



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:09 am GMT

PDB ID : 4V9C  
Title : Allosteric control of the ribosome by small-molecule antibiotics  
Authors : Cate, J.H.D.; Pulk, A.; Blanchard, S.C.; Wang, L.; Feldman, M.B.; Wasserman, M.R.; Altman, R.  
Deposited on : 2012-07-25  
Resolution : 3.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28972

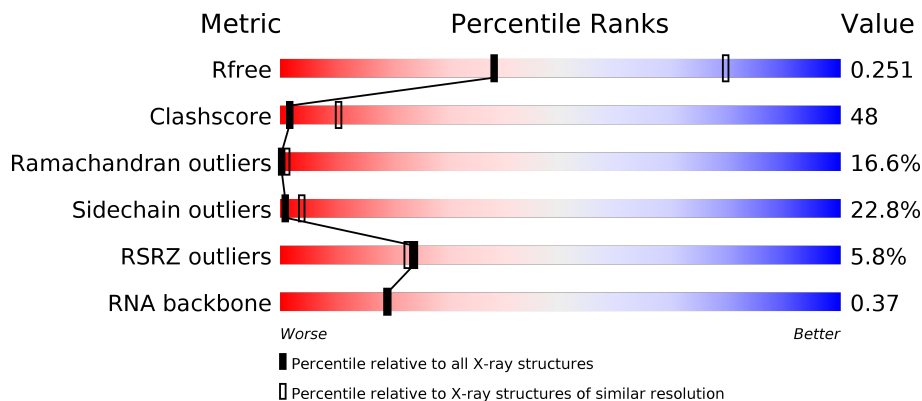
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	100719	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)
RNA backbone	2435	1111 (3.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	CA	1542	
2	AB	241	
2	CB	241	

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Mol	Chain	Length	Quality of chain
3	AC	233	
3	CC	233	
4	AD	206	
4	CD	206	
5	AE	167	
5	CE	167	
6	AF	135	
6	CF	135	
7	AG	179	
7	CG	179	
8	AH	130	
8	CH	130	
9	AI	130	
9	CI	130	
10	AJ	103	
10	CJ	103	
11	AK	129	
11	CK	129	
12	AL	124	
12	CL	124	
13	AM	118	
13	CM	118	
14	AN	101	
14	CN	101	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	82	
16	CP	82	
17	AQ	84	
17	CQ	84	
18	AR	75	
18	CR	75	
19	AS	92	
19	CS	92	
20	AT	87	
20	CT	87	
21	AU	71	
21	CU	71	
22	AV	76	
22	CV	76	
23	AX	24	
23	CX	24	
24	BA	2904	
24	DA	2904	
25	BB	120	
25	DB	120	
26	BC	273	
26	DC	273	
27	BD	209	
27	DD	209	




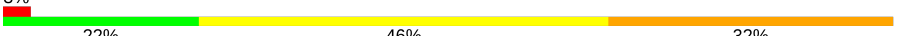
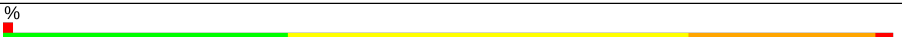
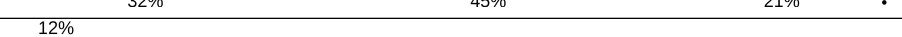
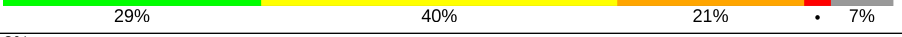


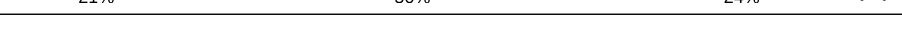
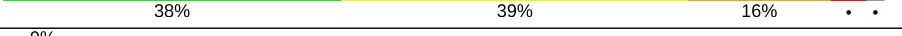
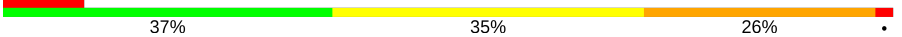
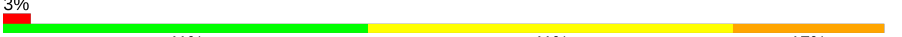
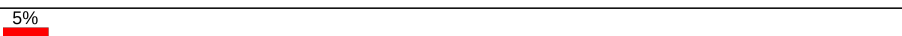
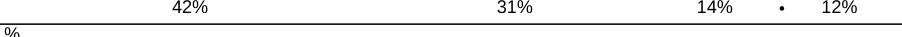
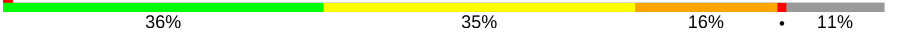
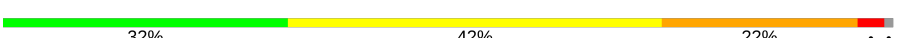

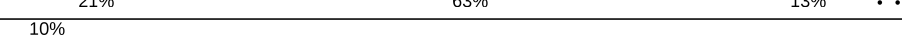
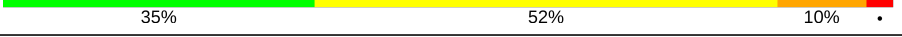




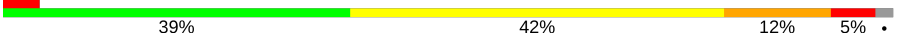
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Mol	Chain	Length	Quality of chain
28	BE	201	
28	DE	201	
29	BF	179	
29	DF	179	
30	BG	177	
30	DG	177	
31	BH	149	
31	DH	149	
32	BI	142	
32	DI	142	
33	BJ	142	
33	DJ	142	
34	BK	123	
34	DK	123	
35	BL	144	
35	DL	144	
36	BM	136	
36	DM	136	
37	BN	127	
37	DN	127	
38	BO	117	
38	DO	117	
39	BP	115	
39	DP	115	
40	BQ	118	

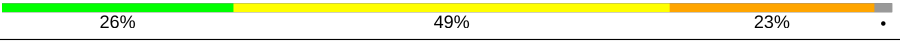
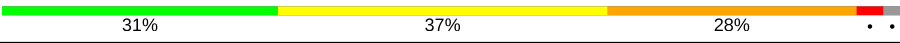
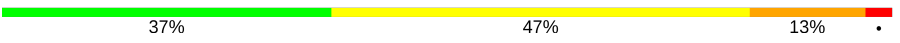
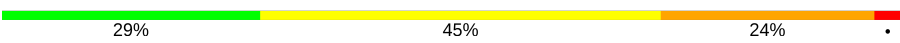

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Mol	Chain	Length	Quality of chain
40	DQ	118	
41	BR	103	
41	DR	103	
42	BS	110	
42	DS	110	
43	BT	100	
43	DT	100	
44	BU	104	
44	DU	104	
45	BV	94	
45	DV	94	
46	BW	85	
46	DW	85	
47	BX	78	
47	DX	78	
48	BY	63	
48	DY	63	
49	BZ	59	
49	DZ	59	
50	B0	57	
50	D0	57	
51	B1	55	
51	D1	55	
52	B2	46	
52	D2	46	

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Mol	Chain	Length	Quality of chain
53	B3	65	
53	D3	65	
54	B4	38	
54	D4	38	
55	CY	185	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1601	-	-	-	X
56	MG	AA	1602	-	-	-	X
56	MG	AA	1608	-	-	-	X
56	MG	AA	1613	-	-	-	X
56	MG	AA	1614	-	-	-	X
56	MG	AA	1617	-	-	-	X
56	MG	AA	1619	-	-	-	X
56	MG	AA	1621	-	-	-	X
56	MG	AA	1626	-	-	-	X
56	MG	AA	1630	-	-	-	X
56	MG	AA	1633	-	-	-	X
56	MG	AA	1638	-	-	-	X
56	MG	AA	1641	-	-	-	X
56	MG	AA	1644	-	-	-	X
56	MG	AA	1652	-	-	-	X
56	MG	AD	301	-	-	-	X
56	MG	BA	3005	-	-	-	X
56	MG	BA	3008	-	-	-	X
56	MG	BA	3011	-	-	-	X
56	MG	BA	3013	-	-	-	X
56	MG	BA	3021	-	-	-	X
56	MG	BA	3022	-	-	-	X
56	MG	BA	3023	-	-	-	X
56	MG	BA	3025	-	-	-	X
56	MG	BA	3027	-	-	-	X
56	MG	BA	3030	-	-	-	X
56	MG	BA	3031	-	-	-	X
56	MG	BA	3044	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3047	-	-	-	X
56	MG	BA	3049	-	-	-	X
56	MG	BA	3054	-	-	-	X
56	MG	BA	3056	-	-	-	X
56	MG	BA	3058	-	-	-	X
56	MG	BA	3063	-	-	-	X
56	MG	BA	3064	-	-	-	X
56	MG	BA	3065	-	-	-	X
56	MG	BA	3070	-	-	-	X
56	MG	BA	3072	-	-	-	X
56	MG	BA	3077	-	-	-	X
56	MG	BA	3078	-	-	-	X
56	MG	BA	3092	-	-	-	X
56	MG	BA	3095	-	-	-	X
56	MG	BA	3103	-	-	-	X
56	MG	BA	3104	-	-	-	X
56	MG	BA	3105	-	-	-	X
56	MG	BA	3106	-	-	-	X
56	MG	BA	3107	-	-	-	X
56	MG	BA	3108	-	-	-	X
56	MG	BA	3109	-	-	-	X
56	MG	BA	3111	-	-	-	X
56	MG	BA	3115	-	-	-	X
56	MG	BA	3119	-	-	-	X
56	MG	BA	3127	-	-	-	X
56	MG	BA	3129	-	-	-	X
56	MG	BA	3130	-	-	-	X
56	MG	BA	3140	-	-	-	X
56	MG	BA	3146	-	-	-	X
56	MG	BA	3147	-	-	-	X
56	MG	BA	3148	-	-	-	X
56	MG	BA	3153	-	-	-	X
56	MG	BA	3168	-	-	-	X
56	MG	BA	3170	-	-	-	X
56	MG	BB	201	-	-	-	X
56	MG	BB	202	-	-	-	X
56	MG	CA	1601	-	-	-	X
56	MG	CA	1602	-	-	-	X
56	MG	CA	1612	-	-	-	X
56	MG	CA	1614	-	-	-	X
56	MG	CA	1617	-	-	-	X
56	MG	CA	1626	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	CA	1636	-	-	-	X
56	MG	CA	1637	-	-	-	X
56	MG	CA	1640	-	-	-	X
56	MG	CA	1641	-	-	-	X
56	MG	CA	1646	-	-	-	X
56	MG	CA	1659	-	-	-	X
56	MG	CA	1669	-	-	-	X
56	MG	DA	3008	-	-	-	X
56	MG	DA	3009	-	-	-	X
56	MG	DA	3012	-	-	-	X
56	MG	DA	3013	-	-	-	X
56	MG	DA	3017	-	-	-	X
56	MG	DA	3020	-	-	-	X
56	MG	DA	3021	-	-	-	X
56	MG	DA	3022	-	-	-	X
56	MG	DA	3028	-	-	-	X
56	MG	DA	3029	-	-	-	X
56	MG	DA	3036	-	-	-	X
56	MG	DA	3038	-	-	-	X
56	MG	DA	3048	-	-	-	X
56	MG	DA	3051	-	-	-	X
56	MG	DA	3057	-	-	-	X
56	MG	DA	3060	-	-	-	X
56	MG	DA	3061	-	-	-	X
56	MG	DA	3064	-	-	-	X
56	MG	DA	3066	-	-	-	X
56	MG	DA	3069	-	-	-	X
56	MG	DA	3071	-	-	-	X
56	MG	DA	3072	-	-	-	X
56	MG	DA	3076	-	-	-	X
56	MG	DA	3079	-	-	-	X
56	MG	DA	3092	-	-	-	X
56	MG	DA	3094	-	-	-	X
56	MG	DA	3098	-	-	-	X
56	MG	DA	3101	-	-	-	X
56	MG	DA	3102	-	-	-	X
56	MG	DA	3104	-	-	-	X
56	MG	DA	3106	-	-	-	X
56	MG	DA	3107	-	-	-	X
56	MG	DA	3111	-	-	-	X
56	MG	DA	3113	-	-	-	X
56	MG	DA	3121	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DA	3127	-	-	-	X
56	MG	DA	3129	-	-	-	X
56	MG	DA	3131	-	-	-	X
56	MG	DA	3142	-	-	-	X
56	MG	DA	3146	-	-	-	X
56	MG	DA	3147	-	-	-	X
56	MG	DA	3153	-	-	-	X
56	MG	DA	3157	-	-	-	X
56	MG	DA	3158	-	-	-	X
56	MG	DA	3167	-	-	-	X
56	MG	DA	3169	-	-	-	X
56	MG	DA	3178	-	-	-	X
56	MG	DA	3181	-	-	-	X
56	MG	DA	3192	-	-	-	X
56	MG	DA	3193	-	-	-	X
56	MG	DB	201	-	-	-	X
56	MG	DB	204	-	-	-	X
56	MG	DO	201	-	-	-	X
57	NMY	AA	1655	-	-	X	-
57	NMY	AA	1656	-	-	-	X
57	NMY	AA	1657	-	-	-	X
57	NMY	BA	3161	-	-	-	X
57	NMY	BA	3162	-	-	-	X
57	NMY	BA	3163	-	-	-	X
57	NMY	BA	3164	-	-	-	X
57	NMY	BA	3165	-	-	X	X
57	NMY	BA	3167	-	-	-	X
57	NMY	CA	1672	-	-	-	X
57	NMY	DA	3184	-	-	-	X
57	NMY	DA	3185	-	-	-	X
57	NMY	DA	3186	-	-	-	X
57	NMY	DA	3187	-	-	-	X
57	NMY	DA	3189	-	-	-	X
57	NMY	DA	3190	-	-	X	X
58	ZN	D4	101	-	-	-	X

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 293103 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- 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	CB	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	CC	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	CD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
5	CE	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	CF	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	CG	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	CH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
13	CM	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	CN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
17	CQ	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	CR	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	CS	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	CT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
21	CU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a RNA chain called Phenylalanine specific transfer RNA, tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
22	CV	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 23 is a RNA chain called Messenger RNA, mRNA.

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

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	12	C	A	SEE REMARK 999	GB AP012306
DB	12	C	A	SEE REMARK 999	GB AP012306

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

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

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

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

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

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

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

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

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

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

- Molecule 31 is a protein called 50S ribosomal protein L9.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	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
36	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	B1	50	Total	C	N	O	0	0	0
			409	263	75	71			
51	D1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	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
52	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

- Molecule 55 is a protein called Ribosome recycling factor, RRF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	CY	183	Total	C	N	O	S	0	0	0
			1423	874	260	283	6			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

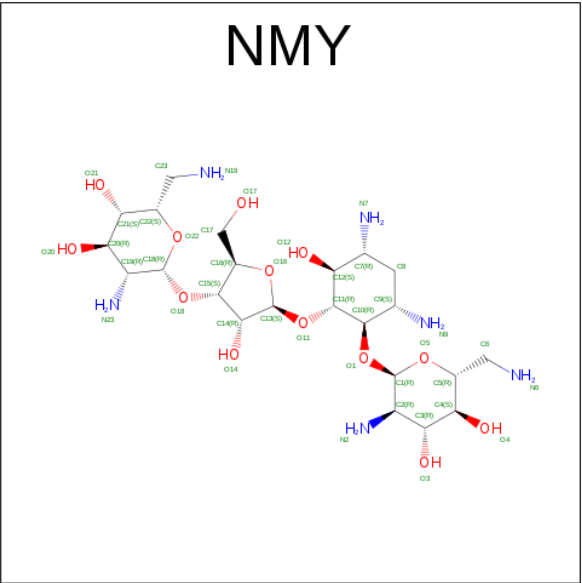
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BB	3	Total	Mg	0	0
			3	3		
56	DE	1	Total	Mg	0	0
			1	1		
56	BA	163	Total	Mg	0	0
			163	163		
56	CA	71	Total	Mg	0	0
			71	71		
56	DO	1	Total	Mg	0	0
			1	1		
56	DL	1	Total	Mg	0	0
			1	1		
56	DA	187	Total	Mg	0	0
			187	187		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	54	Total	Mg	0	0
			54	54		
56	BQ	1	Total	Mg	0	0
			1	1		
56	AN	1	Total	Mg	0	0
			1	1		
56	AD	1	Total	Mg	0	0
			1	1		
56	CX	1	Total	Mg	0	0
			1	1		
56	BC	1	Total	Mg	0	0
			1	1		
56	DB	4	Total	Mg	0	0
			4	4		

- Molecule 57 is NEOMYCIN (three-letter code: NMY) (formula:  $C_{23}H_{46}N_6O_{13}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	AA	1	Total	C	N	O	0	0
			42	23	6	13		
57	AA	1	Total	C	N	O	0	0
			42	23	6	13		
57	AA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	CA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	188	Total	O	0	0
			188	188		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	2	Total 2	O 2	0	0
59	AK	1	Total 1	O 1	0	0
59	AN	4	Total 4	O 4	0	0
59	AT	2	Total 2	O 2	0	0
59	AU	1	Total 1	O 1	0	0
59	BA	616	Total 616	O 616	0	0
59	BB	13	Total 13	O 13	0	0
59	BC	10	Total 10	O 10	0	0
59	BD	4	Total 4	O 4	0	0
59	BL	4	Total 4	O 4	0	0
59	BN	1	Total 1	O 1	0	0
59	BT	3	Total 3	O 3	0	0
59	BU	3	Total 3	O 3	0	0
59	BV	1	Total 1	O 1	0	0
59	B0	1	Total 1	O 1	0	0
59	B3	1	Total 1	O 1	0	0
59	B4	1	Total 1	O 1	0	0
59	CA	192	Total 192	O 192	0	0
59	CC	1	Total 1	O 1	0	0
59	CE	1	Total 1	O 1	0	0
59	CL	1	Total 1	O 1	0	0

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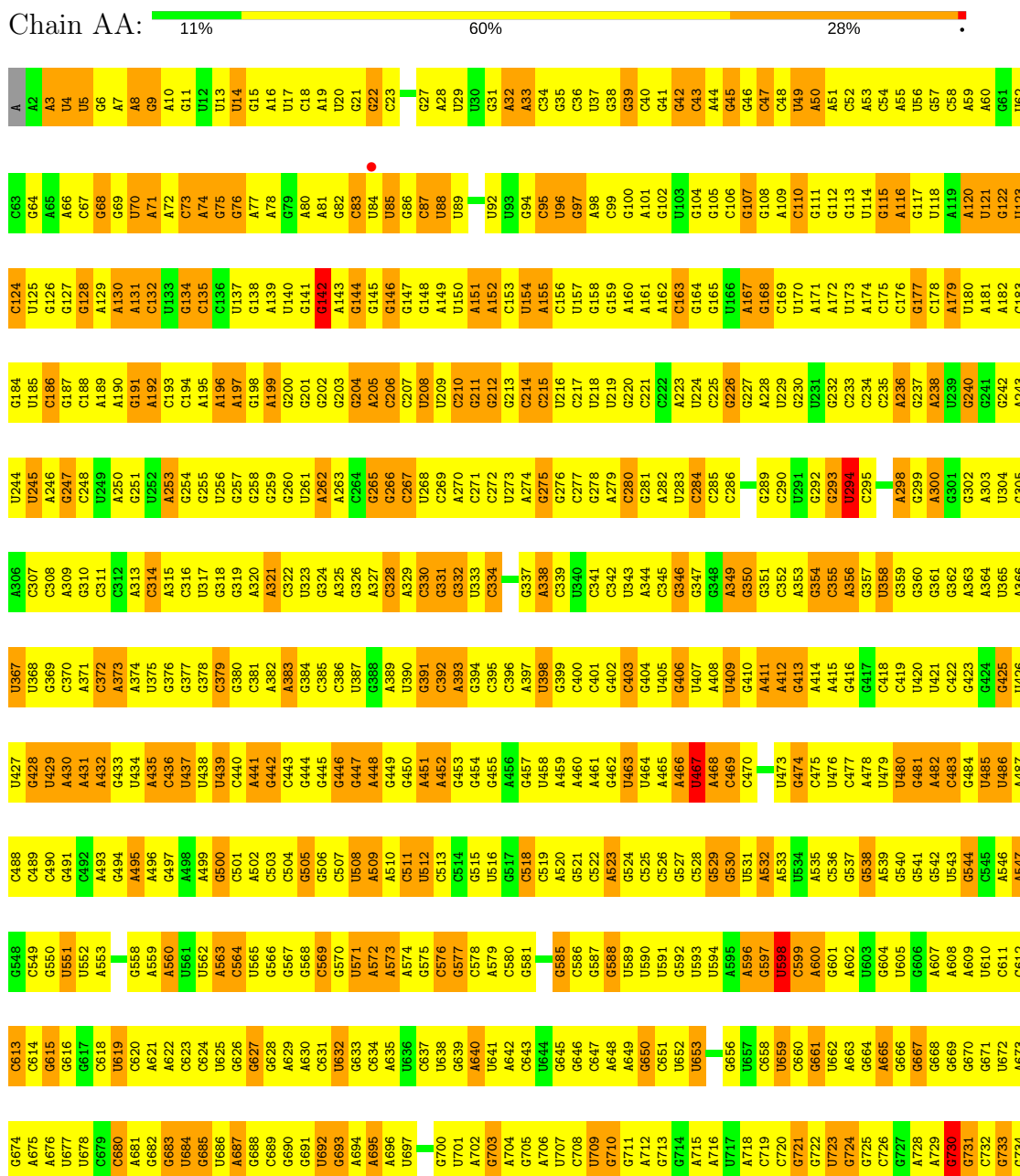
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CN	6	Total 6	O 6	0	0
59	CT	2	Total 2	O 2	0	0
59	DA	627	Total 627	O 627	0	0
59	DB	13	Total 13	O 13	0	0
59	DC	4	Total 4	O 4	0	0
59	DD	2	Total 2	O 2	0	0
59	DE	4	Total 4	O 4	0	0
59	DF	1	Total 1	O 1	0	0
59	DL	7	Total 7	O 7	0	0
59	DN	2	Total 2	O 2	0	0
59	DQ	1	Total 1	O 1	0	0
59	DS	1	Total 1	O 1	0	0
59	DT	1	Total 1	O 1	0	0
59	DU	1	Total 1	O 1	0	0
59	DV	1	Total 1	O 1	0	0
59	D3	2	Total 2	O 2	0	0
59	D4	1	Total 1	O 1	0	0

### 3 Residue-property plots

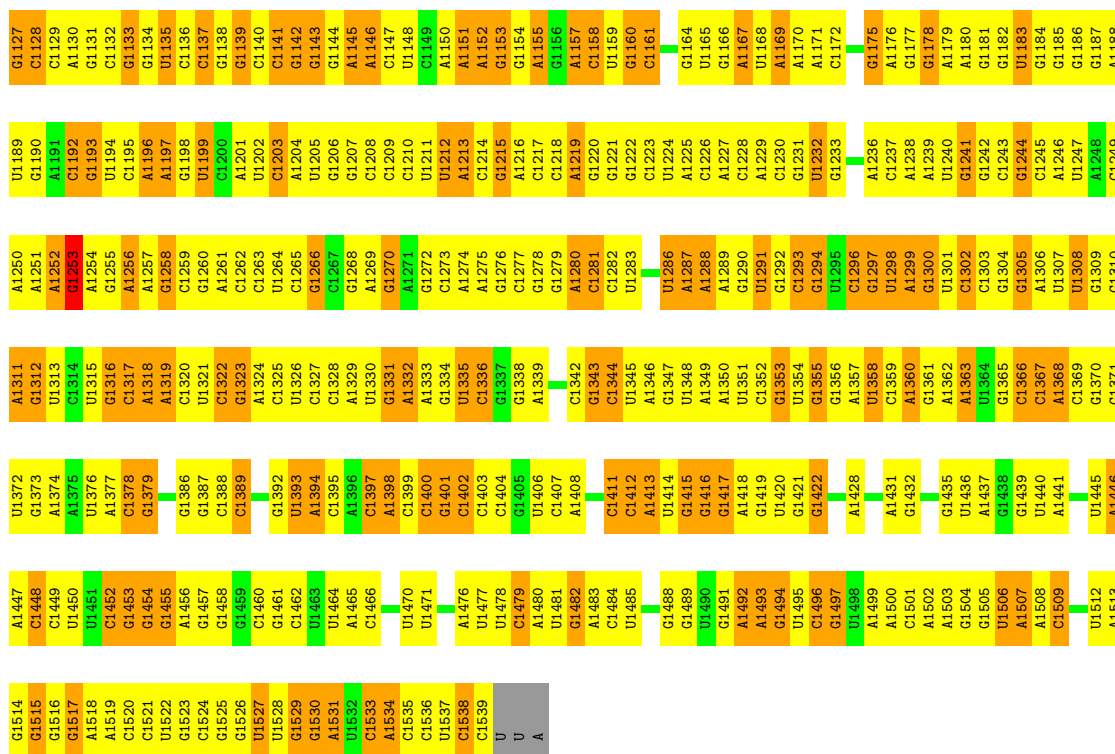
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 16S ribosomal RNA

