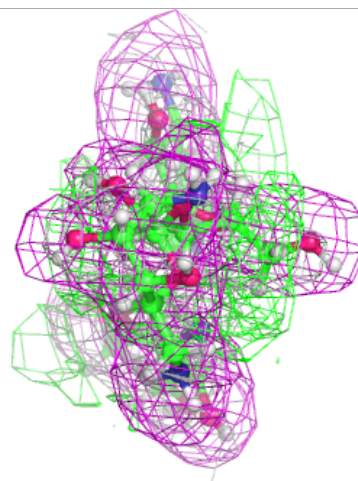
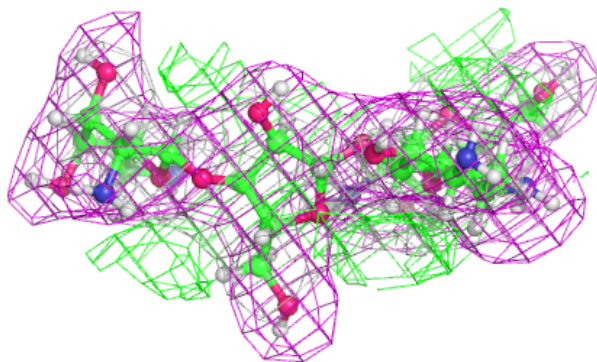
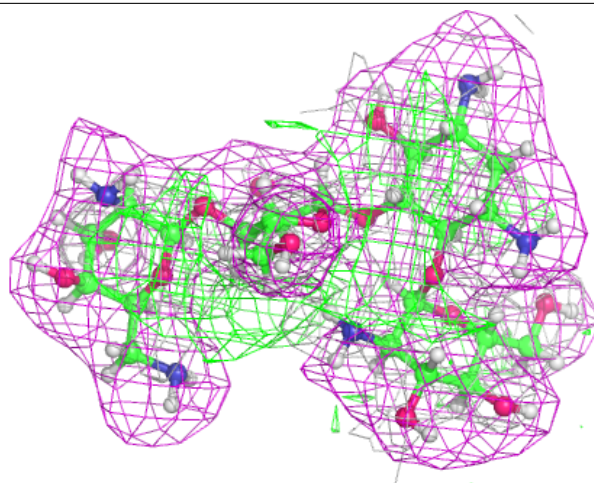
Electron density around PAR CA 3169:

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



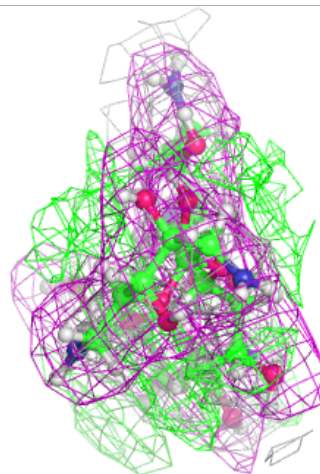
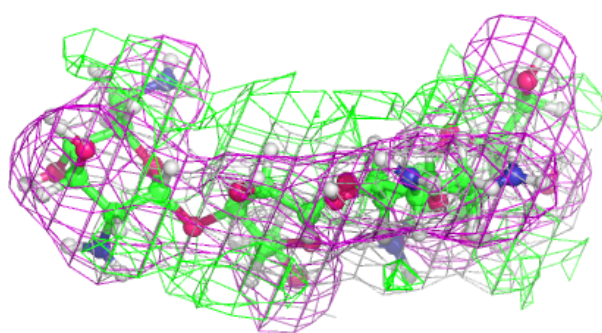
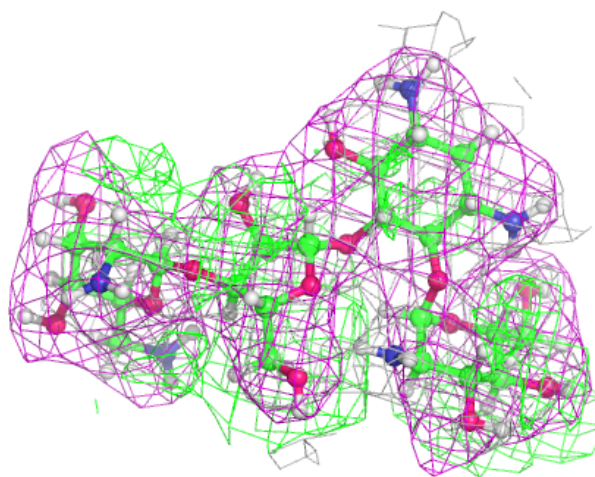
Electron density around PAR CA 3168:

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



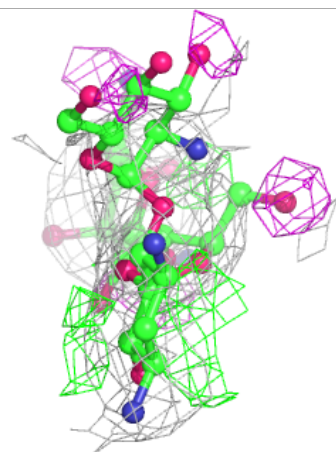
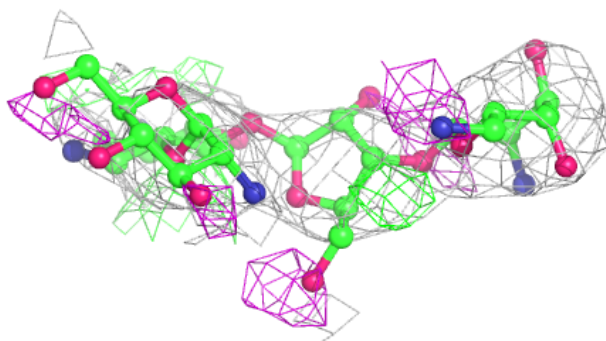
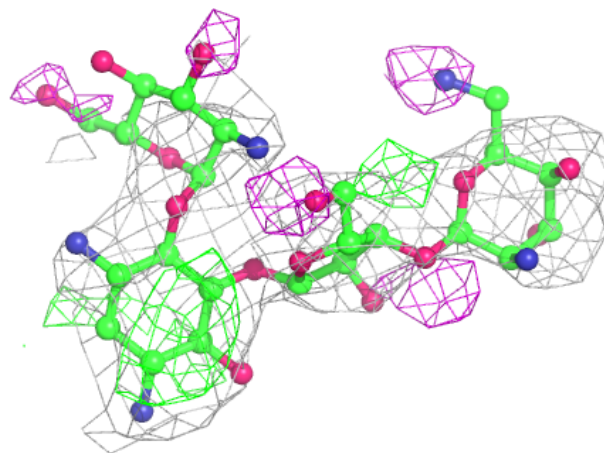
Electron density around PAR DA 1655:

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



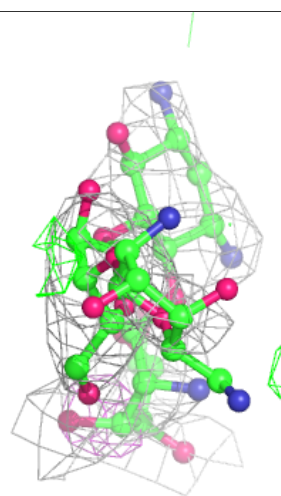
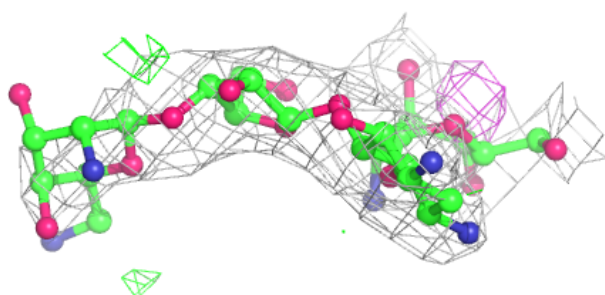
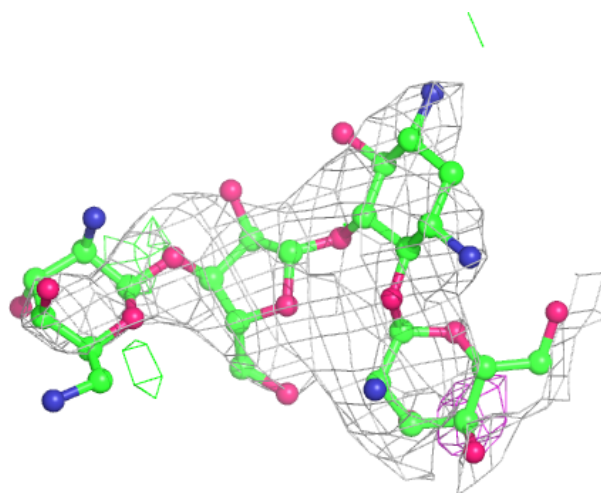
Electron density around PAR CA 3166:

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



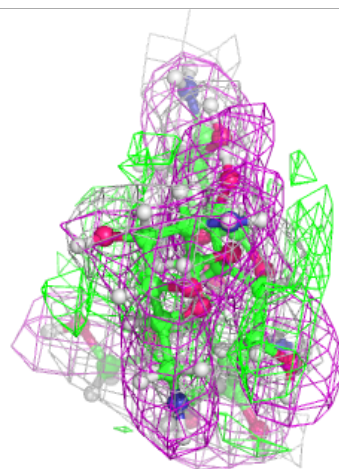
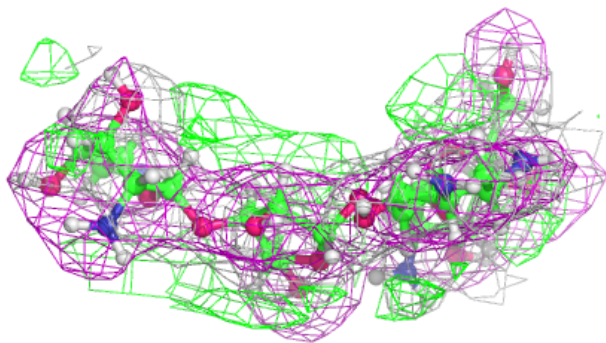
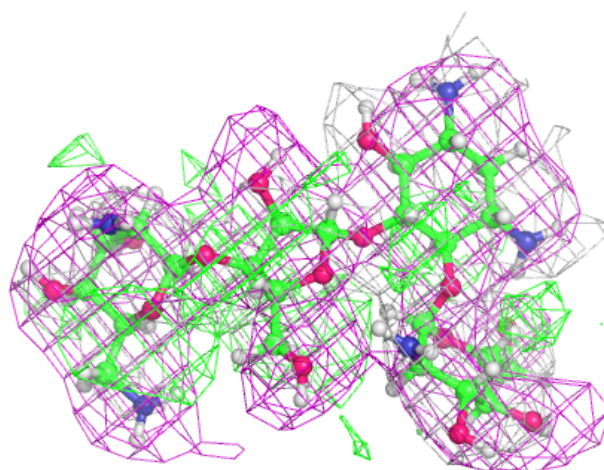
Electron density around PAR BA 3005:

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



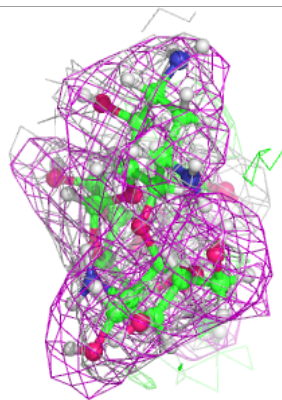
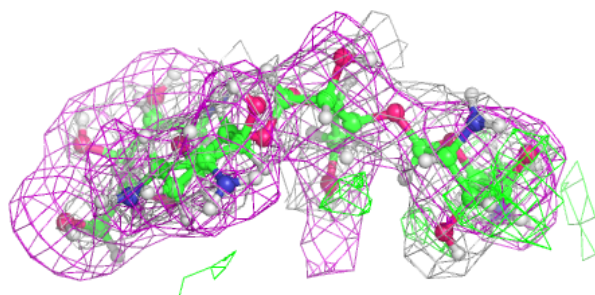
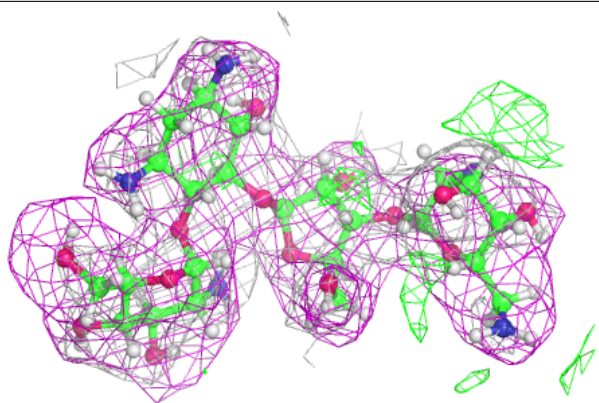
Electron density around PAR CA 3167:

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



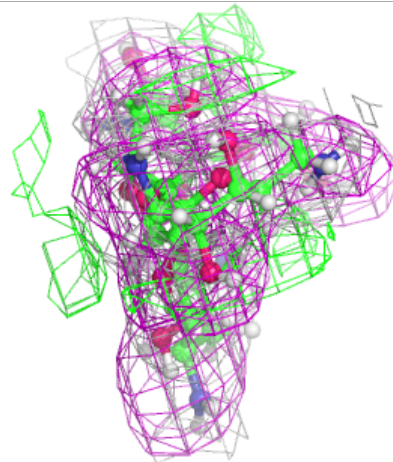
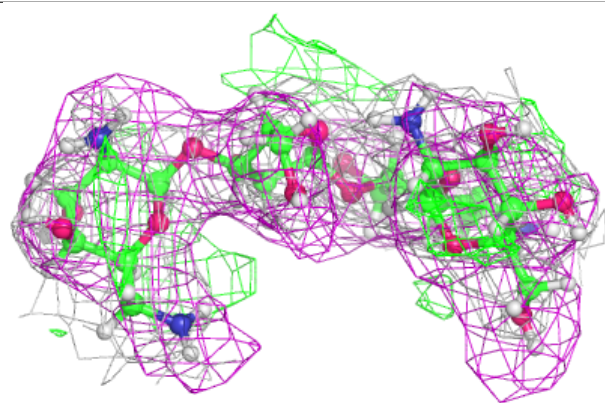
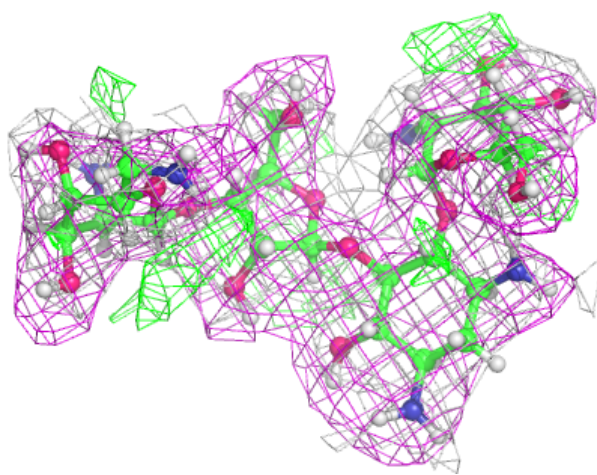
Electron density around PAR BA 3003:

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



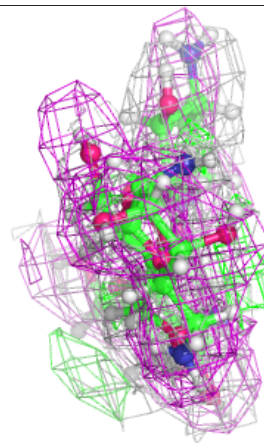
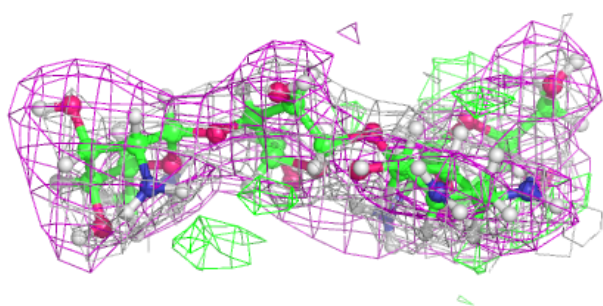
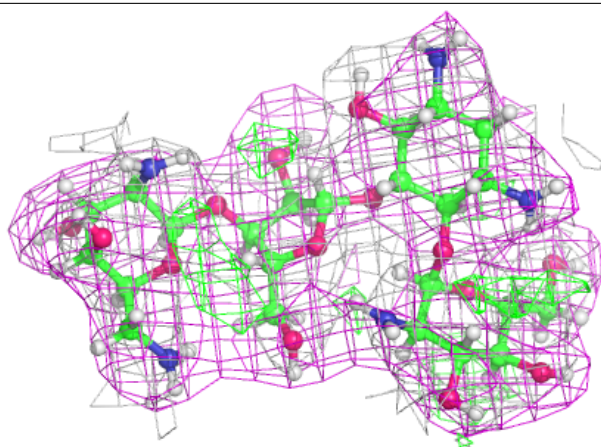
Electron density around PAR CA 3170:

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



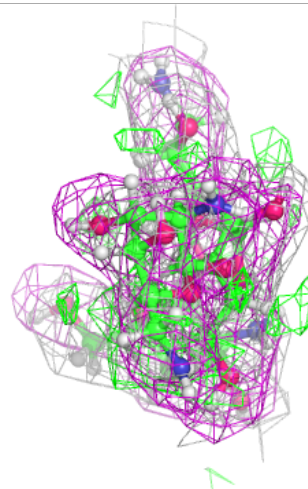
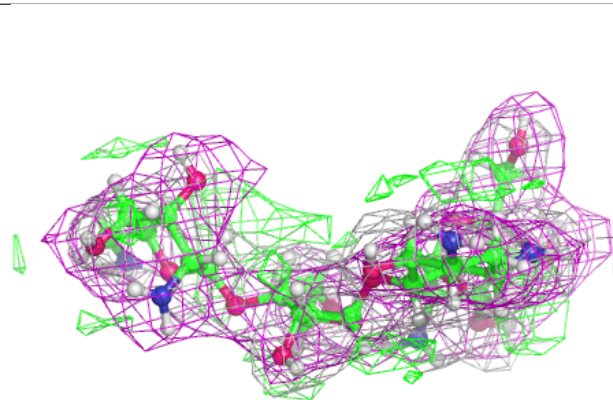
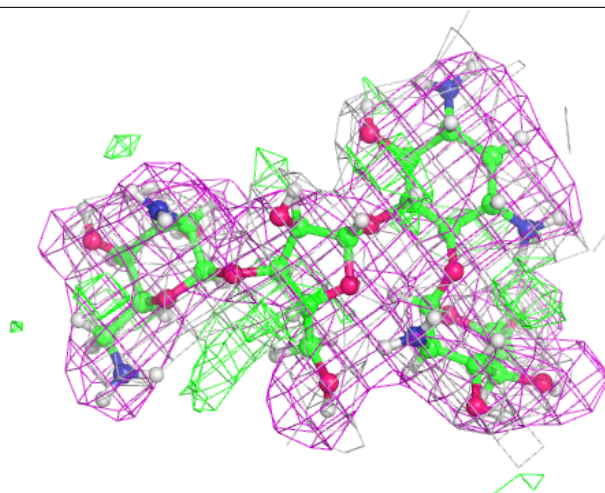
Electron density around PAR DA 1654:

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



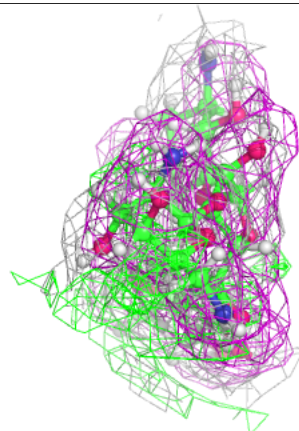
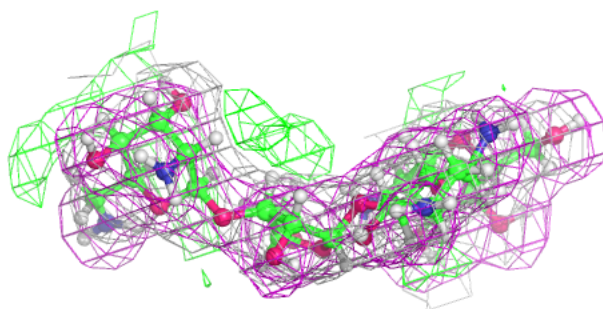
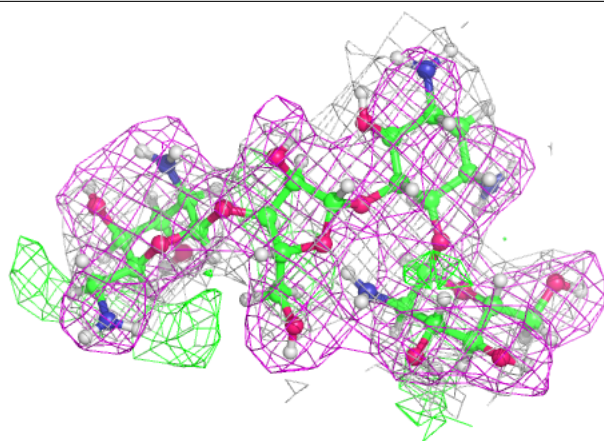
Electron density around PAR BA 3001:

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



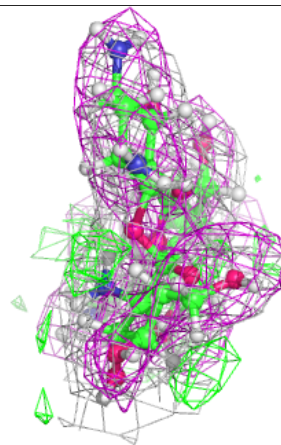
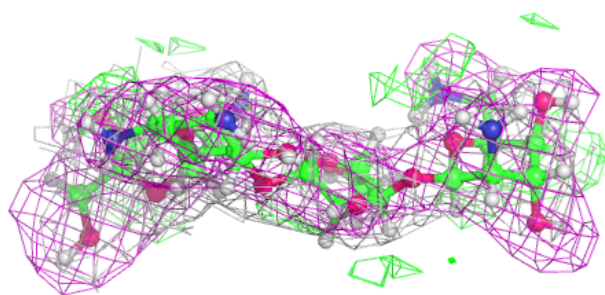
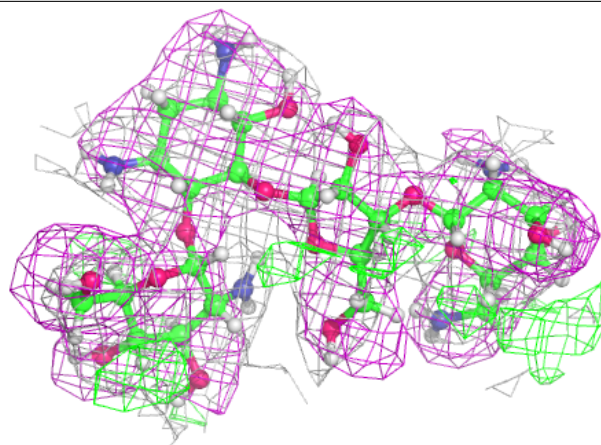
Electron density around PAR BA 3004:

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



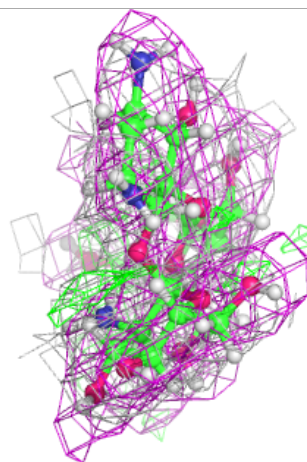
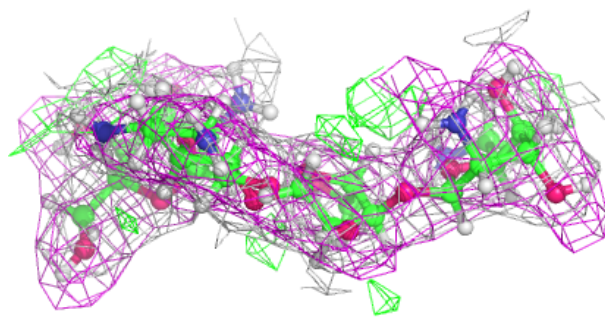
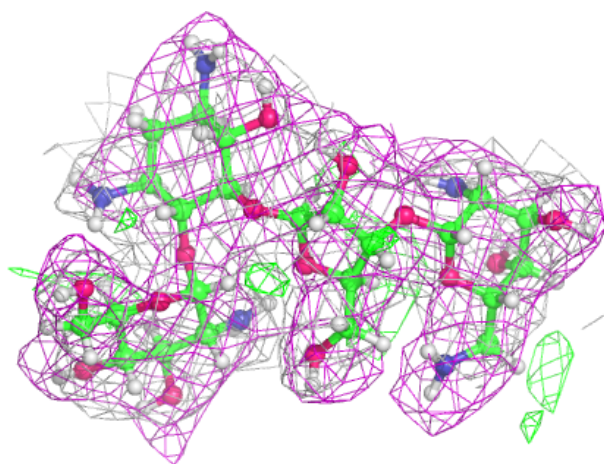
Electron density around PAR AA 1672:

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



Electron density around PAR BA 3002:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.