



# wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 11:04 PM BST

PDB ID : 4V9P  
Title : Control of ribosomal subunit rotation by elongation factor G  
Authors : Pulk, A.; Cate, J.H.D.  
Deposited on : 2013-05-03  
Resolution : 2.90 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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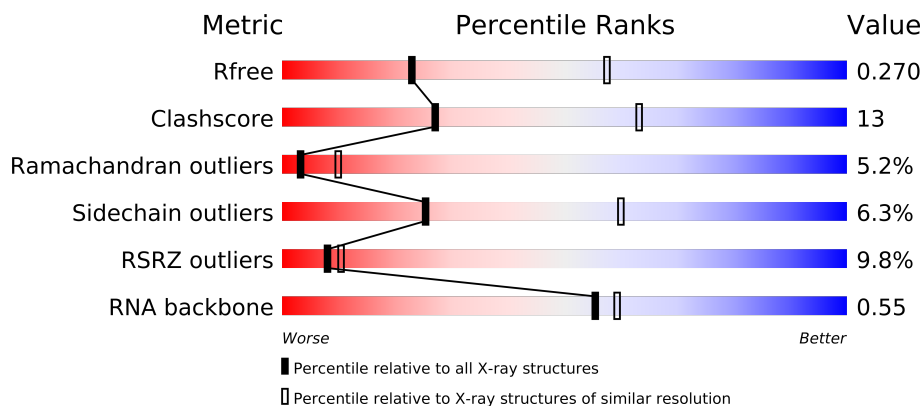
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23397  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23397

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	2904	
1	CA	2904	
1	EA	2904	
1	GA	2904	
2	AB	120	
2	CB	120	
2	EB	120	
2	GB	120	
3	AC	273	
3	CC	273	
3	EC	273	

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Mol	Chain	Length	Quality of chain
3	GC	273	
4	AD	209	
4	CD	209	
4	ED	209	
4	GD	209	
5	AE	201	
5	CE	201	
5	EE	201	
5	GE	201	
6	AF	179	
6	CF	179	
6	EF	179	
6	GF	179	
7	AG	177	
7	CG	177	
7	EG	177	
7	GG	177	
8	AH	50	
8	CH	50	
8	EH	50	
8	GH	50	
9	AI	142	
9	CI	142	
9	EI	142	
9	GI	142	
10	AJ	142	
10	CJ	142	
10	EJ	142	
10	GJ	142	
11	AK	123	
11	CK	123	
11	EK	123	
11	GK	123	
12	AL	144	
12	CL	144	
12	EL	144	
12	GL	144	
13	AM	136	
13	CM	136	
13	EM	136	
13	GM	136	
14	AN	127	

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Mol	Chain	Length	Quality of chain
14	CN	127	
14	EN	127	
14	GN	127	
15	AO	117	
15	CO	117	
15	EO	117	
15	GO	117	
16	AP	115	
16	CP	115	
16	EP	115	
16	GP	115	
17	AQ	118	
17	CQ	118	
17	EQ	118	
17	GQ	118	
18	AR	103	
18	CR	103	
18	ER	103	
18	GR	103	
19	AS	110	
19	CS	110	
19	ES	110	
19	GS	110	
20	AT	100	
20	CT	100	
20	ET	100	
20	GT	100	
21	AU	104	
21	CU	104	
21	EU	104	
21	GU	104	
22	AV	94	
22	CV	94	
22	EV	94	
22	GV	94	
23	AW	85	
23	CW	85	
23	EW	85	
23	GW	85	
24	AX	78	
24	CX	78	
24	EX	78	

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Mol	Chain	Length	Quality of chain
24	GX	78	
25	AY	63	
25	CY	63	
25	EY	63	
25	GY	63	
26	AZ	59	
26	CZ	59	
26	EZ	59	
26	GZ	59	
27	A0	57	
27	C0	57	
27	E0	57	
27	G0	57	
28	A1	55	
28	C1	55	
28	E1	55	
28	G1	55	
29	A2	46	
29	C2	46	
29	E2	46	
29	G2	46	
30	A3	65	
30	C3	65	
30	E3	65	
30	G3	65	
31	A4	38	
31	C4	38	
31	E4	38	
31	G4	38	
32	A5	165	
32	E5	165	
33	BA	1542	
33	DA	1542	
33	FA	1542	
33	HA	1542	
34	BB	241	
34	DB	241	
34	FB	241	
34	HB	241	
35	BC	233	
35	DC	233	
35	FC	233	

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Mol	Chain	Length	Quality of chain
35	HC	233	
36	BD	206	
36	DD	206	
36	FD	206	
36	HD	206	
37	BE	167	
37	DE	167	
37	FE	167	
37	HE	167	
38	BF	135	
38	DF	135	
38	FF	135	
38	HF	135	
39	BG	179	
39	DG	179	
39	FG	179	
39	HG	179	
40	BH	130	
40	DH	130	
40	FH	130	
40	HH	130	
41	BI	130	
41	DI	130	
41	FI	130	
41	HI	130	
42	BJ	103	
42	DJ	103	
42	FJ	103	
42	HJ	103	
43	BK	129	
43	DK	129	
43	FK	129	
43	HK	129	
44	BL	124	
44	DL	124	
44	FL	124	
44	HL	124	
45	BM	118	
45	DM	118	
45	FM	118	
45	HM	118	
46	BN	101	