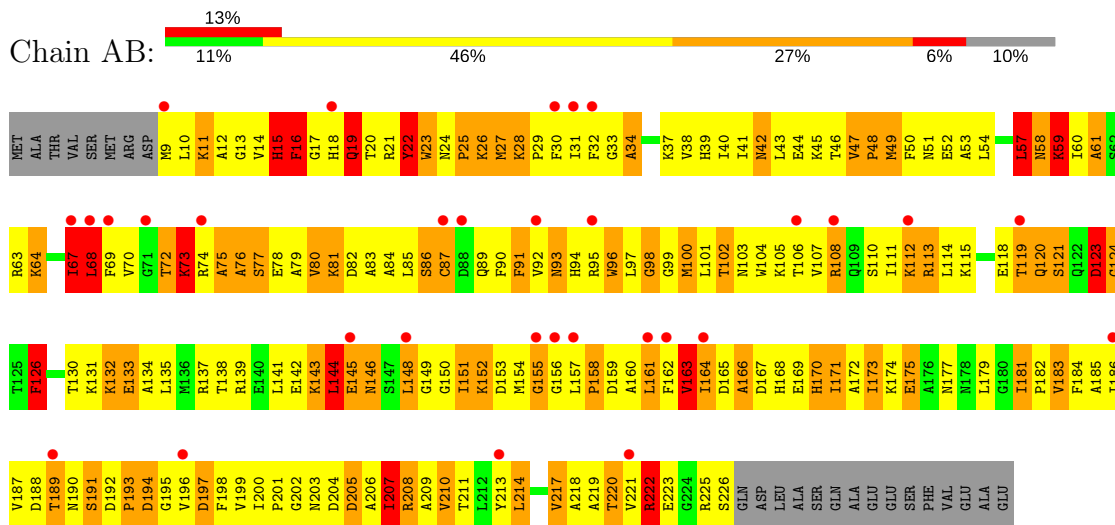


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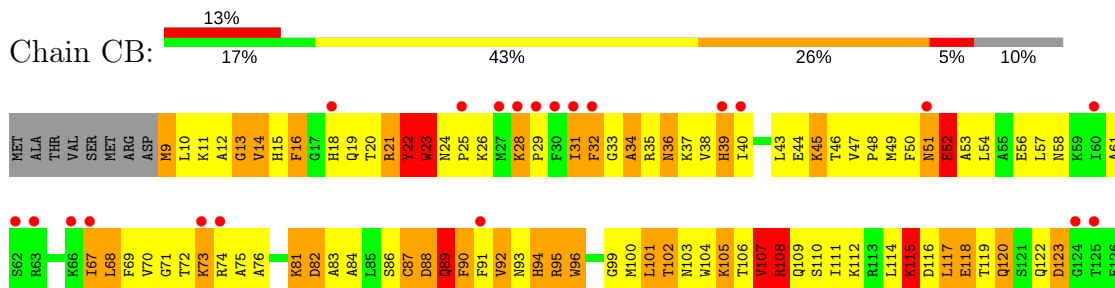


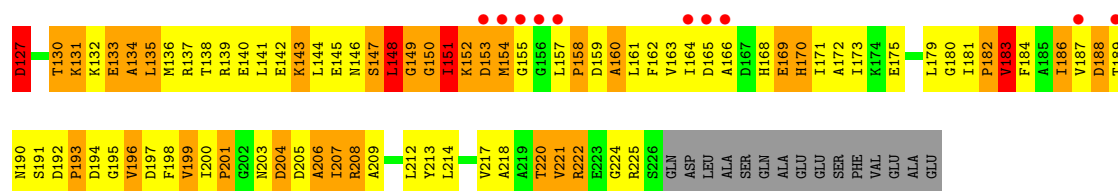


### • Molecule 2: 30S ribosomal protein S2



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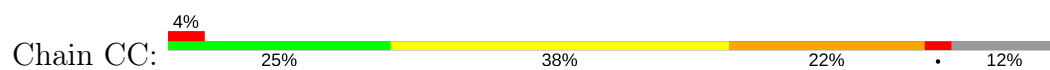




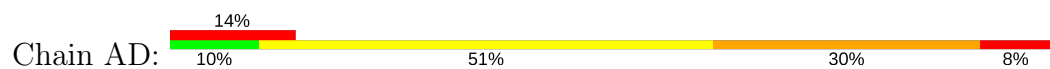
• Molecule 3: 30S ribosomal protein S3

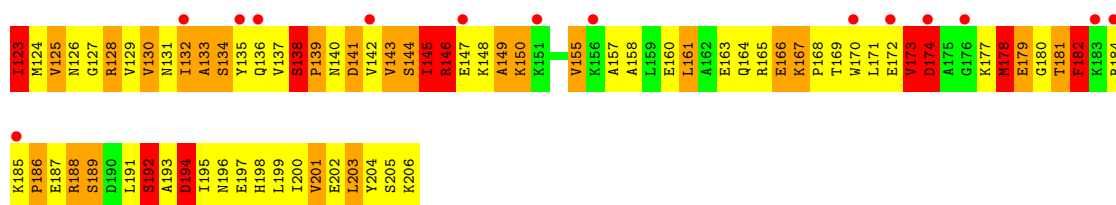


• Molecule 3: 30S ribosomal protein S3

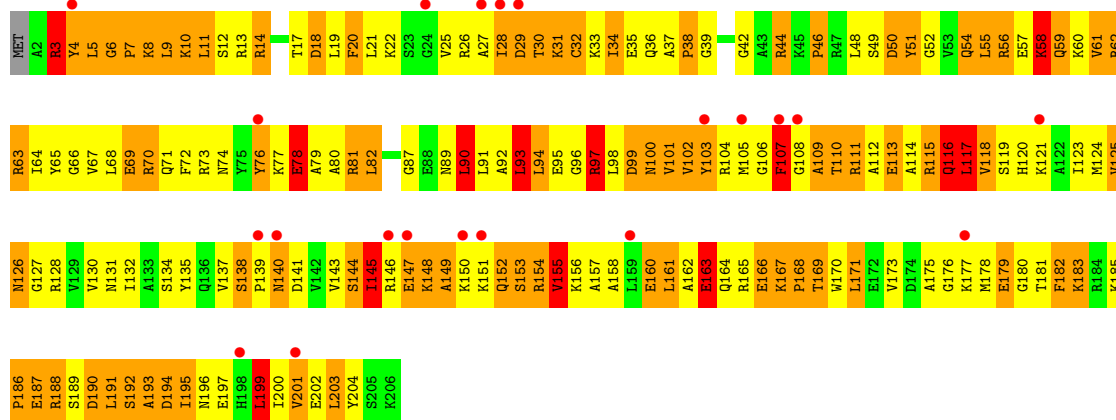
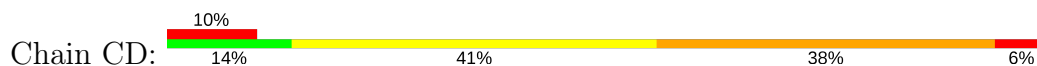


• Molecule 4: 30S ribosomal protein S4

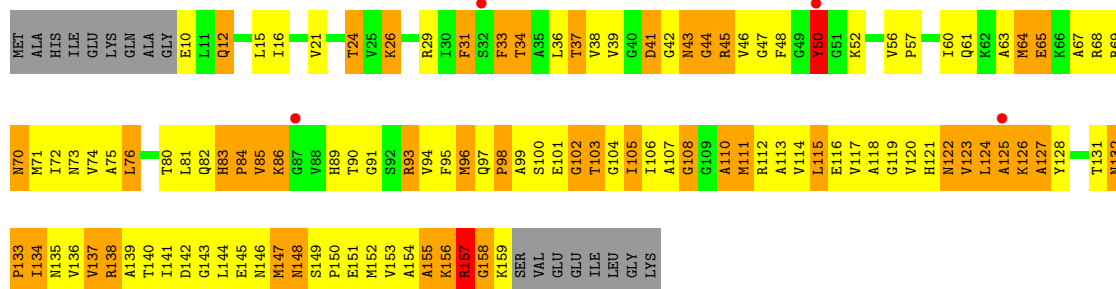
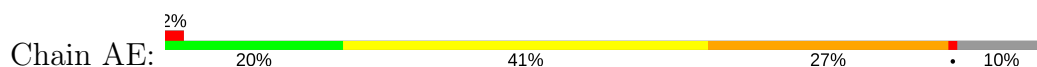




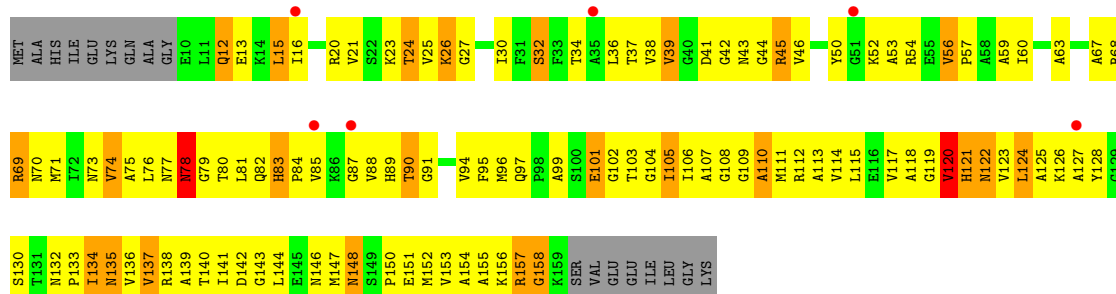
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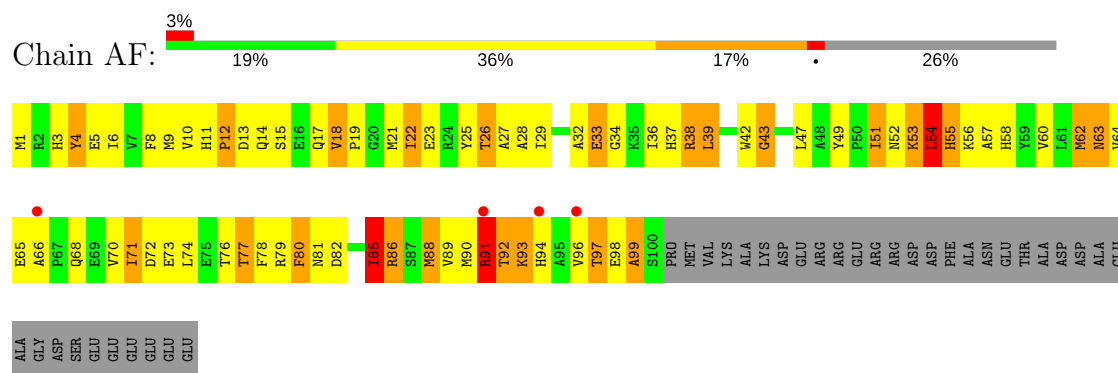
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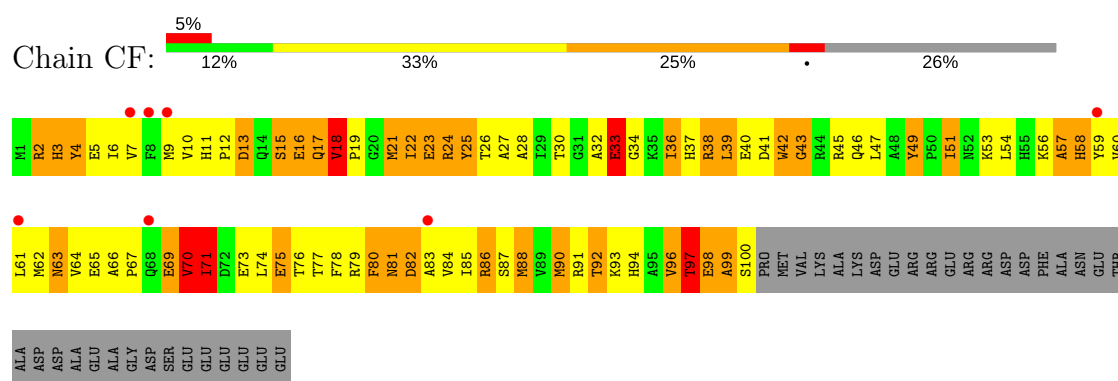
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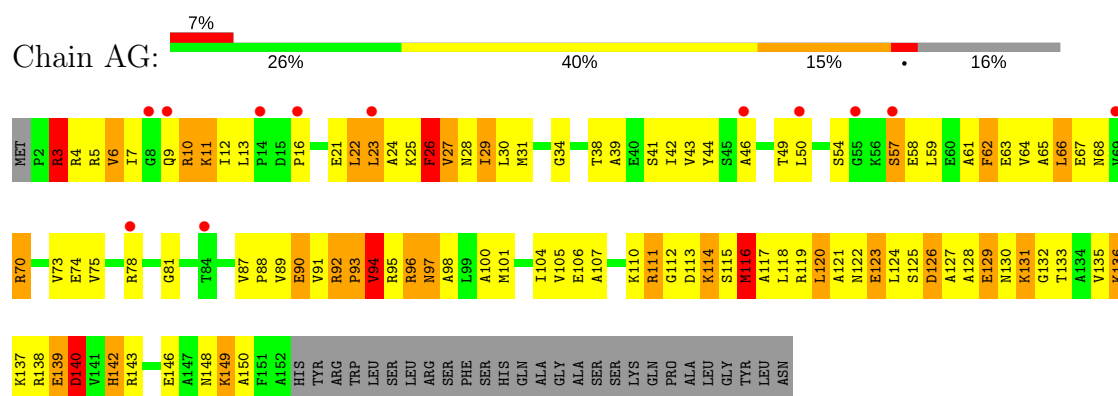
- Molecule 6: 30S ribosomal protein S6



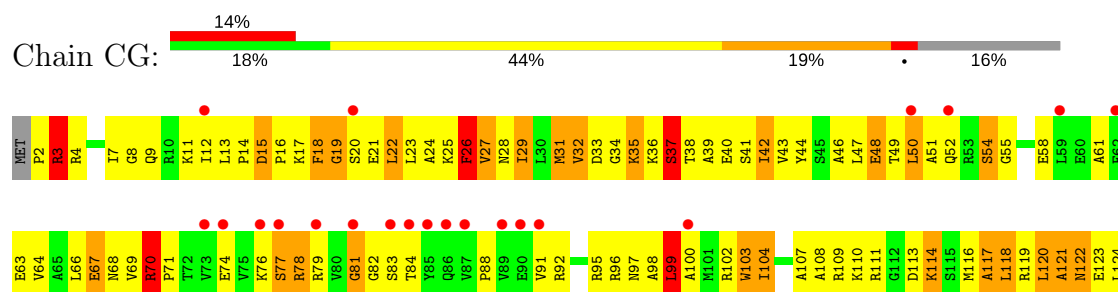
- Molecule 6: 30S ribosomal protein S6

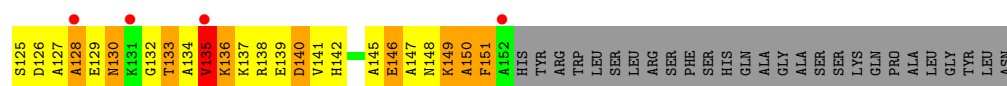


- Molecule 7: 30S ribosomal protein S7

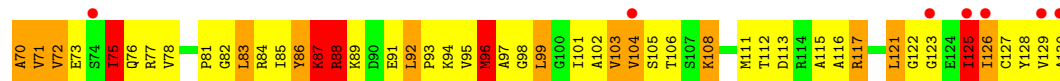
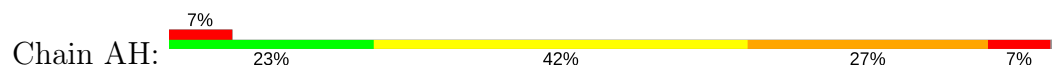


- Molecule 7: 30S ribosomal protein S7

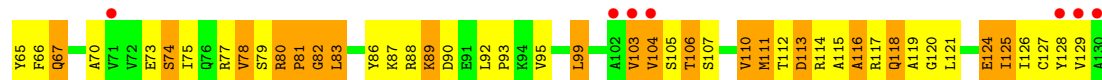




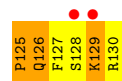
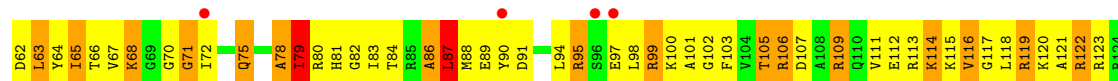
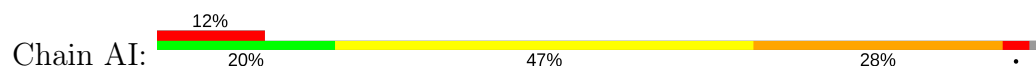
• Molecule 8: 30S ribosomal protein S8



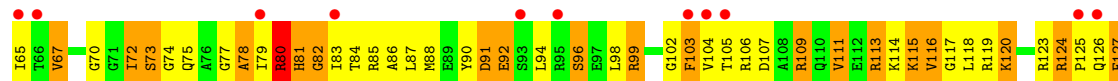
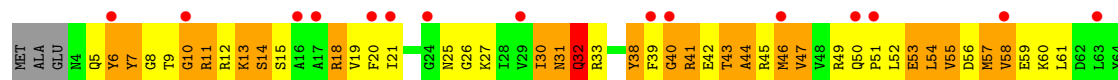
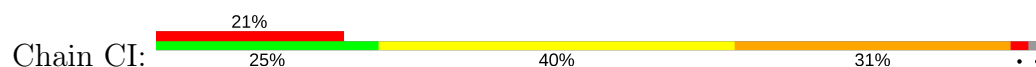
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9

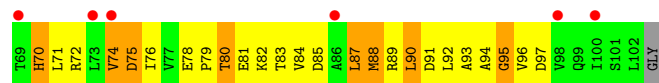


• Molecule 9: 30S ribosomal protein S9

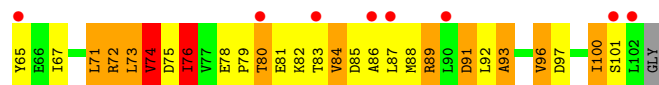
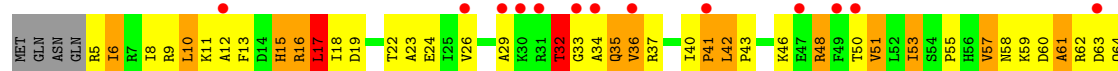




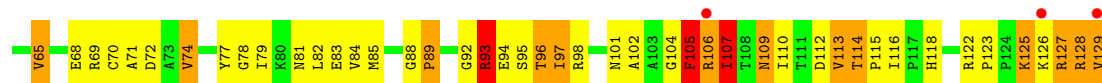
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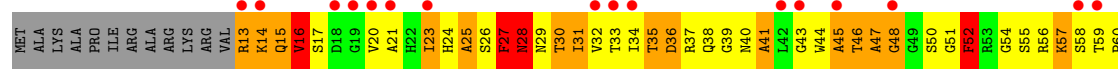
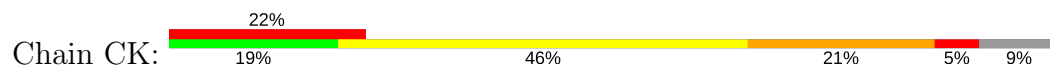
• Molecule 10: 30S ribosomal protein S10



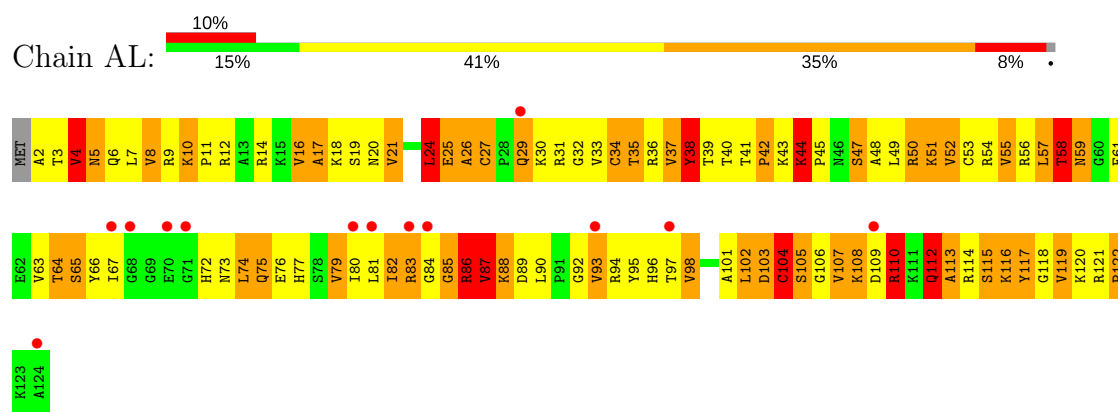
• Molecule 11: 30S ribosomal protein S11



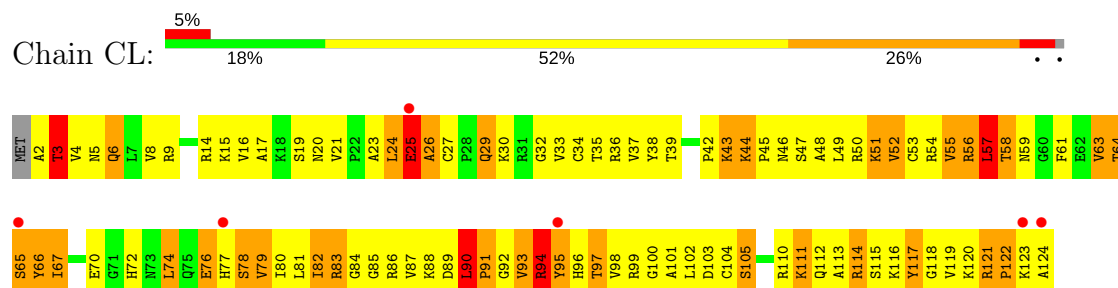
• Molecule 11: 30S ribosomal protein S11



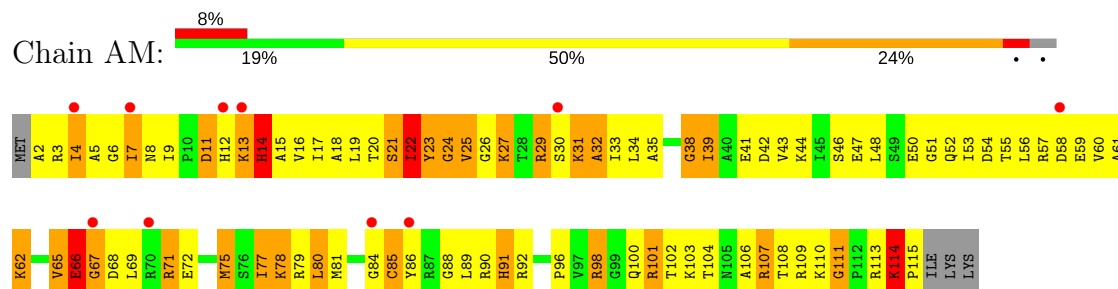
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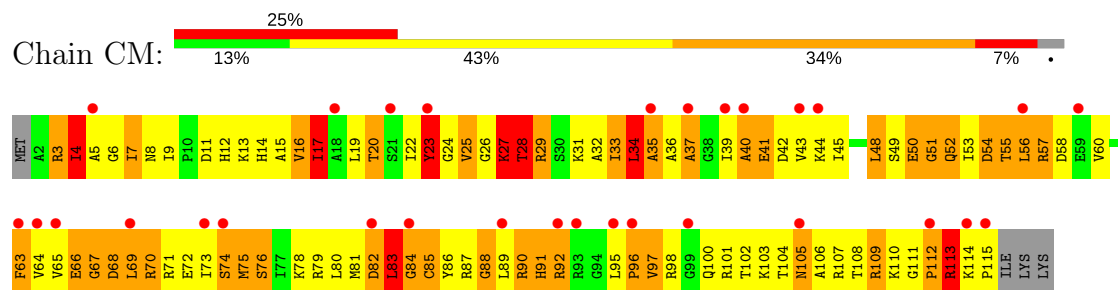
- Molecule 12: 30S ribosomal protein S12



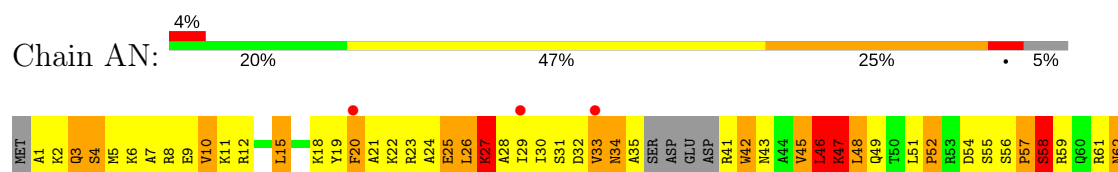
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13

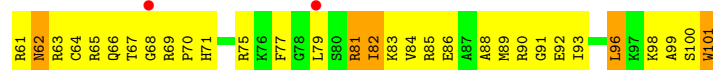
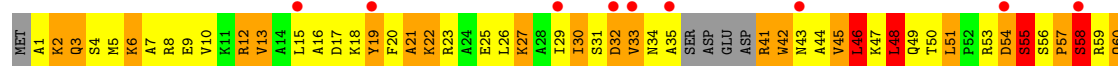
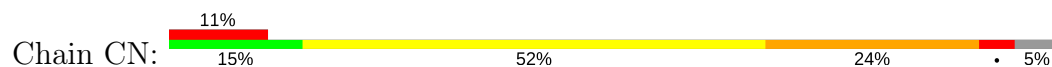


- Molecule 14: 30S ribosomal protein S14





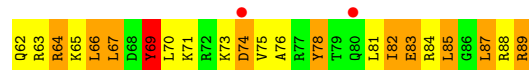
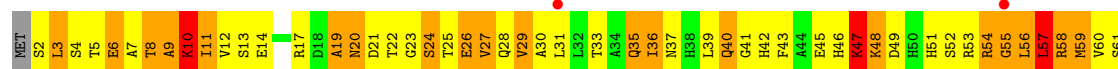
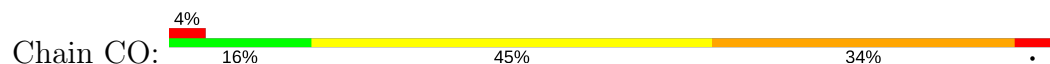
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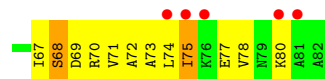
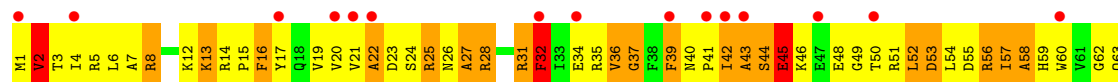
- Molecule 15: 30S ribosomal protein S15



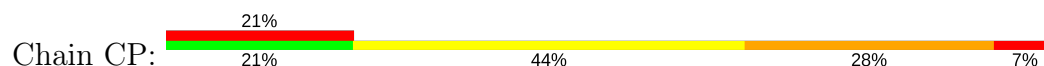
- Molecule 15: 30S ribosomal protein S15



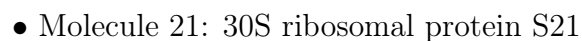
- Molecule 16: 30S ribosomal protein S16

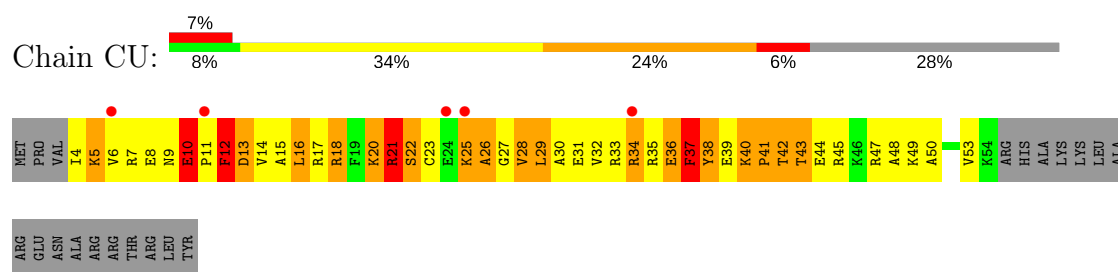


- Molecule 16: 30S ribosomal protein S16

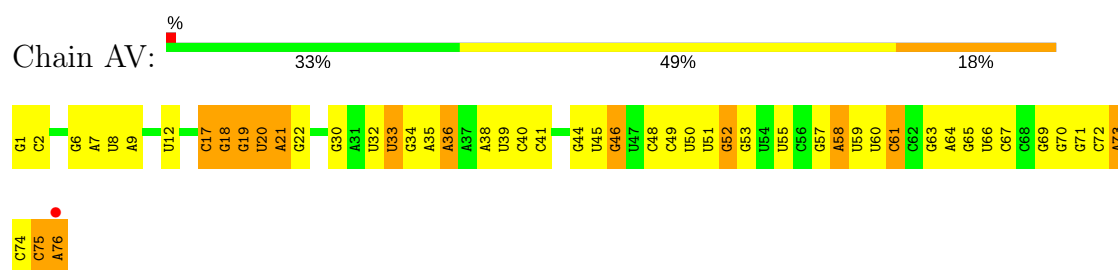




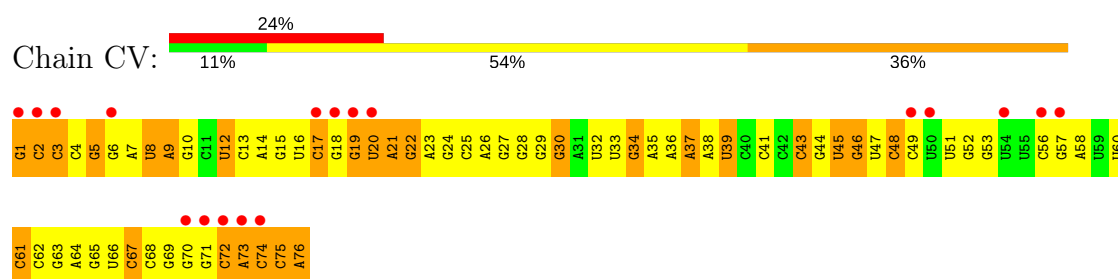




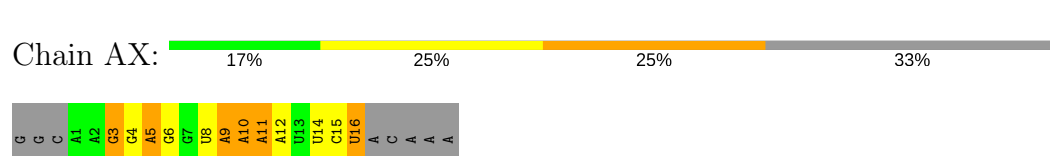
- Molecule 22: Phenylalanine specific transfer RNA, tRNA-Phe



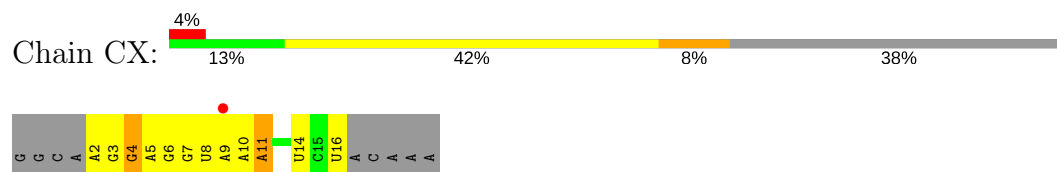
- Molecule 22: Phenylalanine specific transfer RNA, tRNA-Phe



- Molecule 23: Messenger RNA, mRNA



- Molecule 23: Messenger RNA, mRNA



- Molecule 24: 23S ribosomal RNA



C1076	G1011	A947	U884	G822	U762	G695	C635	A575	G512	G450	G386	G325	C257	A196	G132
A1077	U1012	C346	C885	C823	G763	G696	G636	U576	A513	U451	U387	G326	G258	A197	U133
U1078	C1013	G949	A	U824	A764	G	A637	G577	A514	G452	G388	G327	G259	C198	G134
C1079	U1013	G950	U	U825	C765	A699	G638	G578	A515	G453	G389	G328	G260	C199	U135
A1080	G1016	C951	C	U826	U766	G700	U639	G579	C516	U454	U390	G329	G261	U200	U136
U1081	G1017	G952	C	U827	U767	G	U640	U580	C517	U455	A391	A330	G262	C201	G136
U1082	U1018	G953	C	U828	G768	G704	U641	C581	C518	G456	U392	C331	A263	U202	U137
U1083	U1019	G954	G	U829	U769	A705	U642	C582	U519	A457	C393	A332	A265	U203	U138
A1084	A1020	U955	A892	G830	G770	A706	A643	A583	G520	G458	C394	G333	G266	A204	U139
A1085	G1021	G956	U894	G831	G771	G	A644	C584	A521	U459	U395	C334	G205	U206	G141
U1086	G1022	C957	U894	U832	G772	G710	U646	C585	A522	G460	U396	C335	A270	U207	G142
G1087	U1023	U958	U895	A833	U773	G711	U647	A586	C523	G463	U397	C336	G271	A208	A142
A1088	G1024	A959	A896	G834	G774	G712	G648	C587	G524	U464	U398	C337	G272	C208	C143
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G1091	A1027	G962	A899	U837	G777	A715	U650	A590	C527	A466	A401	U340	C275	C211	A146
C1092	U1028	U963	A900	C838	G778	A716	G651	A591	A528	G467	A402	G341	U276	G212	C147
G1093	A1029	C964	C901	U839	U779	C717	U652	A592	A529	G468	U403	A342	G277	U213	U148
U1094	C1030	G	G	U840	G780	A718	U653	U593	G530	G469	A404	C343	A278	G214	A149
A1095	G1031	G969	U906	C841	A781	C719	A654	U594	C531	A470	U405	A344	A279	G215	U150
A1096	U1032	U970	G907	U842	A782	U720	A655	C595	C532	A471	G406	A345	U280	A216	C151
U1097	U1033	G971	C908	G	A783	A721	G656	U596	G533	A472	A407	A346	C281	A217	A152
A1098	G1034	A972	A909	U843	G784	A722	U657	G597	U534	G473	G408	A347	A282	A218	U153
G1099	U1035	A973	A910	A845	U790	C723	U658	U598	G535	G474	G409	A348	G283	A219	U154
C1100	G1037	G974	A911	U846	C786	U724	G659	A599	G536	C475	G410	U349	U284	G220	A155
U1101	G1038	A975	C912	C848	C787	G725	C660	G600	G537	G476	G411	G350	G285	A221	A156
C1102	A1039	G976	U913	A849	A788	G726	A661	C601	A538	A477	A412	C351	G289	A222	U157
A1103	U1040	G977	G914	U850	A789	A727	G662	A602	G539	A478	C413	A352	G290	A223	U158
G1041	G1041	G978	C915	C851	U790	G728	G663	A603	U534	A479	C414	C353	U224	U224	A159
U1105	U1042	G979	C916	U852	G791	G729	G664	G604	G535	A480	A415	A354	U225	C225	A160
G1106	G1044	A980	A917	C853	A792	A730	U665	G605	G543	G481	U416	U355	U292	A226	A161
G1107	U1045	A981	A918	C854	A793	C731	A666	U606	C544	A482	C417	C356	A293	A227	U162
U1108	A1046	C982	U919	G855	A794	G732	U667	U607	C545	A483	C418	C357	A294	C228	C162
G1109	G1047	A983	A920	G856	C795	A733	A668	A608	U546	G484	U419	U358	G295	C229	C164
C1110	U1048	A984	C921	G857	G796	A734	G669	A609	A547	C485	C420	G359	U296	G230	A165
A1111	A1050	C985	C922	G858	G797	A735	A670	C610	G548	C485	C421	U360	G297	A231	U166
G1112	G1051	C986	G923	G859	G798	C736	C671	C611	G549	G488	A422	G361	A300	G232	A167
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C1114	A1054	A988	A925	A861	A800	G	C673	A613	G551	C490	G424	C363	G302	U234	U170
G1115	U1055	G989	G926	G862	G801	C740	G674	A614	G	G491	G425	C364	C305	C237	U171
G1056	G1056	A990	A927	A863	A802	U741	A675	U615	G555	A492	G426	U365	U306	C238	G178
C1117	U1057	C991	A928	G864	U803	A742	A676	A616	A556	G493	U427	C366	U307	C239	C179
G1118	G1058	C992	U929	C865	A804	A743	A677	G617	C557	G494	A428	G367	G307	C240	G180
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U1060	G1060	C994	U931	C867	C806	G745	C679	G619	G559	G496	A430	U369	A309	C242	G181
G1122	U1061	C995	U932	U868	U807	U746	C680	G620	C560	A497	U431	G370	A310	G242	A181
C1123	G1062	A996	A933	G869	G808	U747	G681	A621	U561	G498	A432	A371	A311	U243	A182
G1124	U1063	G997	U934	U870	G809	G748	G682	G622	U562	U499	C433	G372	A312	A244	C183
G1125	C1064	C998	C935	U871	U810	U749	U683	C623	A563	G500	U434	U373	G313	G245	C184
A1126	U1065	U999	A936	U872	U811	A750	G684	C624	C564	A501	C435	A374	C314	G246	G185
U1066	U1066	C999	C937	U873	C812	A751	A685	G625	C565	A502	C436	G375	G315	G247	G186
A1129	U1067	A1001	G938	C876	U813	A752	A686	G626	U566	A503	G442	G376	G316	G248	G187
U1130	G1068	G1002	A939	G877	C814	A753	U686	A627	U567	A504	G443	G377	G317	C249	G188
G1131	A1069	G940	C940	A878	C815	U754	C687	G628	U568	A505	A444	C378	G318	G250	G189
U1132	U1070	C1005	A941	U879	C816	U755	A689	G629	U569	A506	C445	G379	A251	A190	A190
A1133	G1071	C1006	G942	G879	C817	A756	G690	G630	G570	A507	C446	G380	A320	G252	A191
A1134	C1072	C1007	A943	G880	C818	G757	C591	A631	U571	A508	G446	G381	G319	C253	C192
G1135	U1073	A1008	C944	G881	A819	G	C692	A632	A572	C509	A447	G	A322	G254	U193
G1136	G1074	A1009	A945	G882	A820	G760	A693	A633	U573	C510	U448	A384	C323	G255	G194
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A2030	G1964	G1835	C1707	A1570	G1510	G1510	G1447	C1386	U1325	U1263	U1203	A1143
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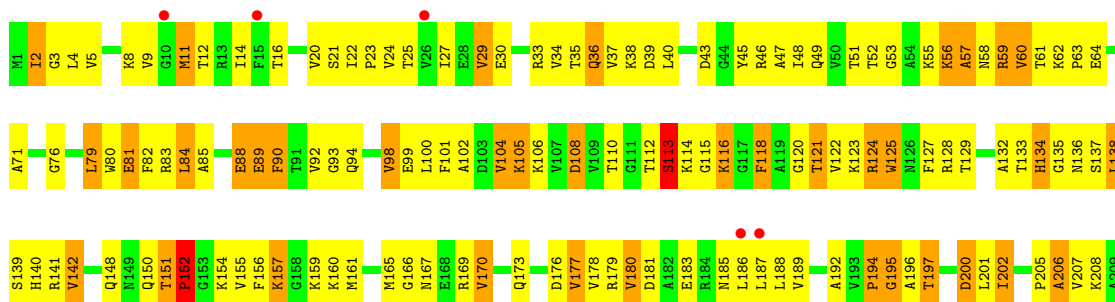


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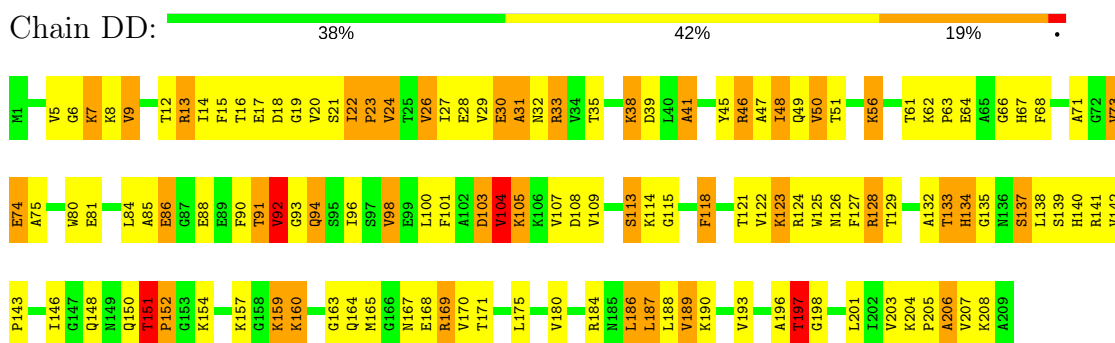
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G2054	G1992	G1929	G1867	A1805	U1667	C1605	A1545	C1480	C1417	G1225	C1291	G1225	G1162
C2055	U1993	G1930	C1868	C1806	G1668	C1606	G1546	U1481	G1418	A1226	G1292	A1226	G1162
U2111	C1994	U1931	G1869	G1807	A1669	C1607	C1547	G1482	A1419	G1227	G1293	G1227	C1164
G2112	U1995	A1932	C1870	A1808	C1741	A1608	G1548	G1483	A1420	G1228	U1294	G1228	G1165
U2113	C1996	G1933	A1871	A1809	U1671	A1609	A1549	U1484	G1421	C1229	C1295	C1229	G1166
A2061	C1997	C1934	A1872	A1810	A1672	A1610	C1550	U1485	G1422	G1232	G1296	G1232	G1167
G2062	U1998	G1935	G1873	G1811	G1673	U1614	A1551	U1486	G1423	G1233	C1297	G1233	G1168
C2063	A1999	A1936	C1874	G1812	G1674	C1615	A1552	U1487	G1424	G1234	C1298	G1234	A1169
U2114	C1999	G1937	G1875	G1813	U1675	A1616	A1553	G1488	G1425	G1235	C1299	U1234	G1170
G2064	C2000	A1937	G1876	C1814	A1676	A1617	U1554	U1489	G1426	G1236	G1300	G1236	G1171
A2065	G2001	U1938	A1876	C1815	C1677	A1618	G1555	A1490	A1427	A1237	A1301	A1237	U1174
C2066	C2002	U1939	C1877	C1816	U1677	A1619	C1556	G1491	G1428	G1238	A1302	G1238	U1175
U2115	A2003	U1940	G1878	G1817	A1678	A1618	G1557	G1492	G1429	G1239	A1303	G1239	G1176
G2067	G2004	C1941	U1879	U1818	A1679	G1620	C1558	G1493	G1430	G1240	U1306	G1240	G1177
U2116	C2005	C1942	U1880	A1819	G1680	G1621	U1559	A1494	G1432	G1241	G1306	G1241	G1178
A2068	U2006	U1943	C1881	U1820	G1681	G1621	U1559	A1494	G1432	G1242	G1306	G1242	G1179



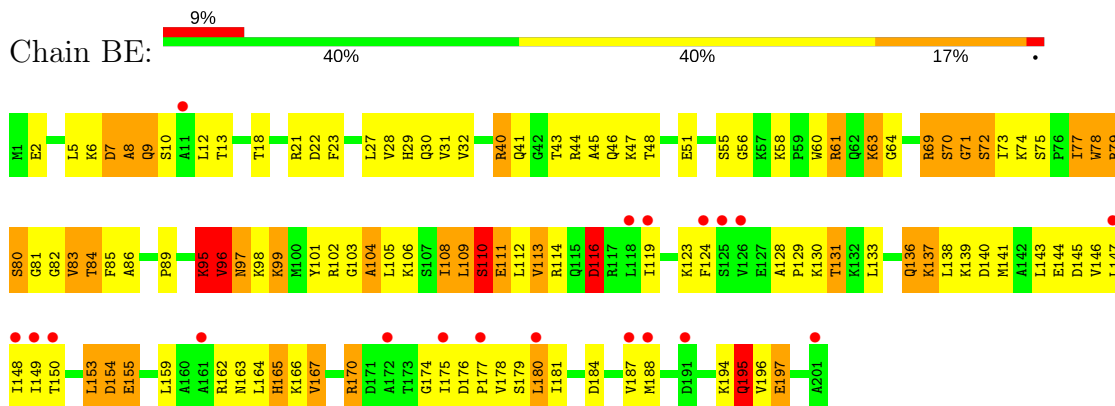




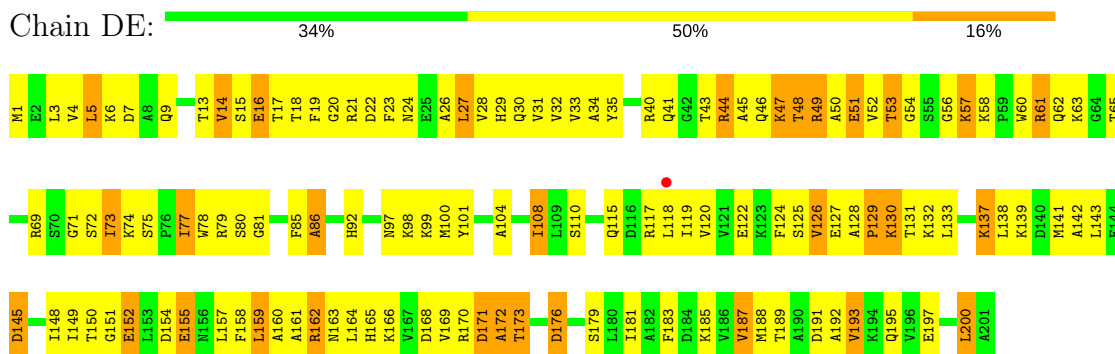
• Molecule 27: 50S ribosomal protein L3



• Molecule 28: 50S ribosomal protein L4



• Molecule 28: 50S ribosomal protein L4

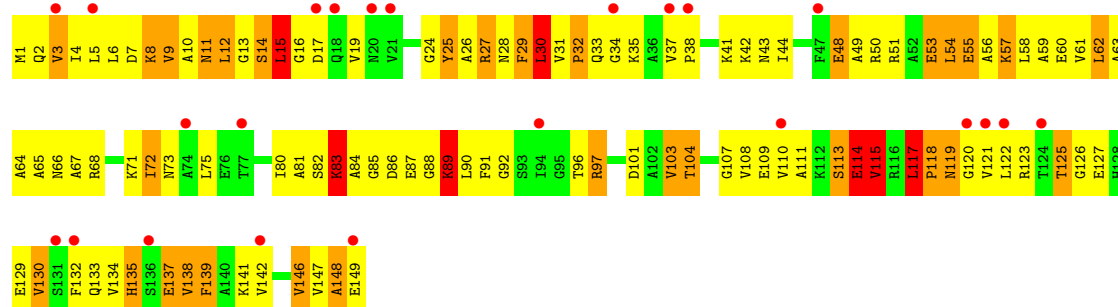


• Molecule 29: 50S ribosomal protein L5

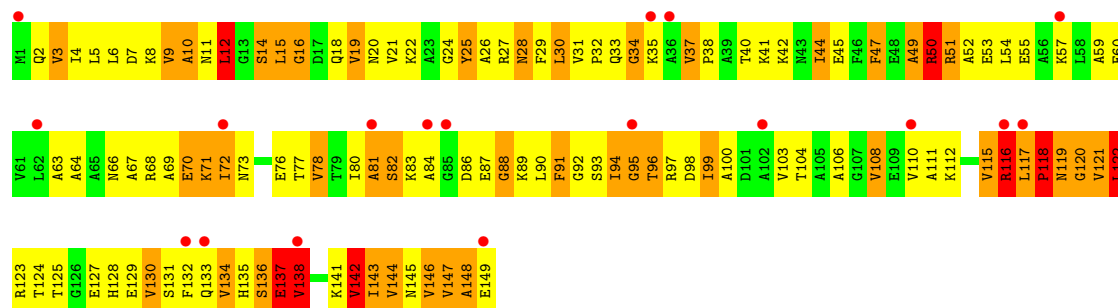
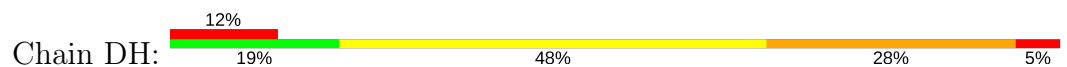