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Mol	Chain	Length	Quality of chain
46	DN	101	
46	FN	101	
46	HN	101	
47	BO	89	
47	DO	89	
47	FO	89	
47	HO	89	
48	BP	82	
48	DP	82	
48	FP	82	
48	HP	82	
49	BQ	84	
49	DQ	84	
49	FQ	84	
49	HQ	84	
50	BR	75	
50	DR	75	
50	FR	75	
50	HR	75	
51	BS	92	
51	DS	92	
51	FS	92	
51	HS	92	
52	BT	87	
52	DT	87	
52	FT	87	
52	HT	87	
53	BU	71	
53	DU	71	
53	FU	71	
53	HU	71	
54	BV	704	
54	DV	704	
54	FV	704	
54	HV	704	
55	BW	6	
55	DW	6	
55	FW	6	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
56	MG	AA	3005	-	X
56	MG	AA	3007	-	X
56	MG	AA	3009	-	X
56	MG	AA	3010	-	X
56	MG	AA	3018	-	X
56	MG	AA	3028	-	X
56	MG	AA	3033	-	X
56	MG	AA	3035	-	X
56	MG	AA	3041	-	X
56	MG	AA	3042	-	X
56	MG	AA	3055	-	X
56	MG	AA	3059	-	X
56	MG	AA	3060	-	X
56	MG	AA	3062	-	X
56	MG	AA	3078	-	X
56	MG	AA	3083	-	X
56	MG	AA	3084	-	X
56	MG	AA	3091	-	X
56	MG	AA	3093	-	X
56	MG	AA	3098	-	X
56	MG	AA	3102	-	X
56	MG	AA	3107	-	X
56	MG	AA	3109	-	X
56	MG	AA	3115	-	X
56	MG	AA	3117	-	X
56	MG	AA	3123	-	X
56	MG	AC	301	-	X
56	MG	AC	303	-	X
56	MG	BA	1606	-	X
56	MG	BA	1607	-	X
56	MG	BA	1612	-	X
56	MG	BA	1614	-	X
56	MG	BA	1615	-	X
56	MG	BA	1618	-	X
56	MG	BA	1619	-	X
56	MG	BA	1622	-	X
56	MG	BA	1625	-	X
56	MG	BA	1635	-	X
56	MG	BA	1637	-	X
56	MG	BA	1638	-	X
56	MG	BV	802	-	X
56	MG	CA	3005	-	X
56	MG	CA	3010	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
56	MG	CA	3011	-	X
56	MG	CA	3016	-	X
56	MG	CA	3028	-	X
56	MG	CA	3030	-	X
56	MG	CA	3037	-	X
56	MG	CA	3039	-	X
56	MG	CA	3040	-	X
56	MG	CA	3051	-	X
56	MG	CA	3066	-	X
56	MG	CA	3073	-	X
56	MG	CA	3077	-	X
56	MG	CA	3079	-	X
56	MG	CA	3085	-	X
56	MG	CA	3091	-	X
56	MG	CA	3096	-	X
56	MG	CA	3097	-	X
56	MG	CA	3107	-	X
56	MG	CA	3114	-	X
56	MG	CA	3118	-	X
56	MG	CA	3119	-	X
56	MG	CA	3121	-	X
56	MG	CA	3123	-	X
56	MG	CE	301	-	X
56	MG	DA	1602	-	X
56	MG	DA	1612	-	X
56	MG	DA	1616	-	X
56	MG	DA	1621	-	X
56	MG	DA	1628	-	X
56	MG	DA	1629	-	X
56	MG	DA	1631	-	X
56	MG	DA	1636	-	X
56	MG	DA	1640	-	X
56	MG	EA	3009	-	X
56	MG	EA	3011	-	X
56	MG	EA	3015	-	X
56	MG	EA	3020	-	X
56	MG	EA	3025	-	X
56	MG	EA	3027	-	X
56	MG	EA	3031	-	X
56	MG	EA	3034	-	X
56	MG	EA	3042	-	X
56	MG	EA	3049	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
56	MG	EA	3050	-	X
56	MG	EA	3052	-	X
56	MG	EA	3053	-	X
56	MG	EA	3055	-	X
56	MG	EA	3060	-	X
56	MG	EA	3061	-	X
56	MG	EA	3064	-	X
56	MG	EA	3067	-	X
56	MG	EA	3069	-	X
56	MG	EA	3073	-	X
56	MG	EA	3078	-	X
56	MG	EA	3079	-	X
56	MG	EA	3085	-	X
56	MG	EA	3087	-	X
56	MG	EA	3088	-	X
56	MG	EA	3099	-	X
56	MG	EA	3102	-	X
56	MG	EA	3107	-	X
56	MG	EA	3108	-	X
56	MG	EA	3114	-	X
56	MG	EA	3118	-	X
56	MG	EA	3120	-	X
56	MG	EA	3121	-	X
56	MG	EA	3122	-	X
56	MG	EA	3123	-	X
56	MG	EA	3126	-	X
56	MG	EA	3129	-	X
56	MG	EA	3131	-	X
56	MG	EA	3132	-	X
56	MG	ED	301	-	X
56	MG	EQ	201	-	X
56	MG	FA	1605	-	X
56	MG	FA	1608	-	X
56	MG	FA	1609	-	X
56	MG	FA	1610	-	X
56	MG	FA	1611	-	X
56	MG	FA	1612	-	X
56	MG	FA	1615	-	X
56	MG	FA	1621	-	X
56	MG	FA	1623	-	X
56	MG	FA	1624	-	X
56	MG	FA	1627	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
56	MG	FA	1628	-	X
56	MG	FA	1636	-	X
56	MG	FA	1639	-	X
56	MG	FA	1640	-	X
56	MG	FE	201	-	X
56	MG	GA	3004	-	X
56	MG	GA	3005	-	X
56	MG	GA	3009	-	X
56	MG	GA	3010	-	X
56	MG	GA	3014	-	X
56	MG	GA	3020	-	X
56	MG	GA	3029	-	X
56	MG	GA	3030	-	X
56	MG	GA	3033	-	X
56	MG	GA	3034	-	X
56	MG	GA	3037	-	X
56	MG	GA	3039	-	X
56	MG	GA	3040	-	X
56	MG	GA	3042	-	X
56	MG	GA	3044	-	X
56	MG	GA	3045	-	X
56	MG	GA	3047	-	X
56	MG	GA	3048	-	X
56	MG	GA	3051	-	X
56	MG	GA	3052	-	X
56	MG	GA	3059	-	X
56	MG	GA	3060	-	X
56	MG	GA	3061	-	X
56	MG	GA	3063	-	X
56	MG	GA	3067	-	X
56	MG	GA	3068	-	X
56	MG	GA	3070	-	X
56	MG	GA	3072	-	X
56	MG	GA	3073	-	X
56	MG	GA	3078	-	X
56	MG	GA	3080	-	X
56	MG	GA	3081	-	X
56	MG	GA	3083	-	X
56	MG	GA	3084	-	X
56	MG	GA	3087	-	X
56	MG	GA	3088	-	X
56	MG	GA	3091	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
56	MG	GA	3094	-	X
56	MG	GA	3100	-	X
56	MG	GA	3102	-	X
56	MG	GA	3103	-	X
56	MG	GA	3106	-	X
56	MG	GA	3108	-	X
56	MG	GA	3110	-	X
56	MG	GA	3111	-	X
56	MG	GA	3114	-	X
56	MG	GA	3115	-	X
56	MG	GA	3118	-	X
56	MG	GA	3120	-	X
56	MG	GA	3123	-	X
56	MG	GA	3129	-	X
56	MG	GA	3131	-	X
56	MG	GA	3133	-	X
56	MG	GB	1202	-	X
56	MG	GS	201	-	X
56	MG	HA	1601	-	X
56	MG	HA	1602	-	X
56	MG	HA	1603	-	X
56	MG	HA	1604	-	X
56	MG	HA	1607	-	X
56	MG	HA	1610	-	X
56	MG	HA	1611	-	X
56	MG	HA	1612	-	X
56	MG	HA	1613	-	X
56	MG	HA	1615	-	X
56	MG	HA	1621	-	X
56	MG	HA	1625	-	X
56	MG	HA	1626	-	X
56	MG	HA	1630	-	X
56	MG	HA	1632	-	X
56	MG	HA	1639	-	X
56	MG	HT	101	-	X

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 590573 atoms, of which 0 are hydrogen and 0 are deuterium.

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 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
1	CA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
1	EA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
1	GA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
2	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
2	EB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
2	GB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
3	CC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
3	EC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
3	GC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	GG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	CH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	EH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	GH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	CI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	EI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	GI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	CJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	EJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	GJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	CK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	EK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	GK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	CL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	EL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	GL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	GN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	116	Total	C	N	O		0	0	0
			892	552	178	162				
15	CO	116	Total	C	N	O		0	0	0
			892	552	178	162				
15	EO	116	Total	C	N	O		0	0	0
			892	552	178	162				
15	GO	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	CP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	EP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	GP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
17	CQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
17	EQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
17	GQ	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	CR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	ER	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	GR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	CS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	ES	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	GS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	CT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	ET	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	GT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	102	Total	C	N	O	0	0	0
			779	492	146	141			
21	CU	102	Total	C	N	O	0	0	0
			779	492	146	141			
21	EU	102	Total	C	N	O	0	0	0
			779	492	146	141			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	GU	102	Total	C	N	O	0	0	0
			779	492	146	141			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	CV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	EV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	GV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	CW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	EW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	GW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	CX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	EX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	GX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	CY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	EY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	GY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	CZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	EZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	GZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	E0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	G0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	A1	50	Total	C	N	O	0	0	0
			409	263	75	71			
28	C1	50	Total	C	N	O	0	0	0
			409	263	75	71			
28	E1	50	Total	C	N	O	0	0	0
			409	263	75	71			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	G1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	E2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	G2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	E3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	G3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	A4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	E4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	G4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	A5	148	Total	C	N	O	S	0	0	0
			1117	705	196	209	7			
32	E5	144	Total	C	N	O	S	0	0	0
			1092	691	192	202	7			

- Molecule 33 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
33	DA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
33	FA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
33	HA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	DB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	FB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	HB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
35	DC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
35	FC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
35	HC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
36	DD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
36	FD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
36	HD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
37	DE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
37	FE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
37	HE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
38	DF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
38	FF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
38	HF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
39	DG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
39	FG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	HG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
40	DH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
40	FH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
40	HH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
41	DI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
41	FI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
41	HI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
42	DJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
42	FJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
42	HJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 43 is a protein called 30S ribosomal protein S11.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
43	DK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
43	FK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
43	HK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
44	DL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
44	FL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
44	HL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
45	DM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
45	FM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
45	HM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
46	DN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
46	FN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	HN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
47	DO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
47	FO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
47	HO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
48	DP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
48	FP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
48	HP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
49	DQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
49	FQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
49	HQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BR	55	Total	C	N	O	0	0	0
			455	288	86	81			
50	DR	55	Total	C	N	O	0	0	0
			455	288	86	81			
50	FR	55	Total	C	N	O	0	0	0
			455	288	86	81			
50	HR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
51	DS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
51	FS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
51	HS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
52	DT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
52	FT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
52	HT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
53	DU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
53	FU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	HU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 54 is a protein called elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BV	689	Total	C	N	O	S	0	0	0
			5319	3345	919	1030	25			
54	DV	689	Total	C	N	O	S	0	0	0
			5319	3345	919	1030	25			
54	FV	689	Total	C	N	O	S	0	0	0
			5319	3345	919	1030	25			
54	HV	689	Total	C	N	O	S	0	0	0
			5319	3345	919	1030	25			