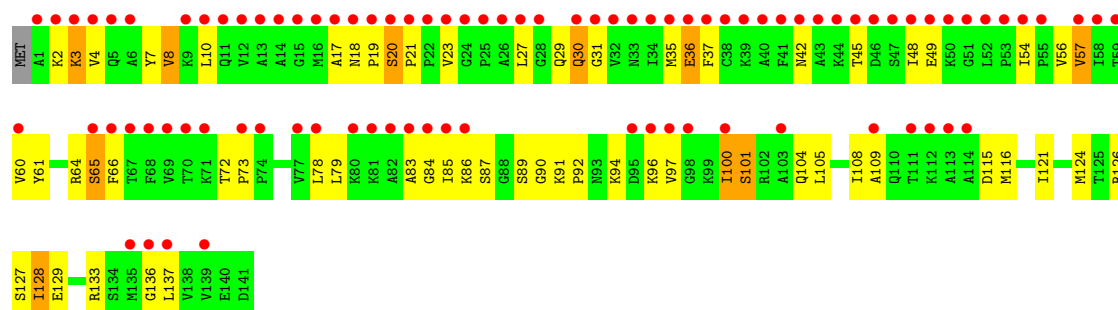
• Molecule 31: 50S ribosomal protein L9



• Molecule 31: 50S ribosomal protein L9

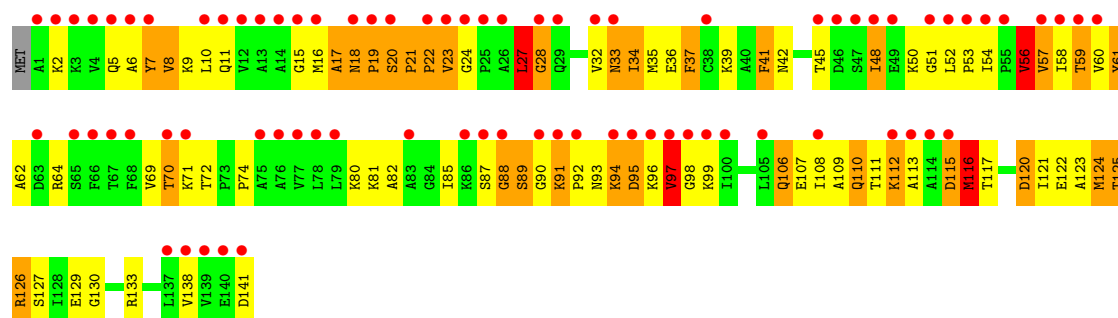


• Molecule 32: 50S ribosomal protein L11

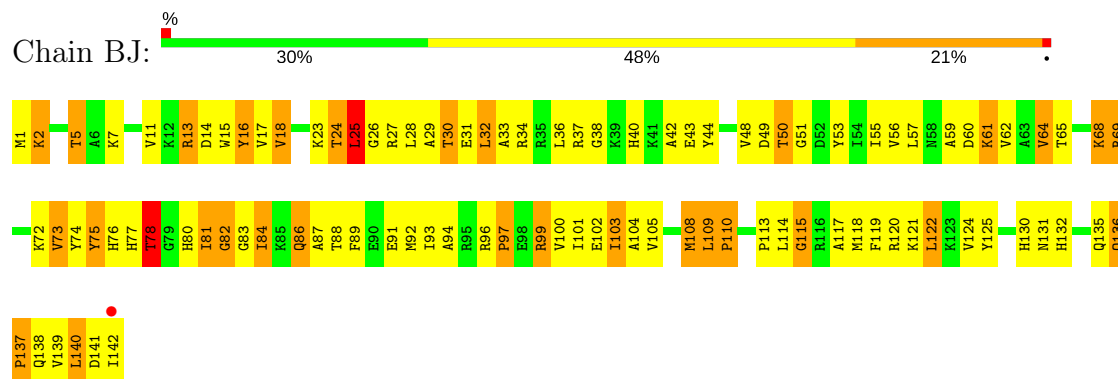


• Molecule 32: 50S ribosomal protein L11

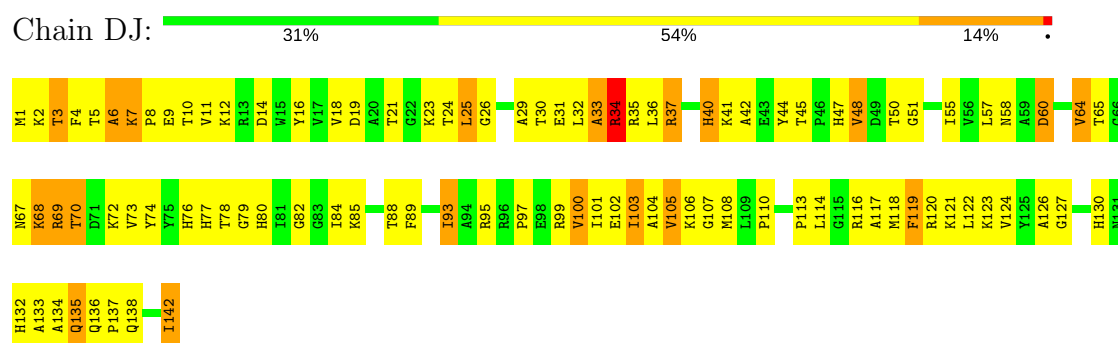




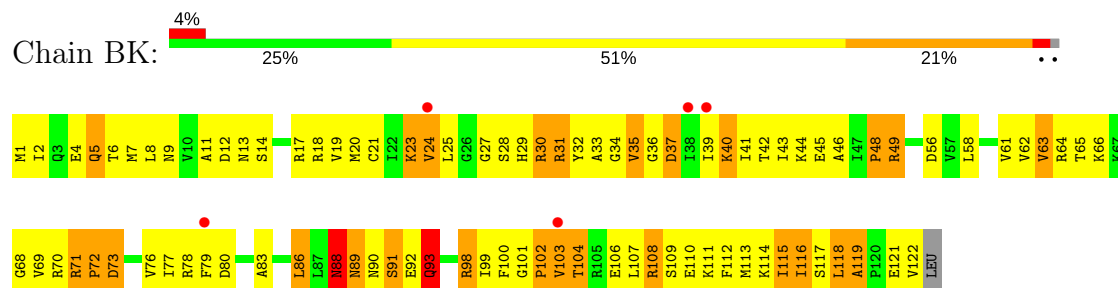
- Molecule 33: 50S ribosomal protein L13



- Molecule 33: 50S ribosomal protein L13

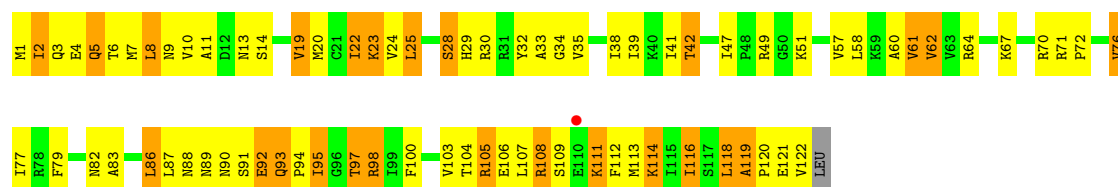


- Molecule 34: 50S ribosomal protein L14

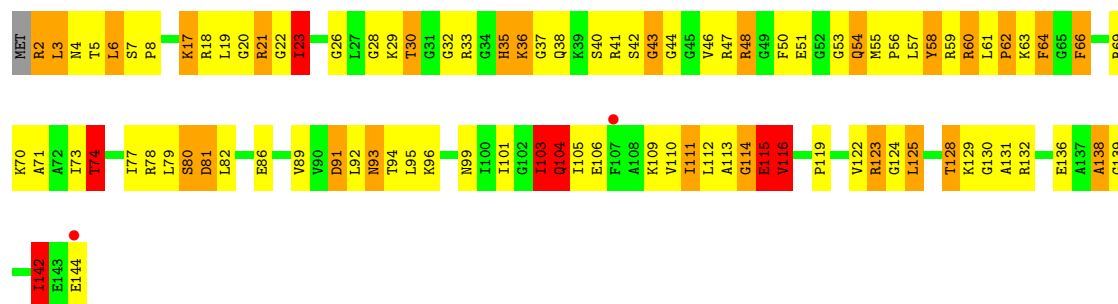


- Molecule 34: 50S ribosomal protein L14

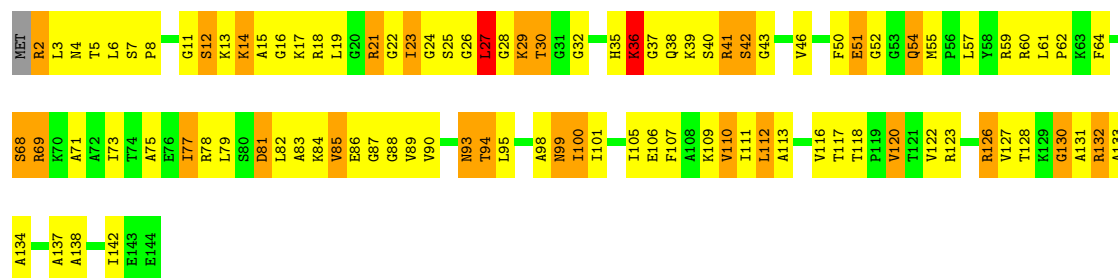




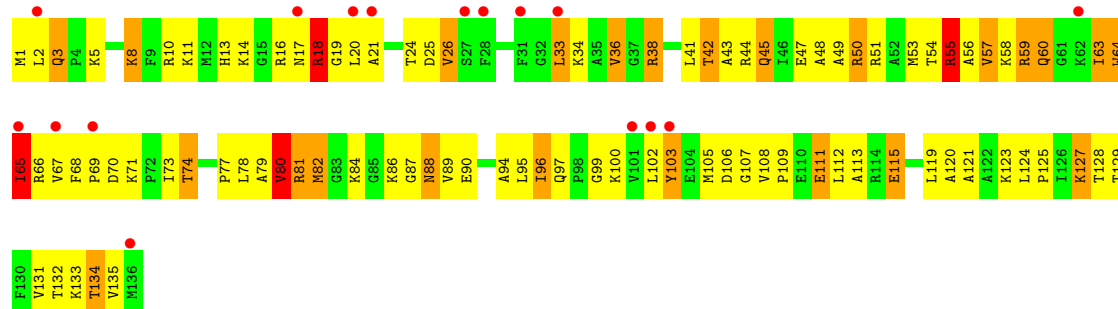
• Molecule 35: 50S ribosomal protein L15



• Molecule 35: 50S ribosomal protein L15



• Molecule 36: 50S ribosomal protein L16

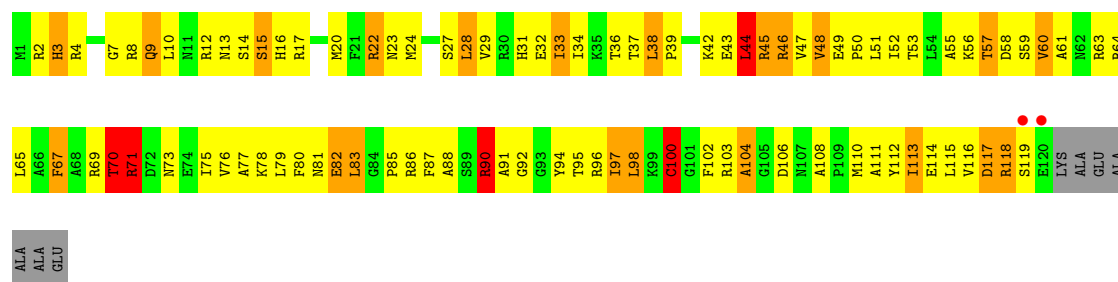


• Molecule 36: 50S ribosomal protein L16

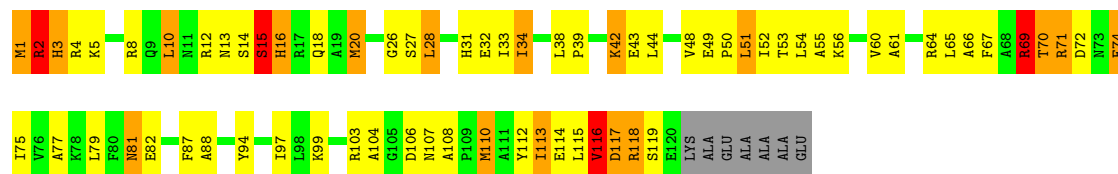




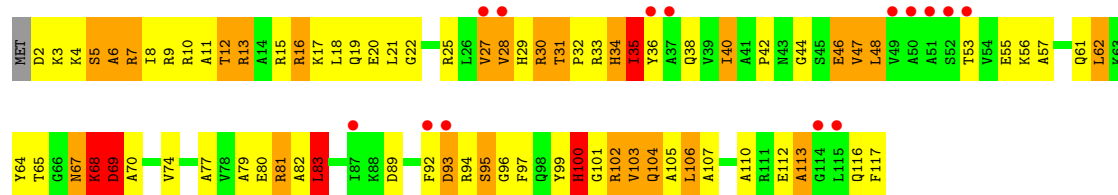
• Molecule 37: 50S ribosomal protein L17



• Molecule 37: 50S ribosomal protein L17



• Molecule 38: 50S ribosomal protein L18

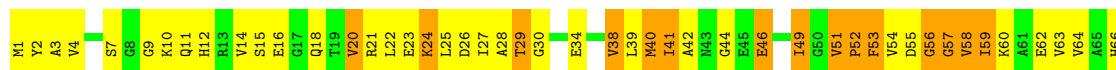






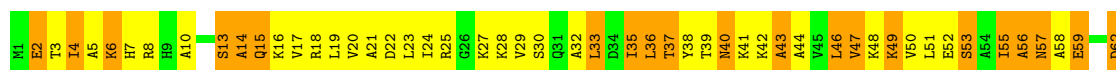
- Molecule 41: 50S ribosomal protein L21

Chain DR: 31% 49% 20%



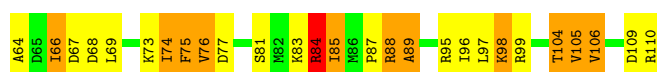
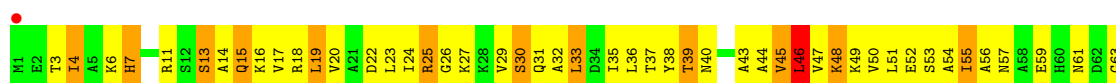
- Molecule 42: 50S ribosomal protein L22

Chain BS: 3% 22% 46% 32%



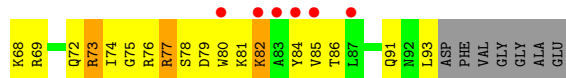
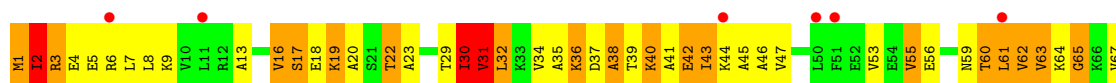
- Molecule 42: 50S ribosomal protein L22

Chain DS: 32% 45% 21%



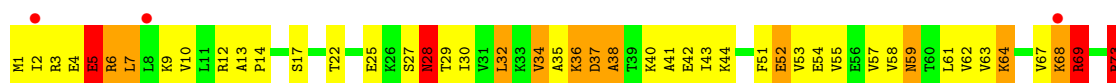
- Molecule 43: 50S ribosomal protein L23

Chain BT: 12% 29% 40% 21% 7%



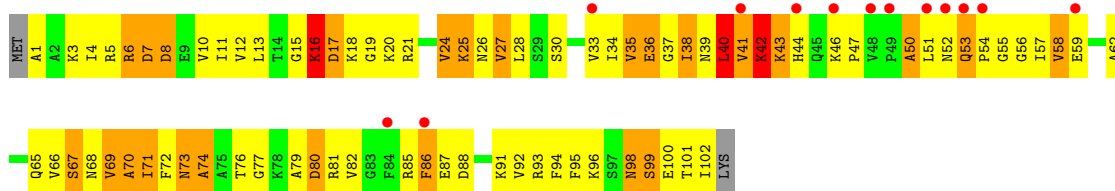
- Molecule 43: 50S ribosomal protein L23

Chain DT: 3% 34% 42% 13% 7%

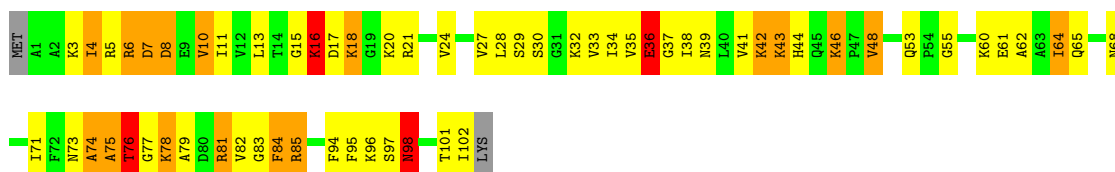




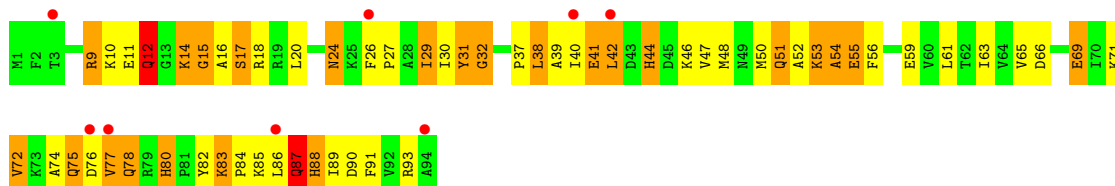
• Molecule 44: 50S ribosomal protein L24



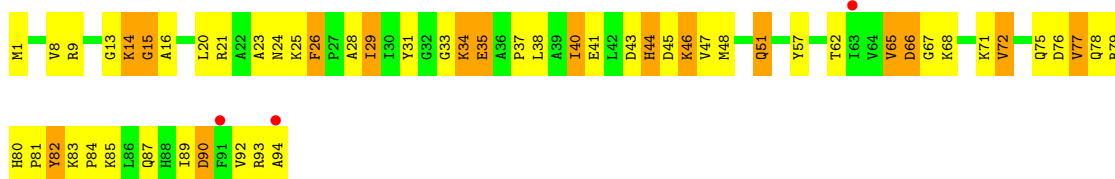
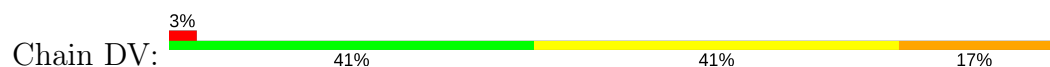
• Molecule 44: 50S ribosomal protein L24



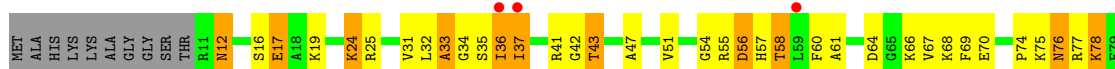
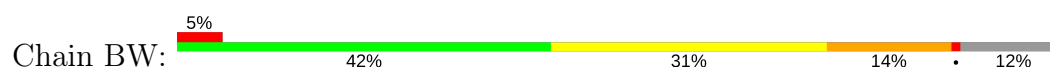
• Molecule 45: 50S ribosomal protein L25

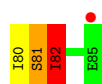


• Molecule 45: 50S ribosomal protein L25



• Molecule 46: 50S ribosomal protein L27





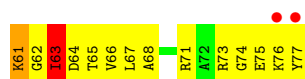
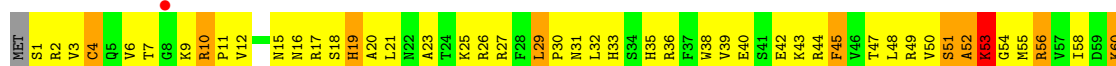
- Molecule 46: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L28



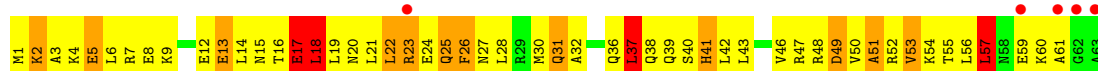
- Molecule 47: 50S ribosomal protein L28



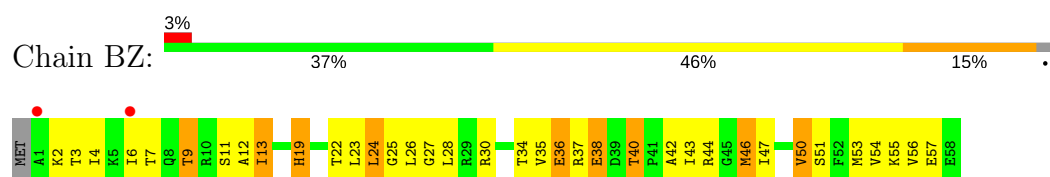
- Molecule 48: 50S ribosomal protein L29



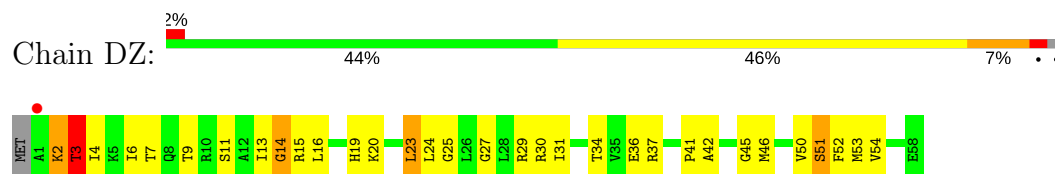
- Molecule 48: 50S ribosomal protein L29



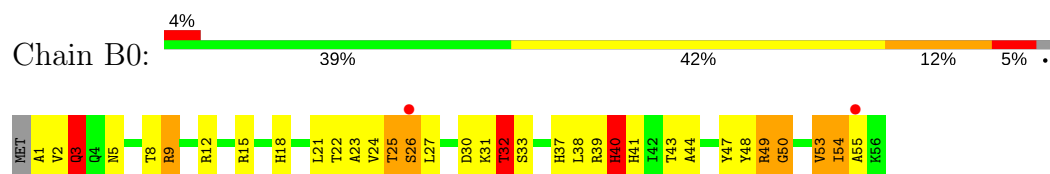
- Molecule 49: 50S ribosomal protein L30



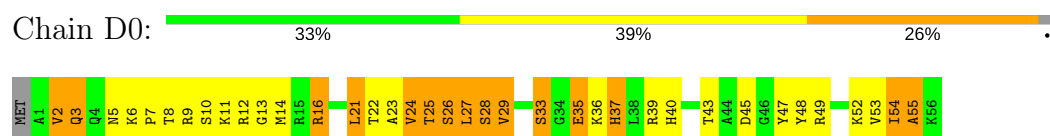
- Molecule 49: 50S ribosomal protein L30