- Molecule 55 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BW	6	Total	C	N	O	0	0	0
			48	25	13	10			
55	DW	6	Total	C	N	O	0	0	0
			48	25	13	10			
55	FW	6	Total	C	N	O	0	0	0
			48	25	13	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	FA	41	Total	Mg	0	0
			41	41		
56	BA	40	Total	Mg	0	0
			40	40		
56	CA	134	Total	Mg	0	0
			134	134		
56	HE	1	Total	Mg	0	0
			1	1		
56	AB	4	Total	Mg	0	0
			4	4		
56	BL	1	Total	Mg	0	0
			1	1		
56	BE	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	GA	134	Total 134	Mg 134	0	0
56	DU	1	Total 1	Mg 1	0	0
56	EB	4	Total 4	Mg 4	0	0
56	FU	1	Total 1	Mg 1	0	0
56	FV	1	Total 1	Mg 1	0	0
56	C4	1	Total 1	Mg 1	0	0
56	AE	1	Total 1	Mg 1	0	0
56	AA	130	Total 130	Mg 130	0	0
56	FE	1	Total 1	Mg 1	0	0
56	GB	4	Total 4	Mg 4	0	0
56	DV	1	Total 1	Mg 1	0	0
56	EA	133	Total 133	Mg 133	0	0
56	BU	1	Total 1	Mg 1	0	0
56	GC	1	Total 1	Mg 1	0	0
56	AD	1	Total 1	Mg 1	0	0
56	HT	1	Total 1	Mg 1	0	0
56	GL	1	Total 1	Mg 1	0	0
56	DA	42	Total 42	Mg 42	0	0
56	EC	1	Total 1	Mg 1	0	0
56	HC	1	Total 1	Mg 1	0	0
56	BV	1	Total 1	Mg 1	0	0

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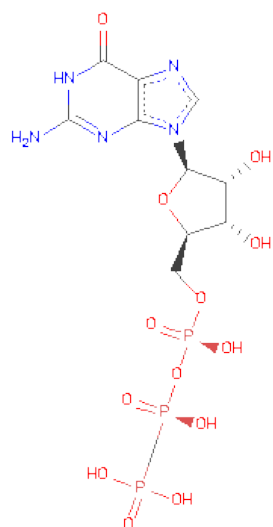
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CB	4	Total 4	Mg 4	0	0
56	GS	1	Total 1	Mg 1	0	0
56	AC	3	Total 3	Mg 3	0	0
56	EQ	1	Total 1	Mg 1	0	0
56	ED	2	Total 2	Mg 2	0	0
56	CD	1	Total 1	Mg 1	0	0
56	AT	1	Total 1	Mg 1	0	0
56	CE	1	Total 1	Mg 1	0	0
56	A3	1	Total 1	Mg 1	0	0
56	HA	40	Total 40	Mg 40	0	0
56	HV	1	Total 1	Mg 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	E4	1	Total 1	Zn 1	0	0
57	G4	1	Total 1	Zn 1	0	0
57	A4	1	Total 1	Zn 1	0	0
57	C4	1	Total 1	Zn 1	0	0

- Molecule 58 is PHOSPHOMETHYLPHOSPHONICACID GUANYLATE ESTER (three-letter code: GCP) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	BV	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
58	DV	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
58	FV	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
58	HV	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	608	Total	O	0	0
			608	608		
59	AB	19	Total	O	0	0
			19	19		
59	AC	10	Total	O	0	0
			10	10		
59	AD	3	Total	O	0	0
			3	3		
59	AE	1	Total	O	0	0
			1	1		
59	AJ	1	Total	O	0	0
			1	1		
59	AL	7	Total	O	0	0
			7	7		
59	AN	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AP	1	Total O 1 1	0	0
59	AQ	1	Total O 1 1	0	0
59	AS	1	Total O 1 1	0	0
59	AU	1	Total O 1 1	0	0
59	A0	1	Total O 1 1	0	0
59	A3	1	Total O 1 1	0	0
59	A4	2	Total O 2 2	0	0
59	BA	197	Total O 197 197	0	0
59	BC	1	Total O 1 1	0	0
59	BD	1	Total O 1 1	0	0
59	BI	1	Total O 1 1	0	0
59	BK	1	Total O 1 1	0	0
59	BN	3	Total O 3 3	0	0
59	BT	2	Total O 2 2	0	0
59	BU	1	Total O 1 1	0	0
59	BV	1	Total O 1 1	0	0
59	CA	604	Total O 604 604	0	0
59	CB	20	Total O 20 20	0	0
59	CC	11	Total O 11 11	0	0
59	CD	3	Total O 3 3	0	0
59	CE	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CF	1	Total 1	O 1	0	0
59	CJ	3	Total 3	O 3	0	0
59	CL	6	Total 6	O 6	0	0
59	CN	4	Total 4	O 4	0	0
59	CS	1	Total 1	O 1	0	0
59	CT	2	Total 2	O 2	0	0
59	C2	1	Total 1	O 1	0	0
59	C3	1	Total 1	O 1	0	0
59	C4	2	Total 2	O 2	0	0
59	DA	193	Total 193	O 193	0	0
59	DC	1	Total 1	O 1	0	0
59	DE	2	Total 2	O 2	0	0
59	DG	1	Total 1	O 1	0	0
59	DK	1	Total 1	O 1	0	0
59	DL	1	Total 1	O 1	0	0
59	DN	6	Total 6	O 6	0	0
59	DQ	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	EA	617	Total 617	O 617	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	EB	20	Total 20	O 20	0	0
59	EC	8	Total 8	O 8	0	0
59	ED	1	Total 1	O 1	0	0
59	EL	4	Total 4	O 4	0	0
59	EN	2	Total 2	O 2	0	0
59	ER	1	Total 1	O 1	0	0
59	ET	1	Total 1	O 1	0	0
59	EU	1	Total 1	O 1	0	0
59	E0	2	Total 2	O 2	0	0
59	E3	2	Total 2	O 2	0	0
59	E4	1	Total 1	O 1	0	0
59	FA	198	Total 198	O 198	0	0
59	FE	1	Total 1	O 1	0	0
59	FK	1	Total 1	O 1	0	0
59	FN	3	Total 3	O 3	0	0
59	FQ	1	Total 1	O 1	0	0
59	FT	4	Total 4	O 4	0	0
59	FV	1	Total 1	O 1	0	0
59	GA	607	Total 607	O 607	0	0
59	GB	19	Total 19	O 19	0	0
59	GC	9	Total 9	O 9	0	0

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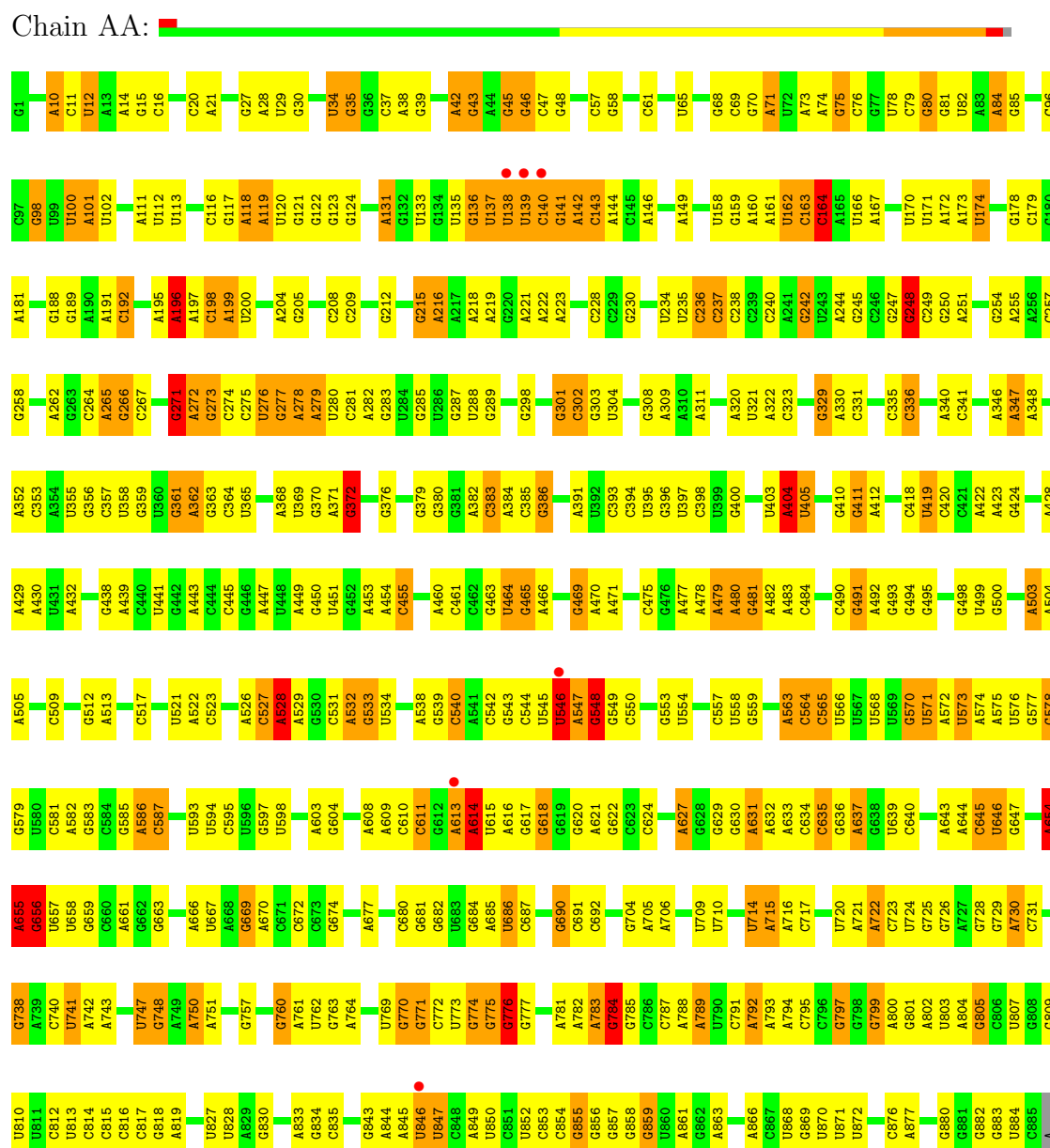
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	GD	4	Total 4	O 4	0	0
59	GE	2	Total 2	O 2	0	0
59	GL	4	Total 4	O 4	0	0
59	GN	3	Total 3	O 3	0	0
59	GQ	1	Total 1	O 1	0	0
59	GR	2	Total 2	O 2	0	0
59	GS	1	Total 1	O 1	0	0
59	GT	1	Total 1	O 1	0	0
59	GU	2	Total 2	O 2	0	0
59	GV	1	Total 1	O 1	0	0
59	G2	2	Total 2	O 2	0	0
59	G3	1	Total 1	O 1	0	0
59	G4	1	Total 1	O 1	0	0
59	HA	197	Total 197	O 197	0	0
59	HD	1	Total 1	O 1	0	0
59	HE	3	Total 3	O 3	0	0
59	HN	5	Total 5	O 5	0	0
59	HT	1	Total 1	O 1	0	0
59	HU	1	Total 1	O 1	0	0
59	HV	1	Total 1	O 1	0	0