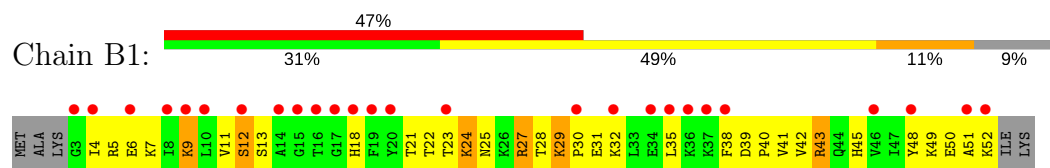
- Molecule 50: 50S ribosomal protein L32



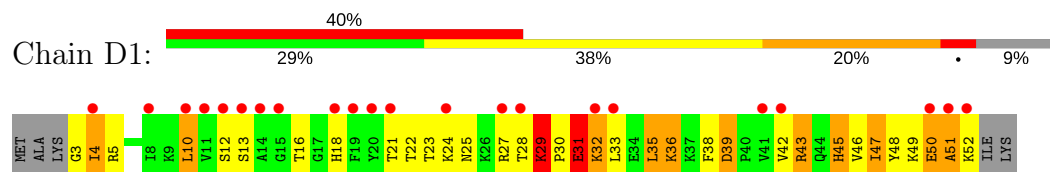
- Molecule 50: 50S ribosomal protein L32



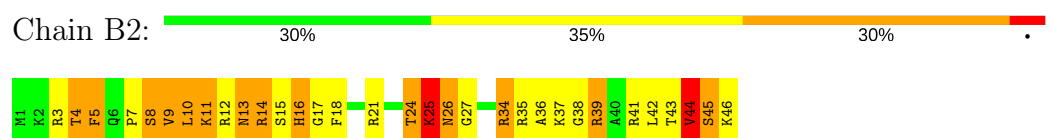
- Molecule 51: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L33

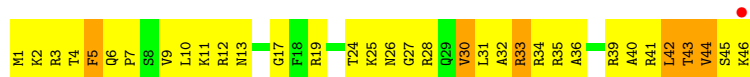


- Molecule 52: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L34





- Molecule 53: 50S ribosomal protein L35



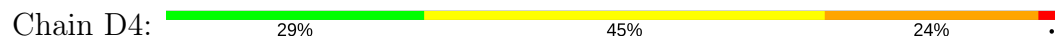
- Molecule 53: 50S ribosomal protein L35



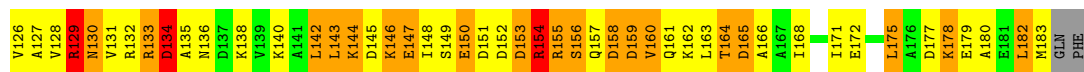
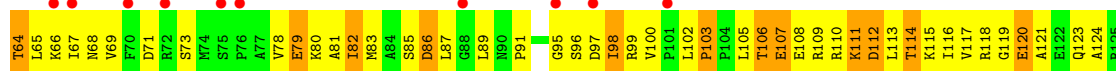
- Molecule 54: 50S ribosomal protein L36



- Molecule 54: 50S ribosomal protein L36



- Molecule 55: Ribosome recycling factor, RRF



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.18Å 433.90Å 608.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.30 69.81 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.30) 94.9 (69.81-3.30)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.206 , 0.255 0.202 , 0.251	Depositor DCC
$R_{free}$ test set	1981 reflections (0.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.3	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 110.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	293103	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, NMY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.34	0/36966	0.95	39/57666 (0.1%)
1	CA	0.33	0/36944	0.93	15/57632 (0.0%)
2	AB	0.28	0/1735	0.61	0/2338
2	CB	0.26	0/1735	0.57	0/2338
3	AC	0.29	0/1651	0.61	0/2225
3	CC	0.30	0/1651	0.58	0/2225
4	AD	0.35	0/1665	0.69	0/2227
4	CD	0.29	0/1665	0.65	0/2227
5	AE	0.28	0/1118	0.66	0/1504
5	CE	0.30	0/1118	0.63	0/1504
6	AF	0.33	0/835	0.67	0/1128
6	CF	0.32	0/835	0.62	0/1128
7	AG	0.25	0/1195	0.52	0/1602
7	CG	0.27	0/1195	0.56	0/1602
8	AH	0.30	0/989	0.66	0/1326
8	CH	0.29	0/989	0.60	0/1326
9	AI	0.25	0/1034	0.59	0/1375
9	CI	0.27	0/1034	0.58	0/1375
10	AJ	0.26	0/796	0.60	0/1077
10	CJ	0.24	0/796	0.53	0/1077
11	AK	0.33	0/893	0.68	0/1205
11	CK	0.30	0/893	0.63	0/1205
12	AL	0.30	0/969	0.71	0/1300
12	CL	0.35	0/969	0.71	1/1300 (0.1%)
13	AM	0.25	0/892	0.57	0/1193
13	CM	0.26	0/892	0.64	0/1193
14	AN	0.26	0/785	0.55	0/1043
14	CN	0.25	0/785	0.56	0/1043
15	AO	0.35	0/722	0.58	0/964
15	CO	0.27	0/722	0.60	0/964
16	AP	0.32	0/659	0.74	2/884 (0.2%)
16	CP	0.29	0/659	0.63	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.28	0/657	0.61	0/881
17	CQ	0.34	0/657	0.71	0/881
18	AR	0.31	0/462	0.69	0/621
18	CR	0.30	0/462	0.60	0/621
19	AS	0.26	0/652	0.57	0/877
19	CS	0.27	0/652	0.65	0/877
20	AT	0.27	0/671	0.59	0/888
20	CT	0.25	0/671	0.58	0/888
21	AU	0.37	0/430	0.76	0/570
21	CU	0.30	0/430	0.61	0/570
22	AV	0.40	1/1813 (0.1%)	0.89	0/2823
22	CV	0.32	1/1813 (0.1%)	0.77	0/2823
23	AX	0.32	0/388	0.88	0/603
23	CX	0.28	0/363	0.85	0/564
24	BA	0.36	0/69659	0.97	72/108672 (0.1%)
24	DA	0.43	3/69659 (0.0%)	1.07	120/108672 (0.1%)
25	BB	0.28	0/2828	0.84	0/4410
25	DB	0.36	0/2850	0.96	2/4444 (0.0%)
26	BC	0.29	0/2121	0.67	0/2852
26	DC	0.34	0/2121	0.75	2/2852 (0.1%)
27	BD	0.31	0/1586	0.66	0/2134
27	DD	0.36	0/1586	0.68	0/2134
28	BE	0.29	0/1571	0.59	0/2113
28	DE	0.32	0/1571	0.67	1/2113 (0.0%)
29	BF	0.26	0/1434	0.53	0/1926
29	DF	0.29	0/1434	0.66	0/1926
30	BG	0.27	0/1343	0.57	0/1816
30	DG	0.31	0/1343	0.67	1/1816 (0.1%)
31	BH	0.31	0/1121	0.57	1/1515 (0.1%)
31	DH	0.34	1/1121 (0.1%)	0.60	1/1515 (0.1%)
32	BI	0.23	0/1046	0.47	0/1410
32	DI	0.24	0/1046	0.56	0/1410
33	BJ	0.32	0/1152	0.66	0/1551
33	DJ	0.35	0/1152	0.67	0/1551
34	BK	0.32	0/947	0.68	0/1268
34	DK	0.37	0/947	0.71	0/1268
35	BL	0.29	0/1054	0.66	0/1403
35	DL	0.33	0/1054	0.73	0/1403
36	BM	0.28	0/1093	0.61	0/1460
36	DM	0.36	0/1093	0.77	2/1460 (0.1%)
37	BN	0.28	0/973	0.63	0/1301
37	DN	0.36	0/973	0.70	0/1301
38	BO	0.27	0/902	0.55	0/1209

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DO	0.33	0/902	0.62	0/1209
39	BP	0.33	0/929	0.67	0/1242
39	DP	0.37	0/929	0.74	1/1242 (0.1%)
40	BQ	0.32	0/960	0.60	0/1278
40	DQ	0.34	0/960	0.69	0/1278
41	BR	0.32	0/829	0.66	0/1107
41	DR	0.38	0/829	0.75	0/1107
42	BS	0.31	0/864	0.69	0/1156
42	DS	0.35	0/864	0.70	0/1156
43	BT	0.30	0/744	0.63	1/994 (0.1%)
43	DT	0.34	0/744	0.70	2/994 (0.2%)
44	BU	0.29	0/787	0.59	0/1051
44	DU	0.32	0/787	0.68	0/1051
45	BV	0.26	0/766	0.57	0/1025
45	DV	0.32	0/766	0.68	0/1025
46	BW	0.30	0/576	0.58	0/762
46	DW	0.35	0/587	0.72	0/776
47	BX	0.33	0/635	0.65	0/848
47	DX	0.32	0/635	0.65	0/848
48	BY	0.25	0/510	0.59	0/677
48	DY	0.28	0/510	0.70	0/677
49	BZ	0.29	0/453	0.59	0/605
49	DZ	0.29	0/453	0.73	0/605
50	B0	0.29	0/450	0.62	0/599
50	D0	0.32	0/450	0.67	0/599
51	B1	0.33	0/416	0.57	0/554
51	D1	0.29	0/416	0.63	0/554
52	B2	0.28	0/380	0.58	0/498
52	D2	0.31	0/380	0.67	0/498
53	B3	0.29	0/513	0.63	0/676
53	D3	0.33	0/513	0.71	0/676
54	B4	0.31	0/303	0.62	0/397
54	D4	0.34	0/303	0.75	0/397
55	CY	0.28	0/1434	0.66	1/1929 (0.1%)
All	All	0.36	6/315264 (0.0%)	0.91	264/471562 (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

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	CB	0	1
3	CC	0	1
4	CD	0	2
5	AE	0	1
8	AH	0	3
9	CI	0	1
12	AL	0	1
13	CM	0	1
16	AP	0	1
16	CP	0	1
26	BC	0	1
26	DC	0	3
27	BD	0	1
27	DD	0	1
31	BH	0	1
31	DH	0	2
33	DJ	0	1
37	BN	0	1
37	DN	0	1
39	DP	0	1
42	DS	0	1
50	D0	0	1
All	All	0	29

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CV	1	G	OP3-P	-10.55	1.48	1.61
22	AV	1	G	OP3-P	-10.36	1.48	1.61
24	DA	2204	G	N9-C8	7.67	1.43	1.37
24	DA	733	G	N3-C4	-5.30	1.31	1.35
31	DH	118	PRO	N-CD	5.25	1.55	1.47

The worst 5 of 264 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	DA	2204	G	C8-N9-C4	-13.18	101.13	106.40
24	DA	733	G	N3-C4-N9	-11.80	118.92	126.00
24	DA	733	G	C6-C5-N7	10.61	136.76	130.40
24	DA	733	G	N9-C4-C5	10.19	109.47	105.40
1	AA	890	G	O4'-C1'-N9	9.65	115.92	108.20

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	162	PHE	Peptide
5	AE	157	ARG	Peptide
8	AH	125	ILE	Peptide
8	AH	87	LYS	Peptide
8	AH	88	ARG	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	33015	0	16617	2761	0
1	CA	32995	0	16607	2603	2
2	AB	1704	0	1732	275	0
2	CB	1704	0	1732	227	0
3	AC	1624	0	1696	188	0
3	CC	1624	0	1696	185	0
4	AD	1643	0	1707	369	0
4	CD	1643	0	1707	356	0
5	AE	1105	0	1148	164	0
5	CE	1105	0	1148	126	0
6	AF	817	0	808	119	0
6	CF	817	0	808	113	0
7	AG	1181	0	1238	102	0
7	CG	1181	0	1238	150	0
8	AH	979	0	1031	209	0
8	CH	979	0	1031	127	0
9	AI	1022	0	1070	143	0
9	CI	1022	0	1070	161	0
10	AJ	786	0	828	71	0
10	CJ	786	0	828	89	0
11	AK	877	0	887	145	0
11	CK	877	0	887	203	0
12	AL	955	0	1016	153	0
12	CL	955	0	1016	179	0
13	AM	883	0	941	137	0
13	CM	883	0	941	173	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	AN	774	0	827	114	0
14	CN	774	0	827	142	0
15	AO	714	0	734	72	0
15	CO	714	0	734	128	0
16	AP	649	0	666	101	0
16	CP	649	0	666	96	0
17	AQ	648	0	691	78	0
17	CQ	648	0	691	97	0
18	AR	455	0	478	67	0
18	CR	455	0	478	65	0
19	AS	637	0	665	116	0
19	CS	637	0	665	130	0
20	AT	665	0	714	125	0
20	CT	665	0	714	103	0
21	AU	425	0	449	95	0
21	CU	425	0	449	88	0
22	AV	1623	0	821	70	0
22	CV	1623	0	821	171	0
23	AX	346	0	173	39	0
23	CX	324	0	162	15	0
24	BA	62195	0	31280	4102	1
24	DA	62195	0	31280	3371	1
25	BB	2529	0	1281	202	0
25	DB	2549	0	1291	111	0
26	BC	2082	0	2157	284	0
26	DC	2082	0	2157	277	0
27	BD	1565	0	1616	178	0
27	DD	1565	0	1616	153	0
28	BE	1552	0	1619	176	0
28	DE	1552	0	1619	153	0
29	BF	1410	0	1447	208	0
29	DF	1410	0	1447	252	0
30	BG	1323	0	1374	137	0
30	DG	1323	0	1374	105	0
31	BH	1110	0	1148	131	1
31	DH	1110	0	1148	237	0
32	BI	1032	0	1088	42	0
32	DI	1032	0	1088	87	0
33	BJ	1129	0	1162	133	0
33	DJ	1129	0	1162	105	0
34	BK	938	0	1012	122	0
34	DK	938	0	1012	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	BL	1045	0	1117	138	0
35	DL	1045	0	1117	115	0
36	BM	1074	0	1157	117	0
36	DM	1074	0	1157	116	0
37	BN	960	0	1000	133	0
37	DN	960	0	1000	98	0
38	BO	892	0	923	147	0
38	DO	892	0	923	123	0
39	BP	917	0	965	102	0
39	DP	917	0	965	72	0
40	BQ	947	0	1022	96	0
40	DQ	947	0	1022	128	0
41	BR	816	0	839	82	0
41	DR	816	0	839	121	0
42	BS	857	0	922	116	0
42	DS	857	0	922	89	0
43	BT	738	0	807	89	0
43	DT	738	0	807	74	0
44	BU	779	0	834	108	0
44	DU	779	0	834	106	0
45	BV	753	0	780	77	0
45	DV	753	0	780	63	1
46	BW	569	0	581	55	0
46	DW	580	0	594	78	0
47	BX	625	0	655	76	0
47	DX	625	0	655	82	0
48	BY	509	0	543	59	0
48	DY	509	0	543	75	0
49	BZ	449	0	491	53	0
49	DZ	449	0	491	32	0
50	B0	444	0	461	43	0
50	D0	444	0	461	39	0
51	B1	409	0	440	50	0
51	D1	409	0	440	38	0
52	B2	377	0	418	52	0
52	D2	377	0	418	40	0
53	B3	504	0	574	66	0
53	D3	504	0	574	69	0
54	B4	302	0	340	33	0
54	D4	302	0	340	39	0
55	CY	1423	0	1476	166	0
56	AA	54	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AD	1	0	0	0	0
56	AN	1	0	0	0	0
56	BA	163	0	0	0	0
56	BB	3	0	0	0	0
56	BC	1	0	0	0	0
56	BQ	1	0	0	0	0
56	CA	71	0	0	0	0
56	CX	1	0	0	0	0
56	DA	187	0	0	0	0
56	DB	4	0	0	0	0
56	DE	1	0	0	0	0
56	DL	1	0	0	0	0
56	DO	1	0	0	0	0
57	AA	126	0	135	48	0
57	BA	294	0	317	87	0
57	CA	42	0	46	6	0
57	DA	294	0	311	107	0
58	B4	1	0	0	0	0
58	D4	1	0	0	0	0
59	AA	188	0	0	29	0
59	AD	2	0	0	2	0
59	AK	1	0	0	1	0
59	AN	4	0	0	1	0
59	AT	2	0	0	0	0
59	AU	1	0	0	0	0
59	B0	1	0	0	0	0
59	B3	1	0	0	0	0
59	B4	1	0	0	0	0
59	BA	616	0	0	116	0
59	BB	13	0	0	2	0
59	BC	10	0	0	6	0
59	BD	4	0	0	0	0
59	BL	4	0	0	2	0
59	BN	1	0	0	0	0
59	BT	3	0	0	2	0
59	BU	3	0	0	0	0
59	BV	1	0	0	0	0
59	CA	192	0	0	32	0
59	CC	1	0	0	1	0
59	CE	1	0	0	0	0
59	CL	1	0	0	1	0
59	CN	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	CT	2	0	0	1	0
59	D3	2	0	0	0	0
59	D4	1	0	0	0	0
59	DA	627	0	0	120	0
59	DB	13	0	0	4	0
59	DC	4	0	0	0	0
59	DD	2	0	0	1	0
59	DE	4	0	0	2	0
59	DF	1	0	0	0	0
59	DL	7	0	0	4	0
59	DN	2	0	0	0	0
59	DQ	1	0	0	0	0
59	DS	1	0	0	0	0
59	DT	1	0	0	0	0
59	DU	1	0	0	0	0
59	DV	1	0	0	0	0
All	All	293103	0	196267	22971	3

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 48.

The worst 5 of 22971 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BF:96:TRP:CE3	29:BF:99:PHE:CE2	1.79	1.66
29:BF:96:TRP:CZ3	29:BF:99:PHE:HE2	1.31	1.48
31:BH:121:VAL:HB	31:BH:122:LEU:CD2	1.41	1.47
29:BF:96:TRP:CD2	29:BF:99:PHE:CZ	2.03	1.47
31:BH:121:VAL:CB	31:BH:122:LEU:HD23	1.49	1.42

All (3) 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)
31:BH:123:ARG:NH2	1:CA:358:U:OP1[4_555]	2.07	0.13
24:BA:2152:G:N2	1:CA:416:G:OP1[4_555]	2.15	0.05
24:DA:544:C:OP2	45:DV:34:LYS:NZ[4_545]	2.16	0.04

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/241 (90%)	106 (49%)	51 (24%)	59 (27%)	0	0
2	CB	216/241 (90%)	110 (51%)	51 (24%)	55 (26%)	0	0
3	AC	204/233 (88%)	124 (61%)	46 (22%)	34 (17%)	0	1
3	CC	204/233 (88%)	122 (60%)	48 (24%)	34 (17%)	0	1
4	AD	203/206 (98%)	100 (49%)	48 (24%)	55 (27%)	0	0
4	CD	203/206 (98%)	92 (45%)	49 (24%)	62 (30%)	0	0
5	AE	148/167 (89%)	86 (58%)	30 (20%)	32 (22%)	0	0
5	CE	148/167 (89%)	106 (72%)	22 (15%)	20 (14%)	0	2
6	AF	98/135 (73%)	53 (54%)	27 (28%)	18 (18%)	0	1
6	CF	98/135 (73%)	47 (48%)	22 (22%)	29 (30%)	0	0
7	AG	149/179 (83%)	92 (62%)	33 (22%)	24 (16%)	0	1
7	CG	149/179 (83%)	65 (44%)	46 (31%)	38 (26%)	0	0
8	AH	127/130 (98%)	62 (49%)	37 (29%)	28 (22%)	0	0
8	CH	127/130 (98%)	80 (63%)	28 (22%)	19 (15%)	0	1
9	AI	125/130 (96%)	60 (48%)	36 (29%)	29 (23%)	0	0
9	CI	125/130 (96%)	61 (49%)	36 (29%)	28 (22%)	0	0
10	AJ	96/103 (93%)	62 (65%)	22 (23%)	12 (12%)	0	2
10	CJ	96/103 (93%)	55 (57%)	21 (22%)	20 (21%)	0	0
11	AK	115/129 (89%)	76 (66%)	19 (16%)	20 (17%)	0	1
11	CK	115/129 (89%)	52 (45%)	40 (35%)	23 (20%)	0	1
12	AL	121/124 (98%)	58 (48%)	28 (23%)	35 (29%)	0	0
12	CL	121/124 (98%)	72 (60%)	26 (22%)	23 (19%)	0	1
13	AM	112/118 (95%)	65 (58%)	19 (17%)	28 (25%)	0	0
13	CM	112/118 (95%)	55 (49%)	22 (20%)	35 (31%)	0	0
14	AN	92/101 (91%)	50 (54%)	21 (23%)	21 (23%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	92/101 (91%)	64 (70%)	11 (12%)	17 (18%)	0	1
15	AO	86/89 (97%)	52 (60%)	20 (23%)	14 (16%)	0	1
15	CO	86/89 (97%)	42 (49%)	23 (27%)	21 (24%)	0	0
16	AP	80/82 (98%)	35 (44%)	27 (34%)	18 (22%)	0	0
16	CP	80/82 (98%)	39 (49%)	23 (29%)	18 (22%)	0	0
17	AQ	78/84 (93%)	40 (51%)	20 (26%)	18 (23%)	0	0
17	CQ	78/84 (93%)	51 (65%)	12 (15%)	15 (19%)	0	1
18	AR	53/75 (71%)	31 (58%)	8 (15%)	14 (26%)	0	0
18	CR	53/75 (71%)	28 (53%)	12 (23%)	13 (24%)	0	0
19	AS	77/92 (84%)	43 (56%)	23 (30%)	11 (14%)	0	1
19	CS	77/92 (84%)	35 (46%)	23 (30%)	19 (25%)	0	0
20	AT	83/87 (95%)	45 (54%)	23 (28%)	15 (18%)	0	1
20	CT	83/87 (95%)	42 (51%)	22 (26%)	19 (23%)	0	0
21	AU	49/71 (69%)	18 (37%)	16 (33%)	15 (31%)	0	0
21	CU	49/71 (69%)	23 (47%)	14 (29%)	12 (24%)	0	0
26	BC	269/273 (98%)	171 (64%)	48 (18%)	50 (19%)	0	1
26	DC	269/273 (98%)	187 (70%)	51 (19%)	31 (12%)	0	3
27	BD	207/209 (99%)	159 (77%)	29 (14%)	19 (9%)	1	5
27	DD	207/209 (99%)	159 (77%)	33 (16%)	15 (7%)	1	10
28	BE	199/201 (99%)	126 (63%)	49 (25%)	24 (12%)	0	2
28	DE	199/201 (99%)	131 (66%)	53 (27%)	15 (8%)	1	9
29	BF	175/179 (98%)	104 (59%)	44 (25%)	27 (15%)	0	1
29	DF	175/179 (98%)	96 (55%)	39 (22%)	40 (23%)	0	0
30	BG	174/177 (98%)	107 (62%)	43 (25%)	24 (14%)	0	2
30	DG	174/177 (98%)	127 (73%)	27 (16%)	20 (12%)	0	3
31	BH	147/149 (99%)	82 (56%)	39 (26%)	26 (18%)	0	1
31	DH	147/149 (99%)	67 (46%)	37 (25%)	43 (29%)	0	0
32	BI	139/142 (98%)	77 (55%)	45 (32%)	17 (12%)	0	2
32	DI	139/142 (98%)	65 (47%)	39 (28%)	35 (25%)	0	0
33	BJ	140/142 (99%)	108 (77%)	19 (14%)	13 (9%)	1	5
33	DJ	140/142 (99%)	110 (79%)	25 (18%)	5 (4%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BK	120/123 (98%)	77 (64%)	29 (24%)	14 (12%)	0	3
34	DK	120/123 (98%)	95 (79%)	18 (15%)	7 (6%)	2	14
35	BL	141/144 (98%)	84 (60%)	35 (25%)	22 (16%)	0	1
35	DL	141/144 (98%)	98 (70%)	29 (21%)	14 (10%)	1	4
36	BM	134/136 (98%)	94 (70%)	27 (20%)	13 (10%)	1	5
36	DM	134/136 (98%)	94 (70%)	28 (21%)	12 (9%)	1	6
37	BN	118/127 (93%)	72 (61%)	30 (25%)	16 (14%)	0	2
37	DN	118/127 (93%)	84 (71%)	22 (19%)	12 (10%)	1	4
38	BO	114/117 (97%)	65 (57%)	30 (26%)	19 (17%)	0	1
38	DO	114/117 (97%)	64 (56%)	25 (22%)	25 (22%)	0	0
39	BP	112/115 (97%)	80 (71%)	18 (16%)	14 (12%)	0	2
39	DP	112/115 (97%)	92 (82%)	12 (11%)	8 (7%)	1	10
40	BQ	115/118 (98%)	98 (85%)	13 (11%)	4 (4%)	4	26
40	DQ	115/118 (98%)	89 (77%)	16 (14%)	10 (9%)	1	6
41	BR	101/103 (98%)	76 (75%)	18 (18%)	7 (7%)	1	10
41	DR	101/103 (98%)	67 (66%)	23 (23%)	11 (11%)	0	3
42	BS	108/110 (98%)	68 (63%)	22 (20%)	18 (17%)	0	1
42	DS	108/110 (98%)	77 (71%)	21 (19%)	10 (9%)	1	5
43	BT	91/100 (91%)	54 (59%)	26 (29%)	11 (12%)	0	2
43	DT	91/100 (91%)	60 (66%)	18 (20%)	13 (14%)	0	1
44	BU	100/104 (96%)	55 (55%)	21 (21%)	24 (24%)	0	0
44	DU	100/104 (96%)	73 (73%)	12 (12%)	15 (15%)	0	1
45	BV	92/94 (98%)	50 (54%)	26 (28%)	16 (17%)	0	1
45	DV	92/94 (98%)	79 (86%)	4 (4%)	9 (10%)	1	4
46	BW	73/85 (86%)	56 (77%)	9 (12%)	8 (11%)	0	3
46	DW	74/85 (87%)	51 (69%)	14 (19%)	9 (12%)	0	2
47	BX	75/78 (96%)	55 (73%)	10 (13%)	10 (13%)	0	2
47	DX	75/78 (96%)	51 (68%)	14 (19%)	10 (13%)	0	2
48	BY	61/63 (97%)	38 (62%)	17 (28%)	6 (10%)	1	4
48	DY	61/63 (97%)	31 (51%)	19 (31%)	11 (18%)	0	1
49	BZ	56/59 (95%)	42 (75%)	12 (21%)	2 (4%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	DZ	56/59 (95%)	37 (66%)	16 (29%)	3 (5%)	2	15
50	B0	54/57 (95%)	34 (63%)	9 (17%)	11 (20%)	0	1
50	D0	54/57 (95%)	36 (67%)	10 (18%)	8 (15%)	0	1
51	B1	48/55 (87%)	29 (60%)	15 (31%)	4 (8%)	1	7
51	D1	48/55 (87%)	28 (58%)	10 (21%)	10 (21%)	0	0
52	B2	44/46 (96%)	29 (66%)	8 (18%)	7 (16%)	0	1
52	D2	44/46 (96%)	31 (70%)	10 (23%)	3 (7%)	1	10
53	B3	62/65 (95%)	47 (76%)	9 (14%)	6 (10%)	1	5
53	D3	62/65 (95%)	47 (76%)	7 (11%)	8 (13%)	0	2
54	B4	36/38 (95%)	27 (75%)	7 (19%)	2 (6%)	2	14
54	D4	36/38 (95%)	26 (72%)	7 (19%)	3 (8%)	1	7
55	CY	181/185 (98%)	99 (55%)	52 (29%)	30 (17%)	0	1
All	All	11416/12155 (94%)	7014 (61%)	2503 (22%)	1899 (17%)	0	1