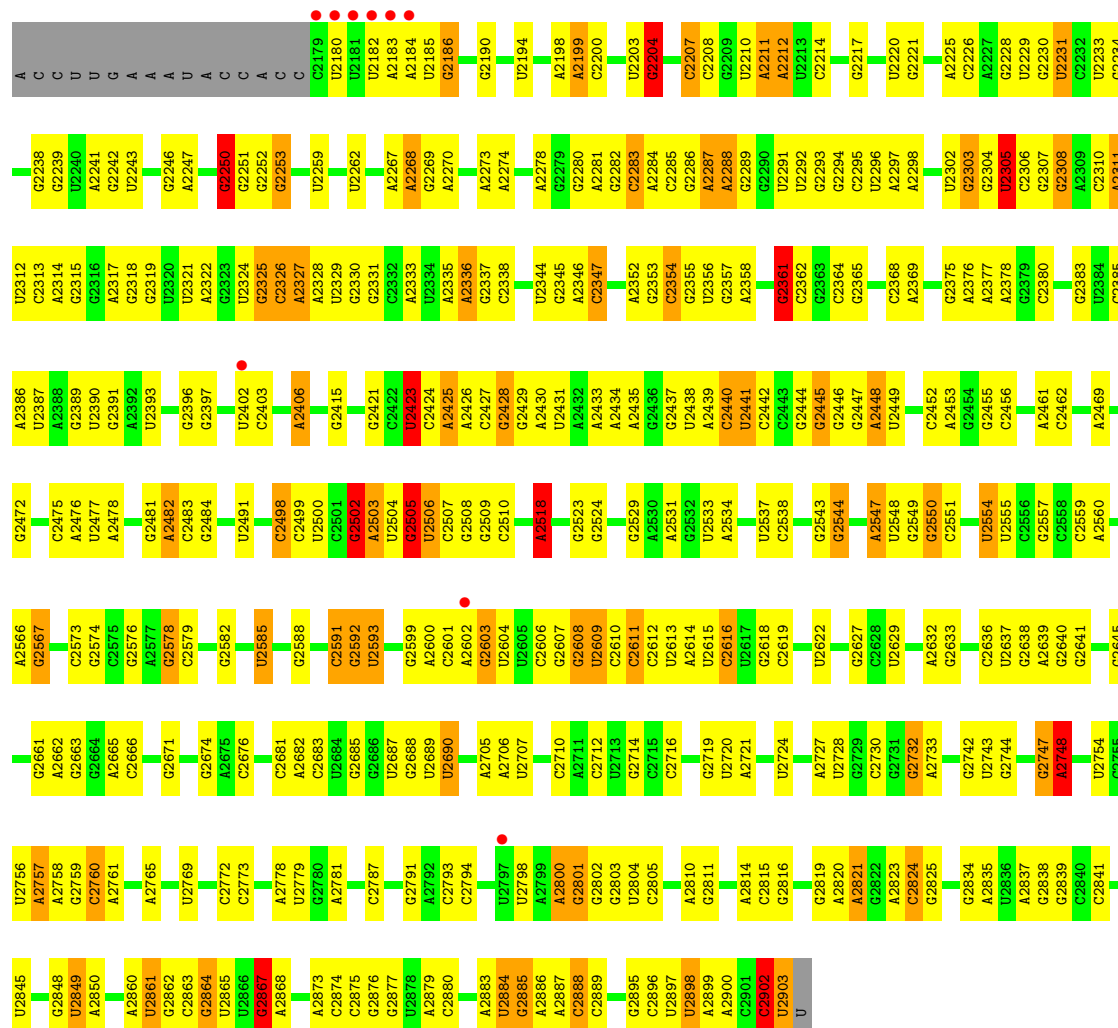
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 23S rRNA