5 of 1899 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	11	LYS
2	AB	16	PHE
2	AB	23	TRP
2	AB	58	ASN
2	AB	64	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%)	128 (71%)	52 (29%)	0	1
2	CB	180/199 (90%)	137 (76%)	43 (24%)	1	3
3	AC	170/190 (90%)	138 (81%)	32 (19%)	2	8
3	CC	170/190 (90%)	130 (76%)	40 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	172/173 (99%)	116 (67%)	56 (33%)	0	1
4	CD	172/173 (99%)	125 (73%)	47 (27%)	0	2
5	AE	113/126 (90%)	91 (80%)	22 (20%)	1	7
5	CE	113/126 (90%)	94 (83%)	19 (17%)	2	12
6	AF	87/116 (75%)	72 (83%)	15 (17%)	2	11
6	CF	87/116 (75%)	65 (75%)	22 (25%)	0	2
7	AG	124/147 (84%)	96 (77%)	28 (23%)	1	4
7	CG	124/147 (84%)	101 (82%)	23 (18%)	2	8
8	AH	104/105 (99%)	81 (78%)	23 (22%)	1	4
8	CH	104/105 (99%)	87 (84%)	17 (16%)	3	13
9	AI	105/107 (98%)	81 (77%)	24 (23%)	1	4
9	CI	105/107 (98%)	84 (80%)	21 (20%)	1	6
10	AJ	86/90 (96%)	73 (85%)	13 (15%)	3	16
10	CJ	86/90 (96%)	67 (78%)	19 (22%)	1	4
11	AK	90/99 (91%)	74 (82%)	16 (18%)	2	10
11	CK	90/99 (91%)	67 (74%)	23 (26%)	0	2
12	AL	103/104 (99%)	69 (67%)	34 (33%)	0	1
12	CL	103/104 (99%)	77 (75%)	26 (25%)	0	2
13	AM	92/96 (96%)	77 (84%)	15 (16%)	3	13
13	CM	92/96 (96%)	63 (68%)	29 (32%)	0	1
14	AN	79/84 (94%)	64 (81%)	15 (19%)	2	8
14	CN	79/84 (94%)	60 (76%)	19 (24%)	1	3
15	AO	76/77 (99%)	55 (72%)	21 (28%)	0	2
15	CO	76/77 (99%)	57 (75%)	19 (25%)	1	2
16	AP	65/65 (100%)	51 (78%)	14 (22%)	1	5
16	CP	65/65 (100%)	41 (63%)	24 (37%)	0	0
17	AQ	74/78 (95%)	59 (80%)	15 (20%)	1	6
17	CQ	74/78 (95%)	54 (73%)	20 (27%)	0	2
18	AR	48/65 (74%)	36 (75%)	12 (25%)	1	2
18	CR	48/65 (74%)	36 (75%)	12 (25%)	1	2
19	AS	70/79 (89%)	53 (76%)	17 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	CS	70/79 (89%)	53 (76%)	17 (24%)	1	3
20	AT	65/66 (98%)	50 (77%)	15 (23%)	1	4
20	CT	65/66 (98%)	50 (77%)	15 (23%)	1	4
21	AU	44/61 (72%)	30 (68%)	14 (32%)	0	1
21	CU	44/61 (72%)	29 (66%)	15 (34%)	0	1
26	BC	216/218 (99%)	164 (76%)	52 (24%)	1	3
26	DC	216/218 (99%)	147 (68%)	69 (32%)	0	1
27	BD	164/164 (100%)	131 (80%)	33 (20%)	1	6
27	DD	164/164 (100%)	125 (76%)	39 (24%)	1	3
28	BE	165/165 (100%)	133 (81%)	32 (19%)	1	7
28	DE	165/165 (100%)	130 (79%)	35 (21%)	1	5
29	BF	148/150 (99%)	115 (78%)	33 (22%)	1	4
29	DF	148/150 (99%)	114 (77%)	34 (23%)	1	4
30	BG	137/138 (99%)	108 (79%)	29 (21%)	1	5
30	DG	137/138 (99%)	111 (81%)	26 (19%)	2	8
31	BH	114/114 (100%)	83 (73%)	31 (27%)	0	2
31	DH	114/114 (100%)	92 (81%)	22 (19%)	1	7
32	BI	109/110 (99%)	101 (93%)	8 (7%)	16	49
32	DI	109/110 (99%)	89 (82%)	20 (18%)	2	9
33	BJ	116/116 (100%)	90 (78%)	26 (22%)	1	4
33	DJ	116/116 (100%)	95 (82%)	21 (18%)	2	9
34	BK	103/104 (99%)	81 (79%)	22 (21%)	1	5
34	DK	103/104 (99%)	77 (75%)	26 (25%)	0	2
35	BL	102/103 (99%)	76 (74%)	26 (26%)	0	2
35	DL	102/103 (99%)	74 (72%)	28 (28%)	0	2
36	BM	109/109 (100%)	80 (73%)	29 (27%)	0	2
36	DM	109/109 (100%)	86 (79%)	23 (21%)	1	5
37	BN	100/103 (97%)	81 (81%)	19 (19%)	2	8
37	DN	100/103 (97%)	83 (83%)	17 (17%)	2	11
38	BO	86/87 (99%)	67 (78%)	19 (22%)	1	4
38	DO	86/87 (99%)	61 (71%)	25 (29%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	BP	99/100 (99%)	81 (82%)	18 (18%)	2	9
39	DP	99/100 (99%)	80 (81%)	19 (19%)	1	7
40	BQ	89/90 (99%)	66 (74%)	23 (26%)	0	2
40	DQ	89/90 (99%)	69 (78%)	20 (22%)	1	4
41	BR	84/84 (100%)	66 (79%)	18 (21%)	1	5
41	DR	84/84 (100%)	70 (83%)	14 (17%)	2	12
42	BS	93/93 (100%)	70 (75%)	23 (25%)	1	2
42	DS	93/93 (100%)	68 (73%)	25 (27%)	0	2
43	BT	80/84 (95%)	57 (71%)	23 (29%)	0	1
43	DT	80/84 (95%)	62 (78%)	18 (22%)	1	4
44	BU	83/85 (98%)	61 (74%)	22 (26%)	0	2
44	DU	83/85 (98%)	63 (76%)	20 (24%)	1	3
45	BV	78/78 (100%)	60 (77%)	18 (23%)	1	4
45	DV	78/78 (100%)	63 (81%)	15 (19%)	1	7
46	BW	56/63 (89%)	45 (80%)	11 (20%)	1	7
46	DW	57/63 (90%)	48 (84%)	9 (16%)	3	14
47	BX	67/68 (98%)	47 (70%)	20 (30%)	0	1
47	DX	67/68 (98%)	56 (84%)	11 (16%)	2	13
48	BY	55/55 (100%)	47 (86%)	8 (14%)	4	18
48	DY	55/55 (100%)	43 (78%)	12 (22%)	1	5
49	BZ	48/49 (98%)	40 (83%)	8 (17%)	2	12
49	DZ	48/49 (98%)	42 (88%)	6 (12%)	5	24
50	B0	47/48 (98%)	39 (83%)	8 (17%)	2	11
50	D0	47/48 (98%)	38 (81%)	9 (19%)	2	7
51	B1	45/49 (92%)	39 (87%)	6 (13%)	4	21
51	D1	45/49 (92%)	36 (80%)	9 (20%)	1	6
52	B2	38/38 (100%)	26 (68%)	12 (32%)	0	1
52	D2	38/38 (100%)	33 (87%)	5 (13%)	5	21
53	B3	51/52 (98%)	37 (72%)	14 (28%)	0	2
53	D3	51/52 (98%)	36 (71%)	15 (29%)	0	1
54	B4	34/34 (100%)	27 (79%)	7 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	D4	34/34 (100%)	23 (68%)	11 (32%)	0	1
55	CY	158/160 (99%)	122 (77%)	36 (23%)	1	4
All	All	9485/9916 (96%)	7325 (77%)	2160 (23%)	1	4

5 of 2160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BX	45	PHE
6	CF	42	TRP
42	DS	4	ILE
50	B0	5	ASN
3	CC	16	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
50	B0	37	HIS
5	CE	121	HIS
40	DQ	43	GLN
51	B1	25	ASN
3	CC	176	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1538/1542 (99%)	503 (32%)	0
1	CA	1537/1542 (99%)	498 (32%)	0
22	AV	75/76 (98%)	19 (25%)	0
22	CV	75/76 (98%)	27 (36%)	0
23	AX	15/24 (62%)	7 (46%)	0
23	CX	14/24 (58%)	6 (42%)	0
24	BA	2895/2904 (99%)	884 (30%)	0
24	DA	2895/2904 (99%)	826 (28%)	0
25	BB	117/120 (97%)	29 (24%)	0
25	DB	118/120 (98%)	24 (20%)	0
All	All	9279/9332 (99%)	2823 (30%)	0

5 of 2823 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	3	A
1	AA	4	U
1	AA	5	U
1	AA	8	A
1	AA	9	G

There are no RNA pucker outliers to report.

## 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, 492 are monoatomic - leaving 18 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	$\# Z  > 2$
57	NMY	AA	1655	-	45,45,45	0.58	0	59,67,67	1.00	4 (6%)
57	NMY	AA	1656	-	45,45,45	2.27	12 (26%)	59,67,67	1.89	20 (33%)
57	NMY	AA	1657	-	45,45,45	2.30	12 (26%)	59,67,67	1.84	17 (28%)
57	NMY	BA	3161	-	45,45,45	0.52	0	59,67,67	1.06	4 (6%)
57	NMY	BA	3162	-	45,45,45	0.52	0	59,67,67	1.08	5 (8%)
57	NMY	BA	3163	-	45,45,45	2.29	10 (22%)	59,67,67	2.37	24 (40%)
57	NMY	BA	3164	-	45,45,45	2.25	11 (24%)	59,67,67	2.40	26 (44%)
57	NMY	BA	3165	-	45,45,45	0.53	0	59,67,67	1.14	5 (8%)
57	NMY	BA	3166	-	45,45,45	2.17	10 (22%)	59,67,67	2.30	16 (27%)
57	NMY	BA	3167	-	45,45,45	2.27	11 (24%)	59,67,67	1.98	14 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	NMY	CA	1672	-	45,45,45	0.55	0	59,67,67	0.94	2 (3%)
57	NMY	DA	3184	-	45,45,45	0.59	0	59,67,67	1.28	5 (8%)
57	NMY	DA	3185	-	45,45,45	2.31	13 (28%)	59,67,67	1.78	16 (27%)
57	NMY	DA	3186	-	45,45,45	2.35	12 (26%)	59,67,67	2.30	15 (25%)
57	NMY	DA	3187	-	45,45,45	2.29	11 (24%)	59,67,67	1.55	14 (23%)
57	NMY	DA	3188	-	45,45,45	2.20	13 (28%)	59,67,67	1.96	21 (35%)
57	NMY	DA	3189	-	45,45,45	2.20	12 (26%)	59,67,67	2.32	23 (38%)
57	NMY	DA	3190	-	45,45,45	2.26	10 (22%)	59,67,67	2.62	26 (44%)

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
57	NMY	AA	1655	-	-	1/18/94/94	0/4/4/4
57	NMY	AA	1656	-	-	0/18/94/94	0/4/4/4
57	NMY	AA	1657	-	-	1/18/94/94	0/4/4/4
57	NMY	BA	3161	-	-	0/18/94/94	0/4/4/4
57	NMY	BA	3162	-	-	0/18/94/94	0/4/4/4
57	NMY	BA	3163	-	-	0/18/94/94	0/4/4/4
57	NMY	BA	3164	-	-	0/18/94/94	0/4/4/4
57	NMY	BA	3165	-	-	0/18/94/94	0/4/4/4
57	NMY	BA	3166	-	-	0/18/94/94	0/4/4/4
57	NMY	BA	3167	-	-	0/18/94/94	0/4/4/4
57	NMY	CA	1672	-	-	0/18/94/94	0/4/4/4
57	NMY	DA	3184	-	-	0/18/94/94	0/4/4/4
57	NMY	DA	3185	-	-	0/18/94/94	0/4/4/4
57	NMY	DA	3186	-	-	0/18/94/94	0/4/4/4
57	NMY	DA	3187	-	-	0/18/94/94	0/4/4/4
57	NMY	DA	3188	-	-	0/18/94/94	0/4/4/4
57	NMY	DA	3189	-	-	0/18/94/94	0/4/4/4
57	NMY	DA	3190	-	-	1/18/94/94	0/4/4/4

The worst 5 of 137 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	DA	3187	NMY	C20-C19	-10.01	1.40	1.53
57	DA	3186	NMY	C20-C19	-9.83	1.41	1.53
57	AA	1657	NMY	C20-C19	-9.81	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	DA	3190	NMY	C20-C19	-9.75	1.41	1.53
57	DA	3185	NMY	C20-C19	-9.70	1.41	1.53

The worst 5 of 257 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	3163	NMY	C1-O1-C10	-6.39	102.42	118.00
57	DA	3190	NMY	C1-O1-C10	-5.75	104.00	118.00
57	DA	3189	NMY	C18-O18-C15	-5.28	105.14	118.00
57	AA	1657	NMY	C18-O18-C15	-5.26	105.18	118.00
57	DA	3186	NMY	O16-C13-C14	-5.16	98.20	104.97

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	AA	1657	NMY	C15-O18-C18-C19
57	DA	3190	NMY	C18-O18-C15-C16
57	AA	1655	NMY	C15-O18-C18-C19

There are no ring outliers.

18 monomers are involved in 248 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	1655	NMY	26	0
57	AA	1656	NMY	12	0
57	AA	1657	NMY	10	0
57	BA	3161	NMY	14	0
57	BA	3162	NMY	16	0
57	BA	3163	NMY	11	0
57	BA	3164	NMY	3	0
57	BA	3165	NMY	25	0
57	BA	3166	NMY	13	0
57	BA	3167	NMY	5	0
57	CA	1672	NMY	6	0
57	DA	3184	NMY	17	0
57	DA	3185	NMY	13	0
57	DA	3186	NMY	19	0
57	DA	3187	NMY	4	0
57	DA	3188	NMY	12	0
57	DA	3189	NMY	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	DA	3190	NMY	32	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	AA	1539/1542 (99%)	-0.49	3 (0%)	94 95	67, 121, 207, 543	0
1	CA	1538/1542 (99%)	-0.50	5 (0%)	93 93	63, 120, 240, 527	0
2	AB	218/241 (90%)	0.70	31 (14%)	3 3	86, 172, 404, 542	0
2	CB	218/241 (90%)	0.62	31 (14%)	3 3	96, 215, 508, 545	0
3	AC	206/233 (88%)	0.47	20 (9%)	8 8	81, 139, 325, 514	0
3	CC	206/233 (88%)	0.25	9 (4%)	35 33	80, 120, 286, 513	0
4	AD	205/206 (99%)	0.64	28 (13%)	3 3	83, 161, 372, 537	0
4	CD	205/206 (99%)	0.40	21 (10%)	7 6	81, 148, 442, 537	0
5	AE	150/167 (89%)	0.01	4 (2%)	55 52	79, 130, 272, 478	0
5	CE	150/167 (89%)	0.29	6 (4%)	39 36	68, 114, 292, 527	0
6	AF	100/135 (74%)	0.04	4 (4%)	39 36	85, 142, 331, 528	0
6	CF	100/135 (74%)	0.50	7 (7%)	17 17	87, 178, 386, 531	0
7	AG	151/179 (84%)	0.21	12 (7%)	13 12	93, 161, 365, 539	0
7	CG	151/179 (84%)	0.79	25 (16%)	2 2	112, 234, 452, 540	0
8	AH	129/130 (99%)	0.26	9 (6%)	17 17	79, 145, 341, 424	0
8	CH	129/130 (99%)	0.54	13 (10%)	8 7	81, 121, 307, 437	0
9	AI	127/130 (97%)	0.50	15 (11%)	5 4	101, 180, 459, 535	0
9	CI	127/130 (97%)	0.93	27 (21%)	1 1	97, 216, 478, 540	0
10	AJ	98/103 (95%)	0.69	12 (12%)	5 4	95, 165, 363, 543	0
10	CJ	98/103 (95%)	1.38	21 (21%)	1 1	101, 202, 530, 543	0
11	AK	117/129 (90%)	0.33	6 (5%)	29 26	75, 112, 337, 492	0
11	CK	117/129 (90%)	1.14	28 (23%)	1 1	83, 243, 494, 531	0
12	AL	123/124 (99%)	0.58	13 (10%)	7 6	75, 109, 299, 403	0
12	CL	123/124 (99%)	-0.04	6 (4%)	30 28	62, 93, 294, 386	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/118 (96%)	0.41	10 (8%) 11 10	106, 239, 498, 530	0
13	CM	114/118 (96%)	1.21	30 (26%) 1 1	122, 312, 536, 547	0
14	AN	96/101 (95%)	0.29	4 (4%) 37 34	89, 175, 381, 527	0
14	CN	96/101 (95%)	0.62	11 (11%) 5 4	95, 183, 535, 545	0
15	AO	88/89 (98%)	0.29	6 (6%) 18 18	90, 136, 315, 374	0
15	CO	88/89 (98%)	0.31	4 (4%) 34 32	94, 176, 350, 510	0
16	AP	82/82 (100%)	1.14	20 (24%) 1 1	76, 125, 380, 528	0
16	CP	82/82 (100%)	1.14	17 (20%) 1 1	75, 115, 387, 524	0
17	AQ	80/84 (95%)	1.29	17 (21%) 1 1	88, 162, 370, 434	0
17	CQ	80/84 (95%)	0.30	3 (3%) 41 37	75, 141, 337, 496	0
18	AR	55/75 (73%)	0.31	3 (5%) 26 24	84, 115, 320, 391	0
18	CR	55/75 (73%)	0.34	6 (10%) 6 5	107, 159, 370, 440	0
19	AS	79/92 (85%)	1.50	21 (26%) 1 1	118, 215, 454, 530	0
19	CS	79/92 (85%)	1.79	31 (39%) 0 0	133, 302, 496, 542	0
20	AT	85/87 (97%)	0.32	2 (2%) 59 56	93, 158, 363, 497	0
20	CT	85/87 (97%)	0.58	10 (11%) 5 4	82, 128, 351, 491	0
21	AU	51/71 (71%)	0.20	2 (3%) 40 37	83, 133, 326, 395	0
21	CU	51/71 (71%)	0.31	5 (9%) 8 7	108, 193, 374, 512	0
22	AV	76/76 (100%)	-0.19	1 (1%) 77 75	63, 117, 160, 255	0
22	CV	76/76 (100%)	1.24	18 (23%) 1 1	61, 257, 424, 542	0
23	AX	16/24 (66%)	-0.21	0 100 100	76, 139, 214, 261	0
23	CX	15/24 (62%)	-0.05	1 (6%) 19 18	83, 191, 269, 339	0
24	BA	2897/2904 (99%)	-0.43	24 (0%) 86 85	54, 96, 294, 544	0
24	DA	2897/2904 (99%)	-0.30	89 (3%) 49 48	37, 67, 231, 547	0
25	BB	118/120 (98%)	-0.81	0 100 100	78, 151, 201, 231	0
25	DB	119/120 (99%)	-0.68	0 100 100	47, 88, 129, 188	0
26	BC	271/273 (99%)	0.25	7 (2%) 56 53	56, 106, 196, 362	0
26	DC	271/273 (99%)	0.04	3 (1%) 80 79	46, 81, 188, 348	0
27	BD	209/209 (100%)	0.00	5 (2%) 59 56	58, 88, 195, 401	0
27	DD	209/209 (100%)	-0.16	0 100 100	38, 57, 129, 253	0
28	BE	201/201 (100%)	0.35	19 (9%) 9 8	59, 105, 224, 424	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DE	201/201 (100%)	0.04	1 (0%) 90 90	40, 72, 155, 487	0
29	BF	177/179 (98%)	1.06	37 (20%) 1 1	125, 257, 446, 539	0
29	DF	177/179 (98%)	0.78	22 (12%) 4 4	76, 147, 367, 520	0
30	BG	176/177 (99%)	0.78	25 (14%) 3 3	93, 155, 360, 507	0
30	DG	176/177 (99%)	0.28	9 (5%) 29 26	54, 94, 190, 439	0
31	BH	149/149 (100%)	0.83	23 (15%) 2 2	15, 223, 436, 532	0
31	DH	149/149 (100%)	0.61	18 (12%) 5 4	25, 213, 475, 538	0
32	BI	141/142 (99%)	3.66	89 (63%) 0 0	126, 471, 546, 549	0
32	DI	141/142 (99%)	3.08	78 (55%) 0 0	123, 380, 542, 548	0
33	BJ	142/142 (100%)	0.17	1 (0%) 87 87	56, 83, 169, 348	0
33	DJ	142/142 (100%)	-0.13	0 100 100	38, 60, 146, 265	0
34	BK	122/123 (99%)	0.33	5 (4%) 38 35	65, 93, 197, 357	0
34	DK	122/123 (99%)	0.02	1 (0%) 86 85	43, 63, 112, 229	0
35	BL	143/144 (99%)	0.04	2 (1%) 75 73	55, 110, 265, 507	0
35	DL	143/144 (99%)	-0.29	0 100 100	41, 68, 170, 291	0
36	BM	136/136 (100%)	0.67	16 (11%) 5 4	65, 99, 208, 340	0
36	DM	136/136 (100%)	0.05	1 (0%) 87 87	47, 67, 153, 262	0
37	BN	120/127 (94%)	0.21	2 (1%) 70 67	66, 107, 190, 466	0
37	DN	120/127 (94%)	-0.16	0 100 100	40, 61, 151, 420	0
38	BO	116/117 (99%)	0.61	14 (12%) 5 4	96, 193, 363, 537	0
38	DO	116/117 (99%)	0.28	5 (4%) 36 34	66, 94, 183, 322	0
39	BP	114/115 (99%)	0.17	2 (1%) 69 66	71, 109, 288, 356	0
39	DP	114/115 (99%)	-0.21	0 100 100	47, 69, 178, 330	0
40	BQ	117/118 (99%)	0.00	0 100 100	55, 76, 170, 304	0
40	DQ	117/118 (99%)	-0.32	0 100 100	38, 54, 156, 310	0
41	BR	103/103 (100%)	0.07	1 (0%) 82 81	57, 92, 180, 286	0
41	DR	103/103 (100%)	-0.06	0 100 100	42, 68, 152, 458	0
42	BS	110/110 (100%)	0.12	3 (2%) 55 52	60, 92, 175, 299	0
42	DS	110/110 (100%)	-0.01	1 (0%) 84 83	38, 56, 115, 161	0
43	BT	93/100 (93%)	0.85	12 (12%) 4 3	93, 155, 337, 441	0
43	DT	93/100 (93%)	0.36	3 (3%) 48 46	56, 90, 192, 530	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BU	102/104 (98%)	0.62	13 (12%) 4 4	78, 133, 337, 443	0
44	DU	102/104 (98%)	-0.13	0 100 100	52, 82, 226, 299	0
45	BV	94/94 (100%)	0.64	8 (8%) 11 11	86, 144, 310, 421	0
45	DV	94/94 (100%)	0.32	3 (3%) 48 46	60, 94, 183, 336	0
46	BW	75/85 (88%)	0.53	4 (5%) 27 25	70, 113, 202, 321	0
46	DW	76/85 (89%)	0.09	1 (1%) 77 75	46, 70, 156, 244	0
47	BX	77/78 (98%)	0.03	0 100 100	62, 110, 268, 318	0
47	DX	77/78 (98%)	0.27	3 (3%) 40 37	48, 83, 165, 320	0
48	BY	63/63 (100%)	0.52	6 (9%) 9 8	95, 176, 353, 521	0
48	DY	63/63 (100%)	0.31	5 (7%) 13 12	58, 106, 283, 388	0
49	BZ	58/59 (98%)	0.39	2 (3%) 46 42	67, 93, 170, 515	0
49	DZ	58/59 (98%)	-0.08	1 (1%) 70 67	44, 59, 141, 198	0
50	B0	56/57 (98%)	0.01	2 (3%) 43 40	59, 98, 294, 405	0
50	D0	56/57 (98%)	-0.38	0 100 100	33, 64, 166, 282	0
51	B1	50/55 (90%)	2.29	26 (52%) 0 0	88, 147, 326, 377	0
51	D1	50/55 (90%)	1.93	22 (44%) 0 0	78, 120, 326, 532	0
52	B2	46/46 (100%)	0.19	0 100 100	70, 95, 239, 293	0
52	D2	46/46 (100%)	0.10	1 (2%) 62 60	54, 67, 171, 292	0
53	B3	64/65 (98%)	-0.03	0 100 100	67, 91, 201, 286	0
53	D3	64/65 (98%)	-0.06	0 100 100	47, 61, 161, 254	0
54	B4	38/38 (100%)	0.05	0 100 100	78, 108, 174, 322	0
54	D4	38/38 (100%)	0.19	0 100 100	53, 67, 150, 295	0
55	CY	183/185 (98%)	0.36	20 (10%) 6 5	53, 148, 442, 539	0
All	All	20909/21487 (97%)	0.07	1213 (5%) 24 23	15, 110, 357, 549	0

The worst 5 of 1213 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	BI	66	PHE	15.7
49	BZ	1	ALA	14.3
32	DI	53	PRO	14.1
32	DI	1	ALA	13.8
51	B1	17	GLY	13.5

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	BA	3058	1/1	0.56	0.95	72.19	108,108,108,108	0
56	MG	CA	1640	1/1	0.91	0.99	60.32	114,114,114,114	0
56	MG	DA	3169	1/1	0.44	0.72	57.15	94,94,94,94	0
56	MG	DA	3057	1/1	0.49	0.84	50.29	114,114,114,114	0
56	MG	CA	1637	1/1	0.71	0.97	45.71	139,139,139,139	0
56	MG	BA	3025	1/1	0.25	0.46	42.95	103,103,103,103	0
56	MG	BA	3103	1/1	0.85	0.95	42.59	105,105,105,105	0
56	MG	CA	1636	1/1	0.78	1.24	42.15	134,134,134,134	0
56	MG	BA	3168	1/1	0.63	0.91	41.55	114,114,114,114	0
56	MG	DA	3113	1/1	0.87	0.49	38.81	106,106,106,106	0
56	MG	AA	1638	1/1	0.81	0.76	37.37	104,104,104,104	0
56	MG	DA	3167	1/1	0.29	0.73	34.24	84,84,84,84	0
56	MG	CA	1602	1/1	0.63	0.49	34.21	105,105,105,105	0
56	MG	BA	3104	1/1	0.94	0.59	33.37	106,106,106,106	0
56	MG	BA	3054	1/1	0.64	1.62	33.11	119,119,119,119	0
56	MG	AD	301	1/1	0.60	0.82	31.45	119,119,119,119	0
56	MG	DB	204	1/1	0.02	0.88	31.25	109,109,109,109	0
56	MG	BA	3013	1/1	0.53	0.54	31.09	114,114,114,114	0
56	MG	DA	3102	1/1	0.49	0.63	29.30	94,94,94,94	0
56	MG	DA	3192	1/1	0.06	0.48	29.22	95,95,95,95	0
56	MG	BA	3127	1/1	0.86	0.42	27.16	95,95,95,95	0
56	MG	DA	3129	1/1	0.70	1.85	26.51	124,124,124,124	0
56	MG	AA	1626	1/1	0.67	0.58	26.37	111,111,111,111	0
56	MG	BA	3107	1/1	0.56	0.45	25.79	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	DA	3061	1/1	0.53	0.63	25.76	106,106,106,106	0
56	MG	BA	3129	1/1	0.70	0.62	23.34	107,107,107,107	0
56	MG	DA	3147	1/1	0.91	0.81	22.92	107,107,107,107	0
56	MG	CA	1659	1/1	0.38	0.65	22.39	110,110,110,110	0
56	MG	BA	3027	1/1	0.73	1.53	22.19	108,108,108,108	0
56	MG	CA	1612	1/1	0.75	0.40	21.31	116,116,116,116	0
56	MG	BA	3147	1/1	0.85	0.52	20.21	95,95,95,95	0
56	MG	DA	3079	1/1	0.65	0.50	19.94	99,99,99,99	0
56	MG	CA	1626	1/1	0.71	0.40	19.64	99,99,99,99	0
56	MG	DA	3013	1/1	0.91	0.47	19.21	107,107,107,107	0
56	MG	DA	3071	1/1	0.76	0.42	18.44	97,97,97,97	0
56	MG	DA	3072	1/1	0.68	0.36	18.40	93,93,93,93	0
56	MG	BA	3148	1/1	0.66	0.47	17.41	101,101,101,101	0
56	MG	BA	3115	1/1	0.74	0.30	17.35	105,105,105,105	0
56	MG	BA	3077	1/1	0.83	0.52	17.35	121,121,121,121	0
56	MG	DA	3193	1/1	0.57	0.53	16.97	95,95,95,95	0
57	NMY	DA	3190	42/42	0.72	0.42	16.60	57,66,70,74	42
56	MG	DA	3106	1/1	0.89	0.52	16.01	100,100,100,100	0
56	MG	CA	1617	1/1	0.03	0.39	15.91	115,115,115,115	0
56	MG	DA	3146	1/1	0.86	0.36	15.77	76,76,76,76	0
56	MG	BA	3153	1/1	0.65	0.57	15.35	112,112,112,112	0
56	MG	DA	3064	1/1	0.45	0.32	15.34	95,95,95,95	0
56	MG	AA	1617	1/1	0.70	0.46	15.04	112,112,112,112	0
56	MG	BA	3109	1/1	0.81	0.38	14.48	106,106,106,106	0
56	MG	DA	3107	1/1	0.78	0.44	14.46	98,98,98,98	0
56	MG	BA	3008	1/1	0.90	0.30	14.44	107,107,107,107	0
56	MG	BA	3063	1/1	0.89	0.64	14.41	106,106,106,106	0
56	MG	AA	1602	1/1	0.80	0.51	14.24	106,106,106,106	0
56	MG	BA	3023	1/1	0.81	0.37	13.56	108,108,108,108	0
56	MG	BB	201	1/1	0.59	0.21	13.18	137,137,137,137	0
56	MG	DA	3094	1/1	0.66	0.35	13.07	87,87,87,87	0
56	MG	AA	1614	1/1	0.71	0.47	13.01	123,123,123,123	0
56	MG	BA	3022	1/1	0.51	0.73	12.40	110,110,110,110	0
56	MG	DA	3101	1/1	0.85	0.36	12.25	86,86,86,86	0
56	MG	BA	3011	1/1	0.81	0.43	11.77	81,81,81,81	0
57	NMY	BA	3164	42/42	0.83	0.33	11.67	90,100,104,105	42
56	MG	DA	3131	1/1	0.66	0.66	11.35	118,118,118,118	0
56	MG	AA	1633	1/1	0.09	0.37	11.29	128,128,128,128	0
56	MG	DO	201	1/1	0.56	0.54	11.23	109,109,109,109	0
56	MG	BB	202	1/1	0.83	0.69	11.08	123,123,123,123	0
56	MG	BA	3049	1/1	0.85	0.28	10.58	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3070	1/1	0.30	0.35	10.42	90,90,90,90	0
56	MG	BA	3072	1/1	0.70	0.31	10.39	103,103,103,103	0
56	MG	DA	3157	1/1	0.86	0.38	10.24	96,96,96,96	0
56	MG	DA	3060	1/1	0.53	0.27	10.22	89,89,89,89	0
56	MG	CA	1646	1/1	0.85	0.32	9.83	95,95,95,95	0
56	MG	BA	3146	1/1	0.66	0.36	9.69	98,98,98,98	0
57	NMY	DA	3187	42/42	0.90	0.32	9.37	106,109,112,114	42
56	MG	BA	3044	1/1	0.84	0.32	9.36	114,114,114,114	0
56	MG	DA	3020	1/1	0.73	0.27	9.13	93,93,93,93	0
56	MG	DA	3009	1/1	0.87	0.36	9.04	102,102,102,102	0
56	MG	DA	3048	1/1	0.88	0.35	8.98	96,96,96,96	0
56	MG	BA	3021	1/1	0.73	0.29	8.92	108,108,108,108	0
57	NMY	AA	1656	42/42	0.84	0.30	8.92	94,99,103,104	42
56	MG	BA	3005	1/1	0.63	0.25	8.82	106,106,106,106	0
56	MG	DA	3098	1/1	0.73	0.24	8.81	99,99,99,99	0
56	MG	DA	3069	1/1	0.52	0.31	8.75	81,81,81,81	0
56	MG	BA	3047	1/1	0.57	0.29	8.71	103,103,103,103	0
56	MG	BA	3095	1/1	0.50	0.35	8.63	107,107,107,107	0
56	MG	AA	1613	1/1	0.70	0.25	8.35	115,115,115,115	0
56	MG	DA	3127	1/1	0.60	0.32	8.33	77,77,77,77	0
56	MG	BA	3031	1/1	0.86	0.24	8.19	87,87,87,87	0
56	MG	AA	1621	1/1	0.85	0.39	8.16	116,116,116,116	0
56	MG	DA	3076	1/1	0.49	0.26	7.96	100,100,100,100	0
56	MG	AA	1652	1/1	0.83	0.37	7.81	101,101,101,101	0
56	MG	DA	3092	1/1	0.75	0.33	7.63	95,95,95,95	0
56	MG	DA	3051	1/1	0.82	0.27	7.63	86,86,86,86	0
56	MG	AA	1608	1/1	0.92	0.38	7.58	114,114,114,114	0
57	NMY	BA	3167	42/42	0.80	0.31	7.36	117,120,124,125	42
57	NMY	AA	1657	42/42	0.80	0.28	7.35	81,84,88,90	42
56	MG	BA	3030	1/1	0.72	0.32	7.27	94,94,94,94	0
57	NMY	BA	3163	42/42	0.81	0.30	7.23	89,98,100,101	42
56	MG	DA	3029	1/1	0.84	0.24	7.07	84,84,84,84	0
56	MG	AA	1630	1/1	0.81	0.31	6.92	105,105,105,105	0
56	MG	DA	3121	1/1	0.79	0.28	6.66	86,86,86,86	0
56	MG	DA	3158	1/1	0.93	0.29	6.62	91,91,91,91	0
56	MG	BA	3065	1/1	0.89	0.31	6.47	101,101,101,101	0
56	MG	BA	3119	1/1	0.89	0.20	6.45	106,106,106,106	0
56	MG	BA	3106	1/1	0.83	0.36	6.43	100,100,100,100	0
56	MG	AA	1644	1/1	0.74	0.41	6.05	106,106,106,106	0
56	MG	DA	3142	1/1	0.67	0.19	6.01	86,86,86,86	0
56	MG	BA	3108	1/1	0.74	0.31	5.95	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3092	1/1	0.59	0.25	5.75	119,119,119,119	0
56	MG	DA	3038	1/1	0.95	0.25	5.71	81,81,81,81	0
56	MG	DA	3181	1/1	0.93	0.39	5.57	77,77,77,77	0
56	MG	BA	3078	1/1	0.65	0.23	5.36	119,119,119,119	0
57	NMY	BA	3165	42/42	0.82	0.30	5.26	79,84,87,90	42
56	MG	BA	3111	1/1	0.86	0.25	5.01	98,98,98,98	0
56	MG	CA	1614	1/1	0.88	0.21	4.95	120,120,120,120	0
56	MG	DA	3008	1/1	0.58	0.24	4.92	88,88,88,88	0
56	MG	BA	3170	1/1	0.88	0.39	4.88	88,88,88,88	0
56	MG	BA	3105	1/1	0.23	0.28	4.76	91,91,91,91	0
56	MG	DA	3021	1/1	0.81	0.36	4.73	108,108,108,108	0
56	MG	DA	3017	1/1	0.87	0.25	4.66	76,76,76,76	0
57	NMY	DA	3186	42/42	0.91	0.27	4.46	53,58,64,71	42
56	MG	BA	3130	1/1	0.91	0.60	4.26	103,103,103,103	0
57	NMY	DA	3185	42/42	0.91	0.22	4.19	46,58,63,67	42
57	NMY	BA	3161	42/42	0.86	0.25	4.14	61,70,77,82	42
57	NMY	BA	3162	42/42	0.85	0.26	4.14	65,79,86,93	42
57	NMY	CA	1672	42/42	0.92	0.24	4.14	54,65,74,77	42
56	MG	DA	3036	1/1	0.83	0.30	4.04	90,90,90,90	0
56	MG	CA	1669	1/1	0.84	0.35	3.94	107,107,107,107	0
56	MG	DA	3111	1/1	0.81	0.44	3.81	102,102,102,102	0
56	MG	DA	3066	1/1	0.71	0.23	3.77	90,90,90,90	0
56	MG	DA	3022	1/1	0.33	0.28	3.62	81,81,81,81	0
57	NMY	DA	3189	42/42	0.91	0.23	3.60	55,63,70,72	42
56	MG	DB	201	1/1	0.40	0.22	3.58	113,113,113,113	0
56	MG	DA	3012	1/1	0.49	0.26	3.56	83,83,83,83	0
56	MG	AA	1619	1/1	0.74	0.22	3.50	95,95,95,95	0
56	MG	DA	3178	1/1	0.96	0.22	2.85	88,88,88,88	0
56	MG	CA	1641	1/1	0.90	0.22	2.81	85,85,85,85	0
57	NMY	DA	3184	42/42	0.88	0.25	2.52	57,71,80,89	42
56	MG	CA	1601	1/1	0.20	0.43	2.46	140,140,140,140	0
56	MG	DA	3028	1/1	0.85	0.31	2.46	85,85,85,85	0
56	MG	BA	3064	1/1	0.86	0.18	2.44	96,96,96,96	0
56	MG	BA	3140	1/1	0.93	0.22	2.36	101,101,101,101	0
56	MG	AA	1601	1/1	0.63	0.36	2.32	132,132,132,132	0
56	MG	BA	3056	1/1	0.79	0.18	2.26	99,99,99,99	0
56	MG	DA	3104	1/1	0.84	0.20	2.10	81,81,81,81	0
56	MG	DA	3153	1/1	0.84	0.20	2.02	95,95,95,95	0
56	MG	DA	3155	1/1	0.74	0.22	1.98	115,115,115,115	0
57	NMY	BA	3166	42/42	0.86	0.25	1.65	68,77,83,90	42
58	ZN	D4	101	1/1	0.94	0.44	1.58	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	AA	1632	1/1	0.59	0.20	1.57	114,114,114,114	0
56	MG	AA	1641	1/1	0.67	0.42	1.56	105,105,105,105	0
57	NMY	DA	3188	42/42	0.94	0.21	1.54	45,60,66,70	42
56	MG	BA	3057	1/1	0.73	0.19	1.50	98,98,98,98	0
56	MG	AA	1637	1/1	0.90	0.23	1.48	103,103,103,103	0
56	MG	CA	1635	1/1	0.78	0.21	1.32	113,113,113,113	0
56	MG	BA	3046	1/1	0.91	0.18	1.28	109,109,109,109	0
56	MG	DA	3047	1/1	0.88	0.20	1.20	76,76,76,76	0
56	MG	DA	3128	1/1	0.78	0.20	1.18	92,92,92,92	0
56	MG	BA	3002	1/1	0.97	0.16	1.09	89,89,89,89	0
56	MG	DA	3005	1/1	0.90	0.16	0.96	88,88,88,88	0
57	NMY	AA	1655	42/42	0.89	0.21	0.93	61,73,90,121	0
56	MG	CA	1621	1/1	0.76	0.18	0.93	111,111,111,111	0
56	MG	CA	1616	1/1	0.52	0.14	0.82	98,98,98,98	0
56	MG	DA	3053	1/1	0.83	0.19	0.70	93,93,93,93	0
56	MG	BA	3035	1/1	0.92	0.18	0.66	94,94,94,94	0
56	MG	BA	3052	1/1	0.59	0.20	0.62	97,97,97,97	0
56	MG	AA	1615	1/1	0.83	0.14	0.50	112,112,112,112	0
56	MG	DA	3133	1/1	0.93	0.22	0.42	100,100,100,100	0
56	MG	BA	3016	1/1	0.84	0.17	0.40	83,83,83,83	0
56	MG	DA	3117	1/1	0.86	0.18	0.32	93,93,93,93	0
56	MG	DA	3056	1/1	0.80	0.16	0.17	86,86,86,86	0
56	MG	DA	3034	1/1	0.75	0.17	0.12	84,84,84,84	0
56	MG	BA	3132	1/1	0.84	0.18	0.09	96,96,96,96	0
56	MG	CA	1630	1/1	0.91	0.24	0.09	118,118,118,118	0
56	MG	DA	3062	1/1	0.71	0.18	0.05	76,76,76,76	0
56	MG	BA	3085	1/1	0.63	0.16	-0.02	95,95,95,95	0
58	ZN	B4	101	1/1	0.95	0.19	-0.29	186,186,186,186	0
56	MG	DE	301	1/1	0.84	0.12	-0.33	100,100,100,100	0
56	MG	DA	3074	1/1	0.64	0.13	-0.37	95,95,95,95	0
56	MG	DA	3046	1/1	0.73	0.15	-0.92	86,86,86,86	0
56	MG	BA	3039	1/1	0.96	0.15	-1.06	96,96,96,96	0
56	MG	BA	3036	1/1	0.89	0.14	-1.07	95,95,95,95	0
56	MG	CA	1662	1/1	0.97	0.12	-1.38	114,114,114,114	0
56	MG	DA	3063	1/1	0.97	0.11	-2.81	69,69,69,69	0
56	MG	BA	3128	1/1	0.90	0.12	-3.26	94,94,94,94	0
56	MG	BA	3048	1/1	0.83	0.09	-3.52	93,93,93,93	0
56	MG	CA	1619	1/1	0.83	0.13	-3.95	93,93,93,93	0
56	MG	AA	1611	1/1	0.94	0.07	-4.96	104,104,104,104	0
56	MG	CA	1604	1/1	0.94	0.10	-5.61	86,86,86,86	0
56	MG	DA	3126	1/1	0.95	0.14	-5.85	60,60,60,60	0
56	MG	DA	3002	1/1	0.88	0.08	-6.03	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3067	1/1	0.84	0.11	-6.83	89,89,89,89	0
56	MG	DA	3037	1/1	0.88	0.25	-	72,72,72,72	0
56	MG	AA	1604	1/1	0.46	0.12	-	102,102,102,102	0
56	MG	DA	3059	1/1	0.38	0.47	-	92,92,92,92	0
56	MG	BA	3081	1/1	0.33	0.33	-	109,109,109,109	0
56	MG	DA	3137	1/1	0.15	0.55	-	93,93,93,93	0
56	MG	CA	1622	1/1	0.80	0.29	-	108,108,108,108	0
56	MG	BA	3157	1/1	0.61	1.00	-	97,97,97,97	0
56	MG	BA	3068	1/1	0.51	0.23	-	126,126,126,126	0
56	MG	DA	3086	1/1	0.82	0.11	-	97,97,97,97	0
56	MG	AA	1612	1/1	0.81	0.13	-	107,107,107,107	0
56	MG	CA	1642	1/1	0.85	0.29	-	106,106,106,106	0
56	MG	DA	3089	1/1	0.96	0.12	-	97,97,97,97	0
56	MG	BA	3088	1/1	0.65	0.31	-	101,101,101,101	0
56	MG	BA	3040	1/1	0.23	0.23	-	112,112,112,112	0
56	MG	DA	3003	1/1	0.51	0.15	-	105,105,105,105	0
56	MG	DA	3083	1/1	0.45	0.32	-	82,82,82,82	0
56	MG	BA	3141	1/1	0.89	0.13	-	114,114,114,114	0
56	MG	CA	1613	1/1	0.72	0.16	-	103,103,103,103	0
56	MG	DA	3140	1/1	0.73	0.33	-	98,98,98,98	0
56	MG	DA	3093	1/1	0.92	0.62	-	105,105,105,105	0
56	MG	DA	3007	1/1	0.73	0.23	-	103,103,103,103	0
56	MG	BA	3001	1/1	0.63	0.18	-	99,99,99,99	0
56	MG	BA	3158	1/1	0.64	0.51	-	106,106,106,106	0
56	MG	BA	3075	1/1	0.52	0.40	-	104,104,104,104	0
56	MG	DA	3001	1/1	0.89	0.12	-	91,91,91,91	0
56	MG	BA	3069	1/1	0.48	0.57	-	129,129,129,129	0
56	MG	BA	3122	1/1	0.73	0.30	-	112,112,112,112	0
56	MG	DA	3032	1/1	0.85	0.52	-	97,97,97,97	0
56	MG	DA	3120	1/1	0.89	0.22	-	98,98,98,98	0
56	MG	BA	3121	1/1	0.74	0.34	-	110,110,110,110	0
56	MG	CA	1670	1/1	0.55	0.69	-	102,102,102,102	0
56	MG	DA	3148	1/1	0.78	0.38	-	60,60,60,60	0
56	MG	DA	3156	1/1	0.71	0.41	-	101,101,101,101	0
56	MG	DA	3068	1/1	0.66	0.89	-	117,117,117,117	0
56	MG	DA	3058	1/1	0.95	0.42	-	96,96,96,96	0
56	MG	AA	1639	1/1	0.79	0.95	-	113,113,113,113	0
56	MG	DA	3149	1/1	0.89	0.33	-	107,107,107,107	0
56	MG	BA	3152	1/1	0.35	0.84	-	115,115,115,115	0
56	MG	DA	3108	1/1	0.74	0.29	-	100,100,100,100	0
56	MG	DB	203	1/1	0.12	0.27	-	100,100,100,100	0
56	MG	CA	1620	1/1	0.49	0.26	-	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3042	1/1	0.95	0.10	-	97,97,97,97	0
56	MG	DB	202	1/1	0.23	0.78	-	122,122,122,122	0
56	MG	CA	1651	1/1	0.08	1.06	-	103,103,103,103	0
56	MG	BA	3136	1/1	0.88	0.49	-	94,94,94,94	0
56	MG	BA	3149	1/1	0.52	0.67	-	85,85,85,85	0
56	MG	AA	1620	1/1	0.89	0.25	-	118,118,118,118	0
56	MG	DA	3122	1/1	0.81	0.28	-	97,97,97,97	0
56	MG	DA	3177	1/1	0.82	0.51	-	96,96,96,96	0
56	MG	CA	1647	1/1	0.38	0.57	-	112,112,112,112	0
56	MG	BA	3004	1/1	0.72	0.20	-	120,120,120,120	0
56	MG	BC	301	1/1	0.41	0.75	-	122,122,122,122	0
56	MG	DA	3067	1/1	0.85	0.38	-	120,120,120,120	0
56	MG	BA	3091	1/1	0.77	0.36	-	115,115,115,115	0
56	MG	BA	3043	1/1	0.88	0.19	-	108,108,108,108	0
56	MG	BA	3033	1/1	0.91	0.51	-	98,98,98,98	0
56	MG	DA	3114	1/1	0.91	0.18	-	77,77,77,77	0
56	MG	DA	3182	1/1	0.54	0.34	-	96,96,96,96	0
56	MG	BA	3097	1/1	0.88	1.23	-	111,111,111,111	0
56	MG	DL	201	1/1	0.82	0.81	-	110,110,110,110	0
56	MG	DA	3050	1/1	0.78	0.24	-	86,86,86,86	0
56	MG	DA	3100	1/1	0.43	0.40	-	96,96,96,96	0
56	MG	DA	3159	1/1	0.88	0.52	-	90,90,90,90	0
56	MG	BA	3017	1/1	0.76	0.14	-	107,107,107,107	0
56	MG	CA	1645	1/1	0.68	0.42	-	96,96,96,96	0
56	MG	AA	1631	1/1	0.61	0.66	-	126,126,126,126	0
56	MG	AA	1634	1/1	0.95	0.51	-	120,120,120,120	0
56	MG	BA	3142	1/1	0.69	0.49	-	103,103,103,103	0
56	MG	BA	3118	1/1	0.73	0.45	-	109,109,109,109	0
56	MG	BA	3099	1/1	0.45	0.38	-	112,112,112,112	0
56	MG	DA	3143	1/1	0.95	1.31	-	79,79,79,79	0
56	MG	BA	3134	1/1	0.80	0.26	-	109,109,109,109	0
56	MG	AA	1645	1/1	0.79	0.33	-	93,93,93,93	0
56	MG	BA	3110	1/1	0.49	0.43	-	110,110,110,110	0
56	MG	BA	3155	1/1	0.66	0.88	-	114,114,114,114	0
56	MG	AA	1606	1/1	0.79	0.34	-	111,111,111,111	0
56	MG	DA	3138	1/1	0.76	0.73	-	81,81,81,81	0
56	MG	DA	3055	1/1	0.55	0.36	-	94,94,94,94	0
56	MG	DA	3011	1/1	0.65	0.53	-	103,103,103,103	0
56	MG	DA	3073	1/1	0.50	0.27	-	99,99,99,99	0
56	MG	AA	1618	1/1	0.81	0.27	-	96,96,96,96	0
56	MG	CA	1618	1/1	0.78	0.39	-	83,83,83,83	0
56	MG	DA	3019	1/1	0.91	0.29	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1653	1/1	-0.28	0.63	-	106,106,106,106	0
56	MG	DA	3039	1/1	0.80	0.33	-	117,117,117,117	0
56	MG	BA	3074	1/1	0.87	0.36	-	115,115,115,115	0
56	MG	CA	1624	1/1	0.31	0.27	-	106,106,106,106	0
56	MG	DA	3082	1/1	0.78	0.26	-	92,92,92,92	0
56	MG	BA	3055	1/1	0.64	0.23	-	101,101,101,101	0
56	MG	DA	3173	1/1	0.79	0.47	-	90,90,90,90	0
56	MG	DA	3045	1/1	0.39	0.12	-	95,95,95,95	0
56	MG	CA	1634	1/1	0.57	0.33	-	120,120,120,120	0
56	MG	BA	3087	1/1	0.38	0.58	-	112,112,112,112	0
56	MG	AA	1650	1/1	-0.01	3.08	-	118,118,118,118	0
56	MG	DA	3124	1/1	0.91	0.26	-	78,78,78,78	0
56	MG	CA	1615	1/1	0.40	0.18	-	112,112,112,112	0
56	MG	BA	3079	1/1	0.79	0.60	-	103,103,103,103	0
56	MG	DA	3150	1/1	0.70	0.70	-	78,78,78,78	0
56	MG	DA	3035	1/1	0.70	0.24	-	94,94,94,94	0
56	MG	CA	1650	1/1	0.85	0.50	-	102,102,102,102	0
56	MG	BA	3156	1/1	0.40	0.68	-	106,106,106,106	0
56	MG	DA	3172	1/1	0.50	0.45	-	109,109,109,109	0
56	MG	CA	1648	1/1	0.82	0.41	-	103,103,103,103	0
56	MG	DA	3077	1/1	0.82	0.41	-	98,98,98,98	0
56	MG	CA	1654	1/1	0.28	1.25	-	116,116,116,116	0
56	MG	BA	3131	1/1	0.37	0.40	-	114,114,114,114	0
56	MG	BA	3050	1/1	0.74	0.38	-	101,101,101,101	0
56	MG	DA	3175	1/1	0.94	0.71	-	75,75,75,75	0
56	MG	CA	1656	1/1	0.66	0.56	-	106,106,106,106	0
56	MG	DA	3164	1/1	0.77	0.67	-	94,94,94,94	0
56	MG	DA	3096	1/1	0.79	0.25	-	75,75,75,75	0
56	MG	BA	3034	1/1	0.76	0.16	-	88,88,88,88	0
56	MG	BA	3080	1/1	0.93	0.15	-	73,73,73,73	0
56	MG	CA	1653	1/1	0.24	0.55	-	99,99,99,99	0
56	MG	BA	3073	1/1	0.83	0.15	-	101,101,101,101	0
56	MG	BA	3100	1/1	0.73	0.36	-	107,107,107,107	0
56	MG	DA	3170	1/1	0.72	0.42	-	94,94,94,94	0
56	MG	DA	3179	1/1	0.39	0.36	-	113,113,113,113	0
56	MG	DA	3024	1/1	0.77	0.24	-	73,73,73,73	0
56	MG	DA	3139	1/1	0.68	0.56	-	77,77,77,77	0
56	MG	BA	3090	1/1	0.72	0.69	-	130,130,130,130	0
56	MG	BA	3084	1/1	0.92	0.19	-	95,95,95,95	0
56	MG	BA	3124	1/1	0.49	0.19	-	114,114,114,114	0
56	MG	DA	3054	1/1	0.90	0.25	-	93,93,93,93	0
56	MG	CA	1606	1/1	0.17	0.16	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AN	201	1/1	0.37	0.58	-	133,133,133,133	0
56	MG	BA	3045	1/1	0.92	0.16	-	118,118,118,118	0
56	MG	CA	1607	1/1	0.73	0.57	-	110,110,110,110	0
56	MG	BA	3151	1/1	0.82	0.66	-	92,92,92,92	0
56	MG	DA	3130	1/1	0.73	0.26	-	96,96,96,96	0
56	MG	AA	1609	1/1	0.76	0.34	-	111,111,111,111	0
56	MG	CA	1660	1/1	0.43	0.49	-	104,104,104,104	0
56	MG	BA	3015	1/1	0.32	0.25	-	115,115,115,115	0
56	MG	BA	3154	1/1	0.64	0.69	-	97,97,97,97	0
56	MG	BA	3143	1/1	0.66	0.53	-	103,103,103,103	0
56	MG	DA	3174	1/1	0.62	0.58	-	105,105,105,105	0
56	MG	BA	3012	1/1	0.67	1.00	-	118,118,118,118	0
56	MG	DA	3031	1/1	0.86	0.28	-	108,108,108,108	0
56	MG	DA	3025	1/1	0.70	0.77	-	118,118,118,118	0
56	MG	BA	3028	1/1	0.96	0.28	-	89,89,89,89	0
56	MG	DA	3090	1/1	0.82	0.23	-	107,107,107,107	0
56	MG	AA	1642	1/1	0.81	0.23	-	94,94,94,94	0
56	MG	BA	3007	1/1	0.05	0.68	-	127,127,127,127	0
56	MG	CA	1655	1/1	0.58	0.31	-	117,117,117,117	0
56	MG	CA	1668	1/1	0.18	0.85	-	107,107,107,107	0
56	MG	DA	3194	1/1	0.75	0.56	-	90,90,90,90	0
56	MG	BA	3096	1/1	0.24	0.76	-	118,118,118,118	0
56	MG	CA	1632	1/1	0.68	1.22	-	128,128,128,128	0
56	MG	CA	1633	1/1	0.49	0.80	-	116,116,116,116	0
56	MG	DA	3075	1/1	0.90	0.42	-	106,106,106,106	0
56	MG	CA	1649	1/1	-0.01	1.11	-	107,107,107,107	0
56	MG	DA	3044	1/1	0.83	0.36	-	105,105,105,105	0
56	MG	DA	3165	1/1	0.80	0.67	-	78,78,78,78	0
56	MG	DA	3161	1/1	0.33	0.30	-	103,103,103,103	0
56	MG	CA	1665	1/1	0.52	0.40	-	112,112,112,112	0
56	MG	DA	3070	1/1	0.85	0.23	-	56,56,56,56	0
56	MG	BA	3019	1/1	0.67	0.23	-	101,101,101,101	0
56	MG	BA	3145	1/1	0.80	0.42	-	99,99,99,99	0
56	MG	AA	1651	1/1	0.72	0.22	-	119,119,119,119	0
56	MG	BA	3032	1/1	0.71	0.68	-	110,110,110,110	0
56	MG	DA	3151	1/1	-0.06	1.03	-	101,101,101,101	0
56	MG	BA	3010	1/1	0.89	0.12	-	85,85,85,85	0
56	MG	DA	3016	1/1	0.87	0.21	-	103,103,103,103	0
56	MG	DA	3118	1/1	0.83	0.28	-	88,88,88,88	0
56	MG	AA	1625	1/1	0.76	0.79	-	117,117,117,117	0
56	MG	CA	1658	1/1	0.83	0.65	-	115,115,115,115	0
56	MG	DA	3081	1/1	0.43	1.04	-	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3163	1/1	0.88	0.26	-	99,99,99,99	0
56	MG	BA	3144	1/1	0.85	0.40	-	87,87,87,87	0
56	MG	BA	3150	1/1	0.92	0.62	-	95,95,95,95	0
56	MG	BA	3086	1/1	0.82	0.12	-	109,109,109,109	0
56	MG	BA	3137	1/1	0.90	0.39	-	82,82,82,82	0
56	MG	BA	3123	1/1	0.50	0.49	-	88,88,88,88	0
56	MG	BA	3139	1/1	0.83	0.77	-	83,83,83,83	0
56	MG	CA	1631	1/1	0.55	0.47	-	120,120,120,120	0
56	MG	AA	1646	1/1	0.51	0.63	-	95,95,95,95	0
56	MG	DA	3023	1/1	0.68	0.69	-	120,120,120,120	0
56	MG	DA	3004	1/1	0.73	0.38	-	99,99,99,99	0
56	MG	BA	3062	1/1	0.83	0.47	-	91,91,91,91	0
56	MG	DA	3084	1/1	0.62	0.25	-	104,104,104,104	0
56	MG	CA	1609	1/1	0.47	0.32	-	117,117,117,117	0
56	MG	DA	3052	1/1	0.62	0.68	-	95,95,95,95	0
56	MG	DA	3014	1/1	0.86	0.23	-	90,90,90,90	0
56	MG	CA	1603	1/1	0.41	0.27	-	120,120,120,120	0
56	MG	BB	203	1/1	0.89	0.13	-	107,107,107,107	0
56	MG	DA	3091	1/1	0.93	0.23	-	104,104,104,104	0
56	MG	DA	3176	1/1	0.62	0.55	-	78,78,78,78	0
56	MG	AA	1654	1/1	-0.38	0.66	-	110,110,110,110	0
56	MG	CA	1638	1/1	0.66	0.70	-	113,113,113,113	0
56	MG	AA	1610	1/1	0.60	0.25	-	120,120,120,120	0
56	MG	BA	3113	1/1	0.94	0.41	-	121,121,121,121	0
56	MG	DA	3180	1/1	0.78	0.41	-	93,93,93,93	0
56	MG	DA	3152	1/1	0.31	0.78	-	105,105,105,105	0
56	MG	DA	3109	1/1	0.81	0.24	-	102,102,102,102	0
56	MG	BA	3133	1/1	0.80	0.36	-	106,106,106,106	0
56	MG	AA	1636	1/1	0.82	0.37	-	103,103,103,103	0
56	MG	AA	1648	1/1	-0.09	1.12	-	116,116,116,116	0
56	MG	DA	3154	1/1	0.86	0.67	-	86,86,86,86	0
56	MG	AA	1603	1/1	0.49	0.20	-	117,117,117,117	0
56	MG	AA	1607	1/1	0.64	0.23	-	116,116,116,116	0
56	MG	DA	3141	1/1	0.96	0.74	-	73,73,73,73	0
56	MG	BA	3098	1/1	0.73	0.36	-	100,100,100,100	0
56	MG	CA	1661	1/1	0.13	0.76	-	101,101,101,101	0
56	MG	BA	3114	1/1	0.67	0.28	-	120,120,120,120	0
56	MG	DA	3095	1/1	0.01	2.06	-	116,116,116,116	0
56	MG	DA	3041	1/1	0.91	0.11	-	81,81,81,81	0
56	MG	DA	3112	1/1	0.83	0.26	-	108,108,108,108	0
56	MG	DA	3168	1/1	0.94	0.20	-	89,89,89,89	0
56	MG	DA	3087	1/1	0.34	0.31	-	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3026	1/1	0.44	0.79	-	134,134,134,134	0
56	MG	DA	3065	1/1	0.62	0.28	-	81,81,81,81	0
56	MG	DA	3110	1/1	0.77	0.26	-	93,93,93,93	0
56	MG	BA	3006	1/1	0.53	0.10	-	101,101,101,101	0
56	MG	BA	3125	1/1	0.28	0.43	-	100,100,100,100	0
56	MG	CA	1667	1/1	0.81	0.65	-	111,111,111,111	0
56	MG	CA	1643	1/1	0.81	0.41	-	103,103,103,103	0
56	MG	DA	3099	1/1	0.96	0.17	-	90,90,90,90	0
56	MG	CA	1605	1/1	0.60	0.17	-	97,97,97,97	0
56	MG	DA	3049	1/1	0.85	0.31	-	97,97,97,97	0
56	MG	DA	3103	1/1	0.85	0.35	-	81,81,81,81	0
56	MG	BA	3159	1/1	0.36	0.75	-	109,109,109,109	0
56	MG	DA	3183	1/1	0.90	0.53	-	87,87,87,87	0
56	MG	BA	3061	1/1	0.74	0.29	-	85,85,85,85	0
56	MG	CA	1644	1/1	0.92	1.25	-	118,118,118,118	0
56	MG	DA	3006	1/1	0.62	0.20	-	92,92,92,92	0
56	MG	CA	1666	1/1	0.86	0.24	-	112,112,112,112	0
56	MG	DA	3105	1/1	0.83	0.40	-	90,90,90,90	0
56	MG	BA	3066	1/1	0.21	0.23	-	96,96,96,96	0
56	MG	CA	1663	1/1	0.81	0.43	-	82,82,82,82	0
56	MG	DA	3080	1/1	0.94	0.31	-	100,100,100,100	0
56	MG	AA	1635	1/1	0.89	0.25	-	105,105,105,105	0
56	MG	BA	3014	1/1	0.88	0.62	-	106,106,106,106	0
56	MG	AA	1629	1/1	0.39	0.53	-	118,118,118,118	0
56	MG	CA	1611	1/1	0.73	0.17	-	110,110,110,110	0
56	MG	BA	3093	1/1	0.88	0.51	-	109,109,109,109	0
56	MG	BA	3135	1/1	0.89	0.72	-	74,74,74,74	0
56	MG	DA	3043	1/1	0.83	0.14	-	90,90,90,90	0
56	MG	AA	1622	1/1	0.57	0.35	-	107,107,107,107	0
56	MG	CA	1627	1/1	0.57	0.32	-	111,111,111,111	0
56	MG	AA	1647	1/1	0.69	0.23	-	109,109,109,109	0
56	MG	BA	3037	1/1	0.95	0.75	-	97,97,97,97	0
56	MG	AA	1624	1/1	0.85	0.40	-	110,110,110,110	0
56	MG	DA	3144	1/1	0.95	0.19	-	108,108,108,108	0
56	MG	DA	3033	1/1	0.91	0.15	-	91,91,91,91	0
56	MG	BA	3138	1/1	0.77	0.71	-	88,88,88,88	0
56	MG	BA	3120	1/1	0.64	0.27	-	94,94,94,94	0
56	MG	DA	3115	1/1	0.46	0.18	-	95,95,95,95	0
56	MG	BA	3059	1/1	0.73	1.36	-	122,122,122,122	0
56	MG	BA	3003	1/1	0.68	0.23	-	115,115,115,115	0
56	MG	CX	101	1/1	0.69	1.13	-	112,112,112,112	0
56	MG	BA	3024	1/1	0.80	0.61	-	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3076	1/1	0.88	0.37	-	120,120,120,120	0
56	MG	CA	1610	1/1	0.74	0.26	-	102,102,102,102	0
56	MG	BA	3041	1/1	0.68	0.16	-	96,96,96,96	0
56	MG	DA	3097	1/1	0.47	0.64	-	105,105,105,105	0
56	MG	DA	3030	1/1	0.77	0.20	-	76,76,76,76	0
56	MG	BA	3051	1/1	0.85	0.38	-	106,106,106,106	0
56	MG	BA	3169	1/1	0.86	0.29	-	101,101,101,101	0
56	MG	BA	3053	1/1	0.76	0.65	-	98,98,98,98	0
56	MG	BA	3083	1/1	0.61	0.21	-	110,110,110,110	0
56	MG	CA	1652	1/1	0.15	0.42	-	106,106,106,106	0
56	MG	BA	3102	1/1	0.76	0.54	-	119,119,119,119	0
56	MG	BA	3094	1/1	0.92	0.23	-	92,92,92,92	0
56	MG	DA	3136	1/1	0.89	0.55	-	74,74,74,74	0
56	MG	DA	3116	1/1	0.77	0.20	-	107,107,107,107	0
56	MG	DA	3119	1/1	0.76	0.23	-	82,82,82,82	0
56	MG	CA	1671	1/1	0.92	0.28	-	96,96,96,96	0
56	MG	DA	3166	1/1	0.70	0.83	-	87,87,87,87	0
56	MG	AA	1640	1/1	0.64	0.45	-	110,110,110,110	0
56	MG	DA	3162	1/1	0.81	0.34	-	95,95,95,95	0
56	MG	BA	3126	1/1	0.48	0.30	-	110,110,110,110	0
56	MG	CA	1628	1/1	0.71	0.35	-	116,116,116,116	0
56	MG	DA	3015	1/1	0.86	0.75	-	124,124,124,124	0
56	MG	BA	3020	1/1	0.81	0.28	-	95,95,95,95	0
56	MG	AA	1643	1/1	0.85	0.18	-	110,110,110,110	0
56	MG	DA	3085	1/1	0.82	0.48	-	108,108,108,108	0
56	MG	DA	3123	1/1	0.59	0.33	-	102,102,102,102	0
56	MG	BA	3117	1/1	0.76	0.15	-	89,89,89,89	0
56	MG	DA	3042	1/1	0.81	0.71	-	105,105,105,105	0
56	MG	BA	3071	1/1	0.51	0.31	-	104,104,104,104	0
56	MG	AA	1616	1/1	0.72	0.49	-	113,113,113,113	0
56	MG	DA	3026	1/1	0.62	0.55	-	98,98,98,98	0
56	MG	BA	3112	1/1	0.80	0.36	-	101,101,101,101	0
56	MG	BQ	201	1/1	0.62	1.42	-	93,93,93,93	0
56	MG	AA	1623	1/1	0.48	1.08	-	119,119,119,119	0
56	MG	BA	3116	1/1	0.56	0.18	-	99,99,99,99	0
56	MG	AA	1628	1/1	0.69	0.36	-	116,116,116,116	0
56	MG	CA	1608	1/1	0.48	0.40	-	115,115,115,115	0
56	MG	DA	3132	1/1	0.85	0.15	-	96,96,96,96	0
56	MG	DA	3191	1/1	0.80	0.14	-	80,80,80,80	0
56	MG	BA	3060	1/1	0.82	0.41	-	106,106,106,106	0
56	MG	BA	3082	1/1	0.78	0.43	-	126,126,126,126	0
56	MG	BA	3029	1/1	0.89	0.23	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3134	1/1	0.50	0.35	-	77,77,77,77	0
56	MG	DA	3160	1/1	0.89	0.77	-	92,92,92,92	0
56	MG	BA	3101	1/1	0.93	0.54	-	102,102,102,102	0
56	MG	AA	1649	1/1	0.61	1.02	-	90,90,90,90	0
56	MG	AA	1627	1/1	0.71	0.48	-	121,121,121,121	0
56	MG	BA	3018	1/1	0.70	0.77	-	118,118,118,118	0
56	MG	DA	3040	1/1	0.72	0.21	-	91,91,91,91	0
56	MG	BA	3038	1/1	0.92	0.22	-	104,104,104,104	0
56	MG	DA	3010	1/1	0.65	0.39	-	106,106,106,106	0
56	MG	CA	1623	1/1	0.38	0.75	-	117,117,117,117	0
56	MG	CA	1657	1/1	0.31	1.34	-	119,119,119,119	0
56	MG	DA	3145	1/1	0.85	0.41	-	91,91,91,91	0
56	MG	DA	3171	1/1	0.47	0.38	-	108,108,108,108	0
56	MG	CA	1629	1/1	0.49	1.03	-	123,123,123,123	0
56	MG	BA	3089	1/1	0.85	0.19	-	109,109,109,109	0
56	MG	DA	3135	1/1	0.87	0.21	-	71,71,71,71	0
56	MG	CA	1625	1/1	0.84	0.20	-	107,107,107,107	0
56	MG	DA	3027	1/1	0.92	0.17	-	79,79,79,79	0
56	MG	DA	3088	1/1	0.60	0.19	-	115,115,115,115	0
56	MG	CA	1639	1/1	0.71	0.12	-	94,94,94,94	0
56	MG	DA	3018	1/1	0.47	0.76	-	102,102,102,102	0
56	MG	DA	3125	1/1	0.94	0.19	-	113,113,113,113	0
56	MG	AA	1605	1/1	0.80	0.36	-	121,121,121,121	0
56	MG	BA	3160	1/1	0.70	0.50	-	102,102,102,102	0
56	MG	DA	3078	1/1	0.86	0.19	-	84,84,84,84	0
56	MG	BA	3009	1/1	0.66	0.30	-	95,95,95,95	0
56	MG	CA	1664	1/1	0.86	0.30	-	112,112,112,112	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.