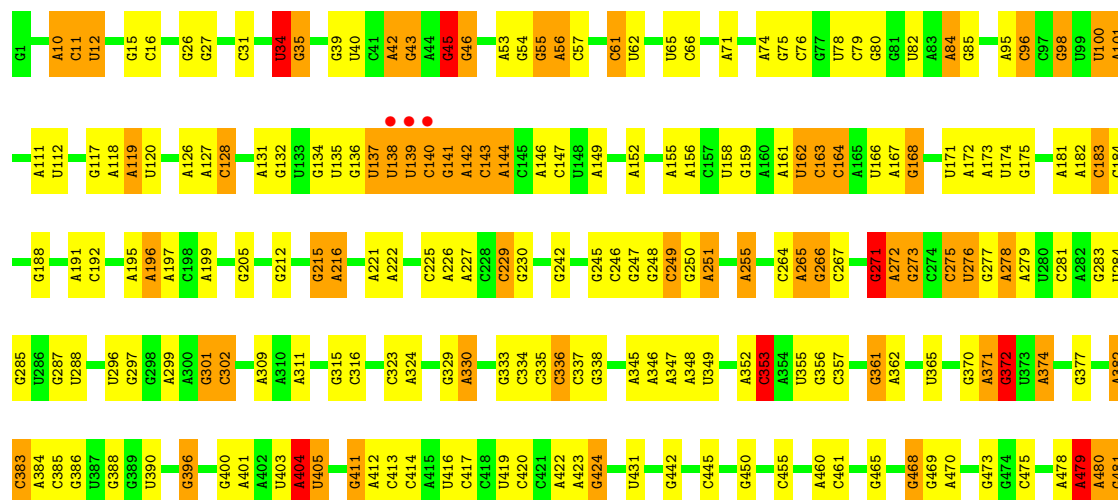


C2103	A2020	G1799	G1723	G1643	G1543	A1469	A1387	C1297	G1136	U1060	A981	C	U
C2104	C2021	C1800	G1724	G1644	A1544	A1470	G1386	C1298	G1137	U1061	C982	C	
U2105	U2022	A1801	U1725	G1645	A1545	A1471	G1389	G1299	G1138	G1062	A983	C	
U2106	C2023	A1802	C1726	G1646	A1546	A1472	U1390	G1300	G1139	G1063	A984	C	
C2107	G2024	A1805	C1727	G1647	A1547	G1473	U1394	A1301	U1141	C1064	C985	G	
A2108	C2025	A1806	G1728	U1647	A1548	G1474	A1395	C1305	U1231	U1065	A892		
U2109	U2026	G1807	U1729	G1648	A1551	A1475	U1396	C1306	G1232	U1066	C993		
U2110	G2027	A1808	C1730	G1649	A1552	A1476	U1397	A1307	U1233	A1067	A990		
U	A2030	G1811	G1731	A1650	G1555	G1477	U1398	G1308	U1234	U1068	C991		
G	A2031	A1812	C1732	G1651	C1556	G1478	U1399	A1309	G1235	A1069	C995		
A	G2032	G1813	G1733	A1652	G1557	U1481	U1400	G1309	G1236	G1071	A996		
G	A2033	G1814	U1734	G1653	C1567	G1482	G1401	C1315	U1237	C1072	A910		
G	G1935	G1815	U1735	A1654	G1567	G1483	U1402	U1316	G1238	A1073	A911		
A	A1936	A1816	U1736	A1655	G1568	U1484	A1403	G1317	U1239	A1009	U999		
U	A1937	C1816	G1737	C1656	A1569	U1486	A1404	U1318	G1074	A1001	A1000		
A	A1938	G1817	U1738	U1657	G1569	U1487	U1405	C1319	A1165	C1075	G914		
G	U1939	U1818	C1739	C1658	C1574	U1487	U1406	A1322	C1176	A1076	C915		
A	C2043	U1819	G1740	A1665	U1578	C1493	G1410	A1327	G1177	C1077	G916		
G	C2047	U1820	C1741	G1666	U1579	A1494	U1411	A1328	A1189	C1078	A917		
U	G1944	U1821	U1742	G1667	U1581	A1495	U1412	U1329	G1178	C1079	A918		
G	G1945	G1823	U1743	A1668	C1582	A1496	U1413	U1330	G1179	U1081	U919		
G	U1955	G1824	A1744	A1669	C1583	G1500	G1416	G1331	U1180	U1082	A920		
G	U1956	A1745	U1746	C1670	U1584	G1501	U1417	C1332	U1181	U1083	C921		
A	C1957	G1828	U1747	U1671	C1585	G1502	G1418	G1333	U1182	C1084	G922		
G	C1958	A1829	C1748	A1672	A1586	U1503	U1419	U1334	U1183	A1085	G923		
C	C1959	C1830	U1749	G1673	G1587	A1504	A1420	U1335	U1184	C1086	A927		
C	G1964	G1831	G1753	G1674	A1591	A1508	G1421	A1336	G1177	U1087	G1017		
U	C1967	C1832	A1754	C1675	A1592	A1509	U1422	G1337	C1178	A1088	U1018		
U	G1968	C1833	A1755	A1677	A1593	G1510	G1423	G1338	U1179	U1089	U932		
G	G1969	U1841	U1756	U1683	C1593	G1511	G1424	G1339	U1180	A1090	A933		
A	A1970	G1842	U1757	G1684	C1595	U1512	G1425	U1340	U1181	G1091	U1020		
G	U1971	C1843	U1758	C1685	G1596	U1513	G1426	G1341	U1182	A1092	U1021		
G	G1972	U1847	U1759	C1686	G1601	U1514	C1427	A1342	G1183	U1093	U1022		
U	C2065	A1848	C1761	G1687	U1602	U1515	G1428	G1343	U1184	U1094	G1023		
G	C2066	A1849	U1765	G1687	A1603	G1516	G1429	U1344	U1263	G1024	A941		
G	C2067	A1853	U1766	A1690	C1604	U1517	A1431	C1350	U1264	U1097	G1025		
G	U2068	U1857	U1767	C1691	C1605	G1518	A1432	C1351	G1185	A1098	G1026		
G	G1980	G1858	C1771	U1692	C1606	U1519	G1433	G1352	G1186	G1099	A945		
A	A2070	A1859	U1772	U1693	C1607	U1520	G1434	U1267	G1187	A1028	C946		
G	C2072	U1865	A1773	C1694	A1608	G1521	C1437	A1268	U1188	A1029	A947		
G	U2076	A1866	C1774	G1695	A1609	U1522	U1438	G1360	G1190	G1030	C948		
G	U1991	U1867	U1775	A1705	A1610	U1523	U1439	G1361	G1193	A1032	G953		
G	G1992	G1869	U1776	C1706	G1613	G1524	G1441	A1364	U1270	U1033	G954		
G	U1993	C1870	U1777	A1713	A1616	A1525	U1442	A1365	G1271	G1110	U958		
G	C1996	A1871	U1781	U1714	G1617	U1526	U1443	G1366	U1272	A1111	A959		
G	C1997	A1872	U1782	G1710	A1618	G1527	G1444	G1367	U1273	G1112	A960		
G	A1998	G1875	A1783	U1711	G1619	U1528	U1445	C1370	A1276	C1114	C962		
G	C2006	G1878	U1784	U1712	G1620	G1529	G1446	G1371	G1202	G1122	U963		
G	U2007	C1879	A1789	U1713	G1621	C1531	U1447	G1377	A1205	G1125	C964		
G	A2015	U1884	U1790	U1714	G1622	A1532	U1448	A1378	G1206	A1126	G971		
G	U2016	G1884	U1791	G1715	G1623	U1533	G1456	C1379	C1207	C1052	A972		
G	U2017	G1906	U1796	U1716	G1624	U1534	U1457	G1380	U1130	C1053	A973		
C	G2100	G2101	U1797	U1717	C1625	A1535	U1458	A1383	G1215	U1131	G974		
G	A2019	G2102	U1798	G1718	A1626	C1536	U1459	A1384	G1216	U1132	A975		
G				U1719	G1627	G1537	G1460	A1385	U1219	A1133	U1057		
G				A1722	C1638	U1538	G1464	C1386	G1220	A1134	U1058		
											G1059		

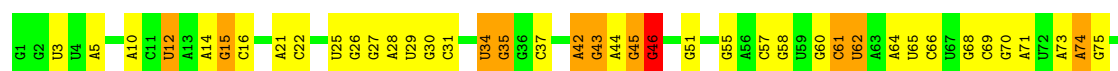


• Molecule 1: 23S rRNA

Chain CA:



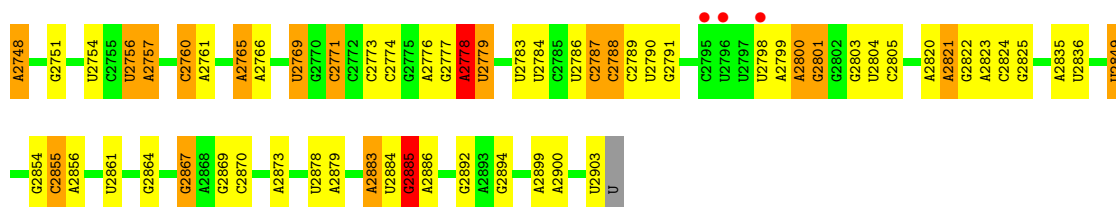
C1732	C1733	G1734	A1735	G1736	G1737	G1738	A1739	G1740	A1744	A1745	G1753	A1754	A1755	G1756	A1757	U1758	A1759	C1760	C1761	A1762	G1763	C1764	U1765	G1770	A1773	C1774	U1775	G1776	U1777	U1778	U1779	A1780	U1781	U1782	A1783	A1784	A1785	A1786	C1790	A1791	G1792	C1793	A1794	G1795	U1796	G1797	U1798	G1799	C1800	A1801	A1802	A1805																																																																																																																																																																																																													
U1621	G1622	G1623	A1626	G1627	A1630	A1635	U1636	A1637	U1647	U1648	G1649	A1652	G1653	A1654	A1655	G1656	G1657	A1658	A1659	A1660	A1661	A1662	A1663	A1664	A1665	A1666	A1667	A1668	A1669	A1670	A1671	A1672	A1673	A1674	A1675	A1676	A1677	A1678	A1679	A1680	A1681	A1682	A1683	A1684	A1685	A1686	A1687	A1688	A1689	A1690	A1691	A1692	A1693	A1694	A1695	A1696	A1697	A1698	A1699	A1700	A1701	A1702	A1703	A1704	A1705	A1706	A1707	A1708	A1709	A1710	A1711	A1712	A1713	A1714	A1715	A1716	A1717	A1718	A1719	A1720	A1721	A1722	A1723	A1724	A1725	A1726	A1727	A1728	A1729	A1730	A1731																																																																																																																																																																						
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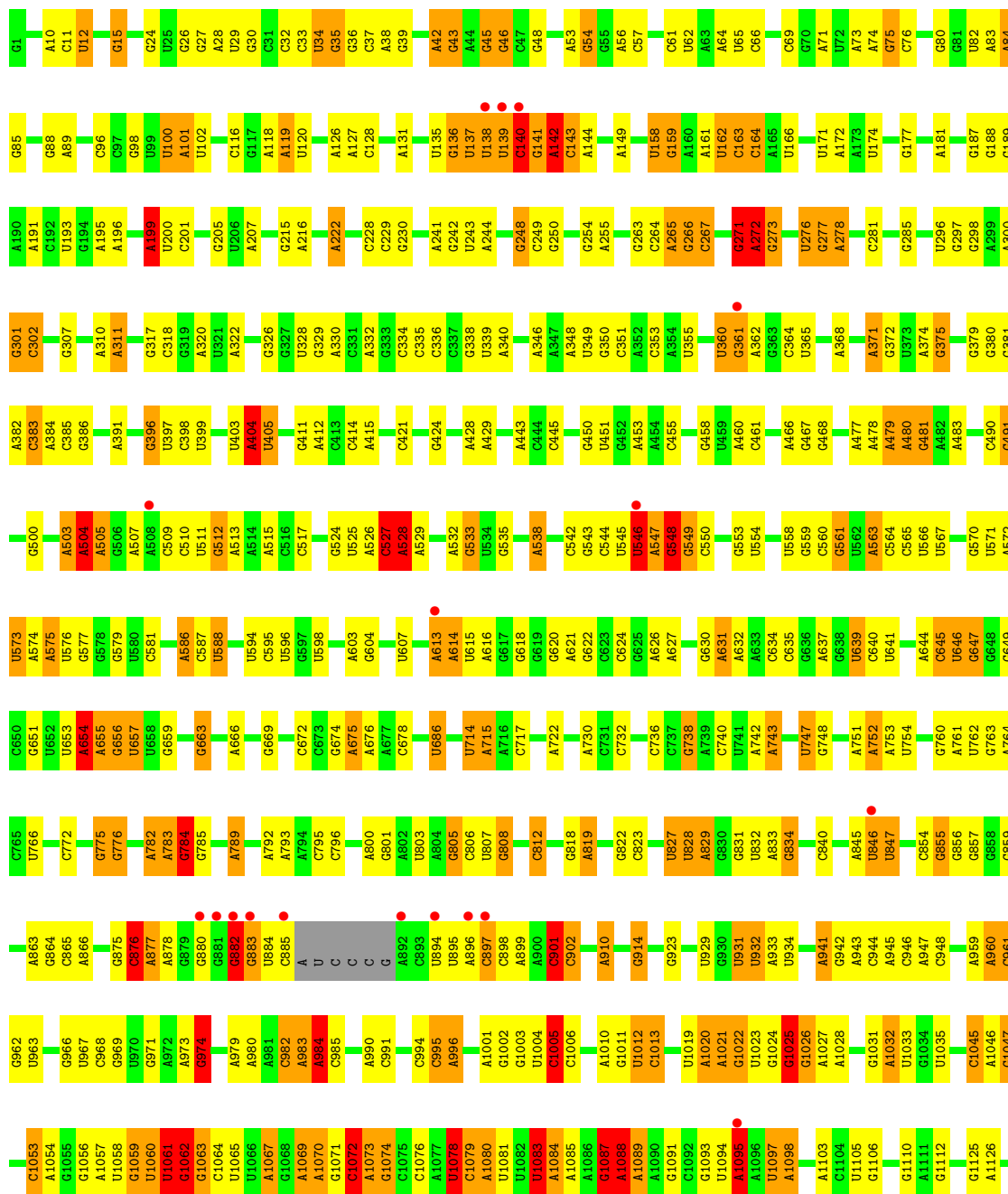
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G1421			A1080	C987	C907	U844	U844	G776	U667	C587	G515	U425	A241		
G1422			A1080	C987	C907	U845	U845	G776	U668	C588	G516	U426	A242		
			A1080	C987	C907	U846	U846	G776	U669	C589	G517	U427	A243		
			A1080	C987	C907	U847	U847	G776	U670	C590	G518	U428	A244		
			A1080	C987	C907	U848	U848	G776	U671	C591	G519	U429	A245		
			A1080	C987	C907	U849	U849	G776	U672	C592	G520	U430	A246		
			A1080	C987	C907	U850	U850	G776	U673	C593	G521	U431	A247		
			A1080	C987	C907	U851	U851	G776	U674	C594	G522	U432	A248		
			A1080	C987	C907	U852	U852	G776	U675	C595	G523	U433	A249		
			A1080	C987	C907	U853	U853	G776	U676	C596	G524	U434	A250		
			A1080	C987	C907	U854	U854	G776	U677	C597	G525	U435	A251		
			A1080	C987	C907	U855	U855	G776	U678	C598	G526	U436	A252		
			A1080	C987	C907	U856	U856	G776	U679	C599	G527	U437	A253		
			A1080	C987	C907	U857	U857	G776	U680	C600	G528	U438	A254		
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			A1080	C987	C907	U861	U861	G776	U684	C604	G532	U442	A258		
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			A1080	C987	C907	U864	U864	G776	U687	C607	G535	U445	A261		
			A1080	C987	C907	U865	U865	G776	U688	C608	G536	U446	A262		
			A1080	C987	C907	U866	U866	G776	U689	C609	G537	U447	A263		
			A1080	C987	C907	U867	U867	G776	U690	C610	G538	U448	A264		
			A1080	C987	C907	U868	U868	G776	U691	C611	G539	U449	A265		
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			A1080	C987	C907	U870	U870	G776	U693	C613	G541	U451	A267		
			A1080	C987	C907	U871	U871	G776	U694	C614	G542	U452	A268		
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			A1080	C987	C907	U873	U873	G776	U696	C616	G544	U454	A270		
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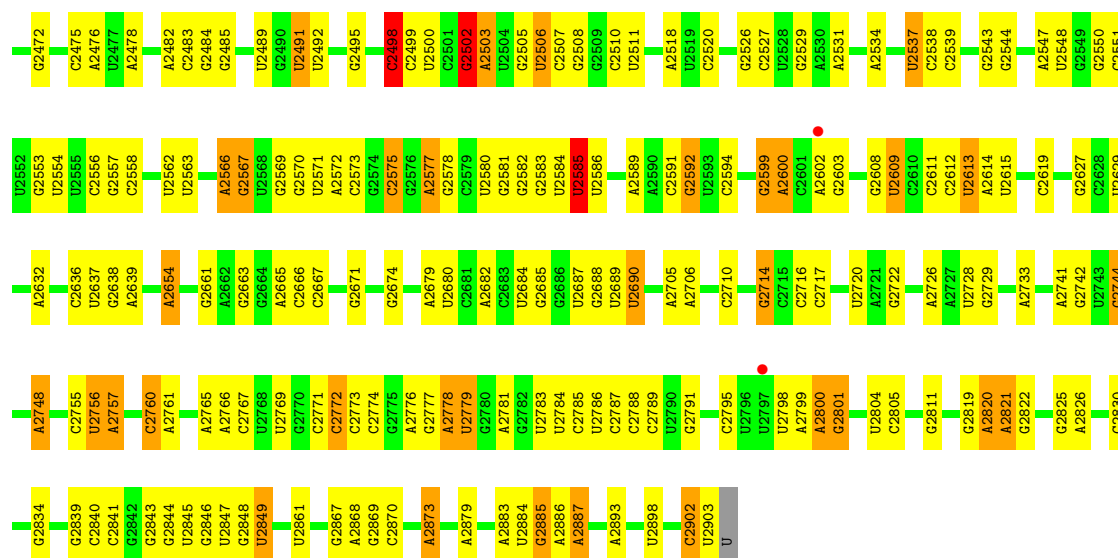


• Molecule 1: 23S rRNA

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U2387	A2388	G2308	U2212	C2145	C2078	G1884	U1797	U1715	A1603	U1476	A1392	G1300	U1231	U1132
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G2328	U2324	U2099	A2020	C2147	U2099	G1891	G1814	G1731	C1617	C1507	A1413	G1317	A1249	A1151
G2329	G2239	A2101	C2021	C2148	A2101	U1915	A1815	G1732	G1619	A1509	G1416	A1321	U1249	G1154
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A2287	A2287	U2109	U2029	U2109	U2109	A1927	U1825	A1744	U1636	G1524	A1427	A1336	U1255	G1186
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G2289	G2289													





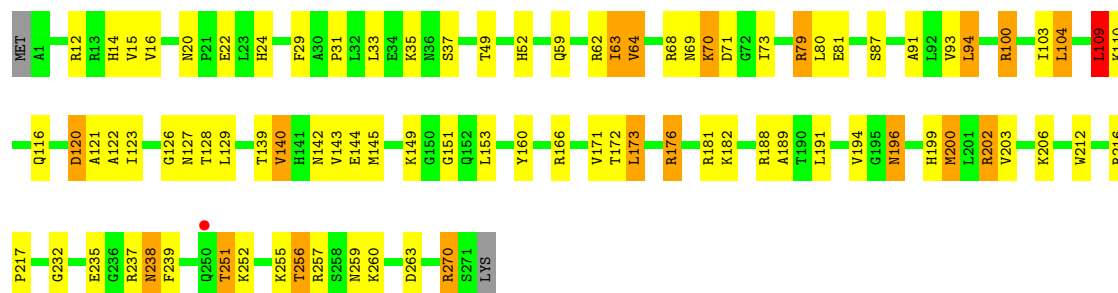
- Molecule 3: 50S ribosomal protein L2

Chain AC:



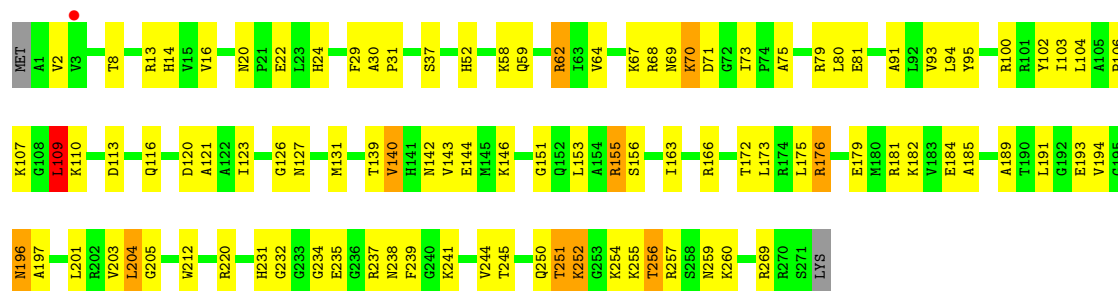
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Chain CC:



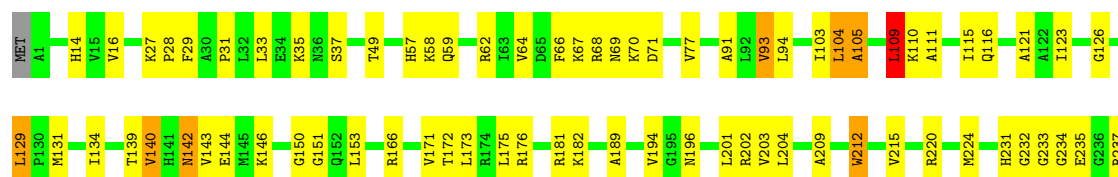
- Molecule 3: 50S ribosomal protein L2

Chain EC:



- Molecule 3: 50S ribosomal protein L2

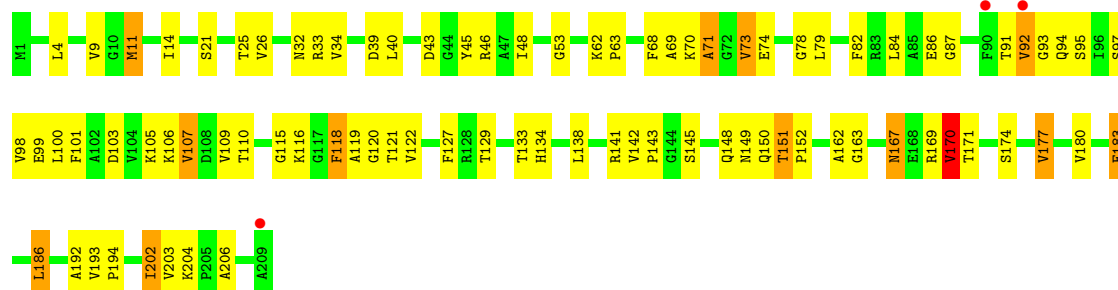
Chain GC:





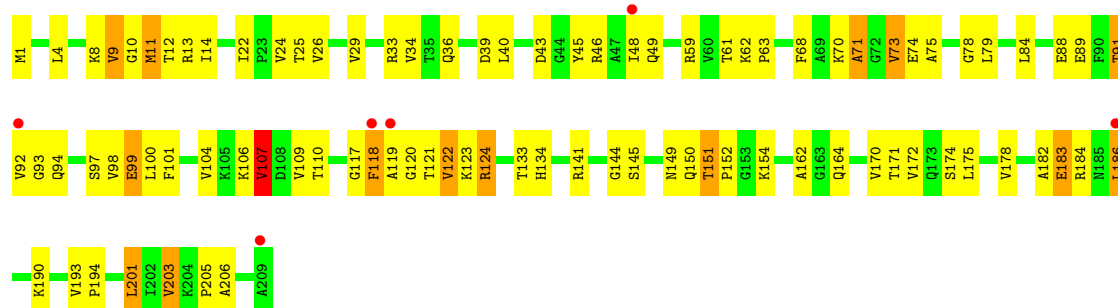
• Molecule 4: 50S ribosomal protein L3

Chain AD:



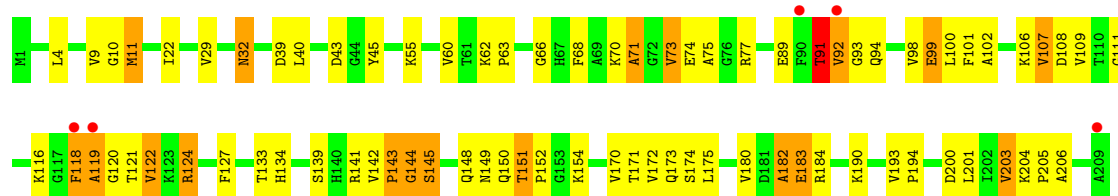
• Molecule 4: 50S ribosomal protein L3

Chain CD:



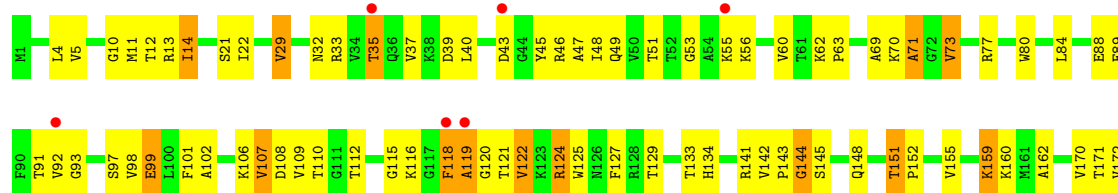
• Molecule 4: 50S ribosomal protein L3

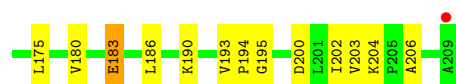
Chain ED:



• Molecule 4: 50S ribosomal protein L3

Chain GD:





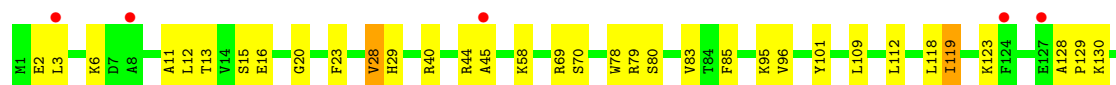
- Molecule 5: 50S ribosomal protein L4

Chain AE:



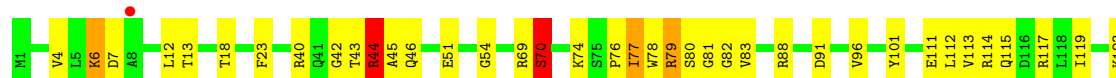
- Molecule 5: 50S ribosomal protein L4

Chain CE:



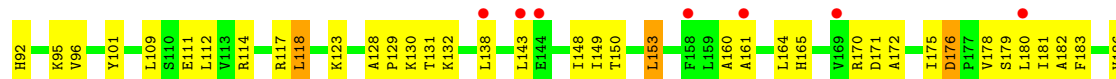
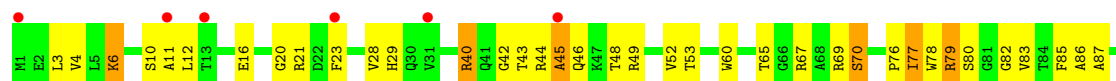
- Molecule 5: 50S ribosomal protein L4

Chain EE:



- Molecule 5: 50S ribosomal protein L4

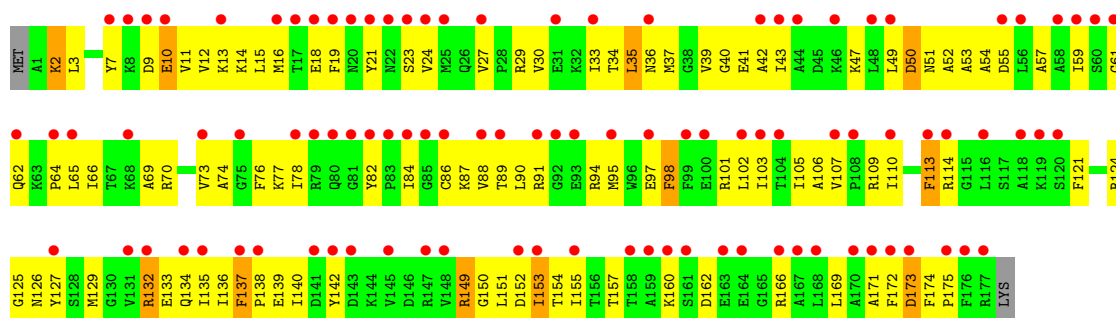
Chain GE:



- Molecule 6: 50S ribosomal protein L5

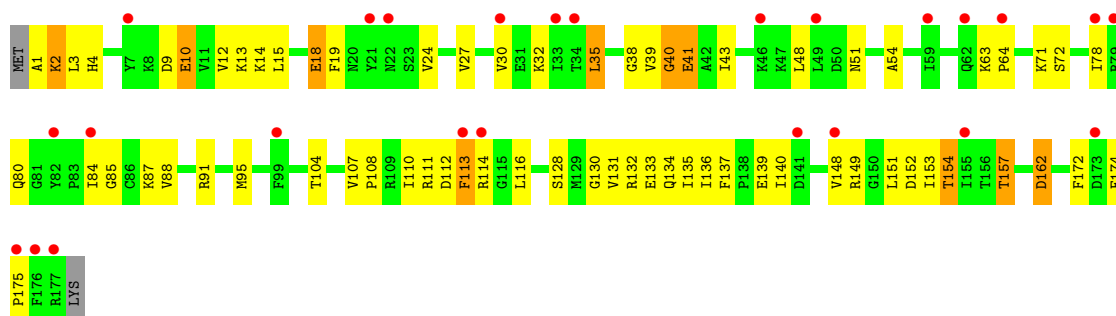
Chain AF:





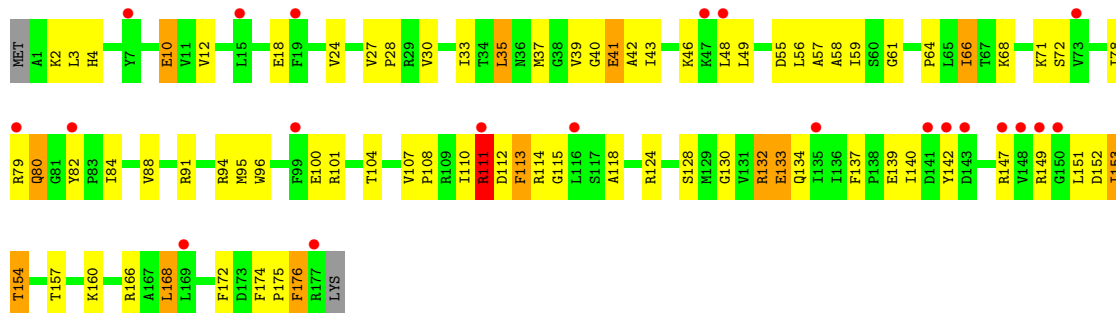
• Molecule 6: 50S ribosomal protein L5

Chain CF:



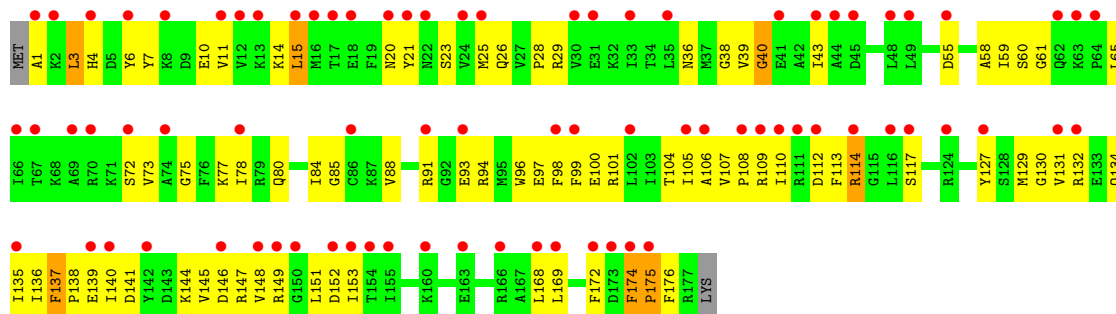
• Molecule 6: 50S ribosomal protein L5

Chain EF:



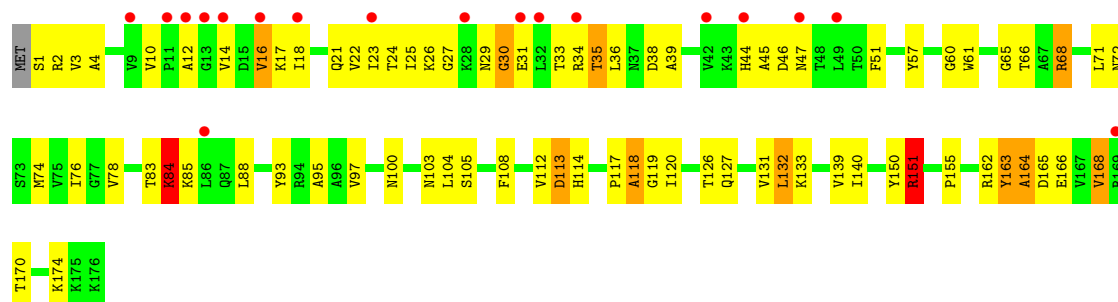
• Molecule 6: 50S ribosomal protein L5

Chain GF:



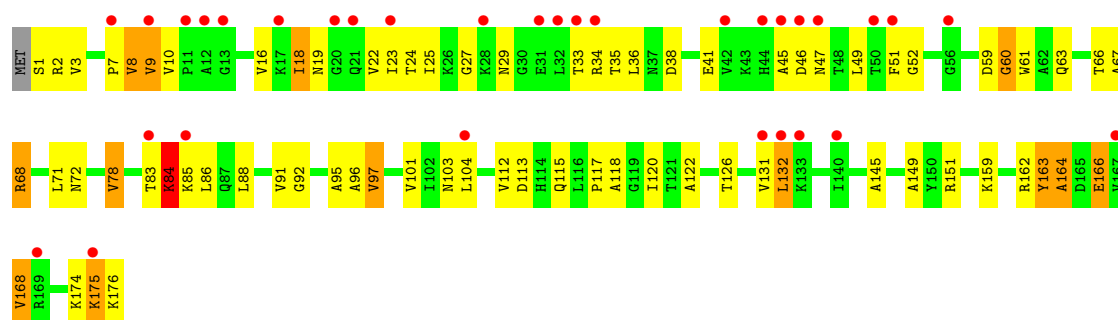
• Molecule 7: 50S ribosomal protein L6

Chain AG:



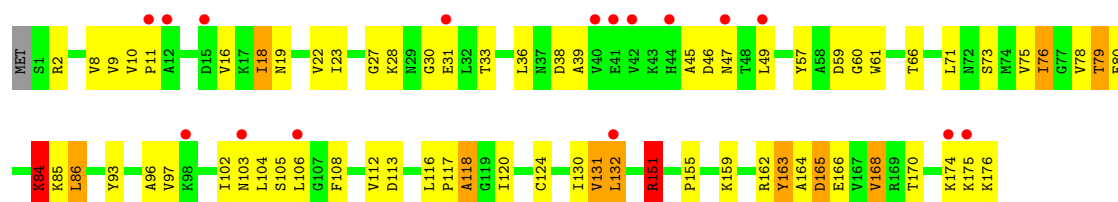
- Molecule 7: 50S ribosomal protein L6

Chain CG:



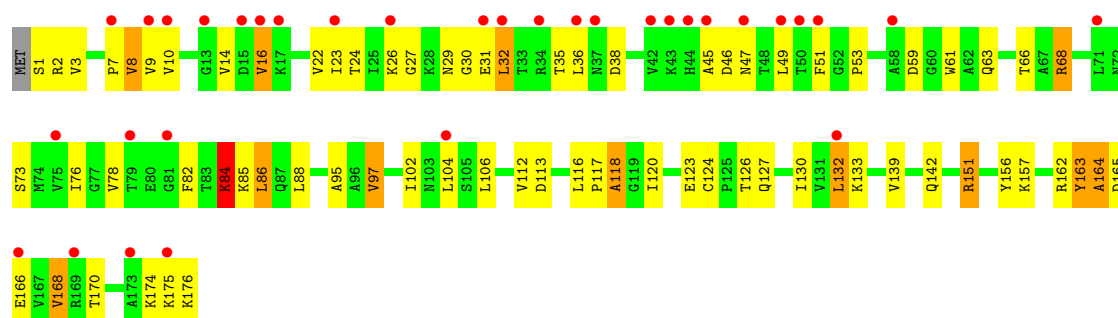
- Molecule 7: 50S ribosomal protein L6

Chain EG:



- Molecule 7: 50S ribosomal protein L6

Chain GG:



- Molecule 8: 50S ribosomal protein L9

Chain AH:



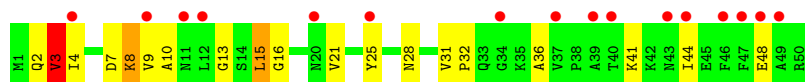
- Molecule 8: 50S ribosomal protein L9

Chain CH:



- Molecule 8: 50S ribosomal protein L9

Chain EH:



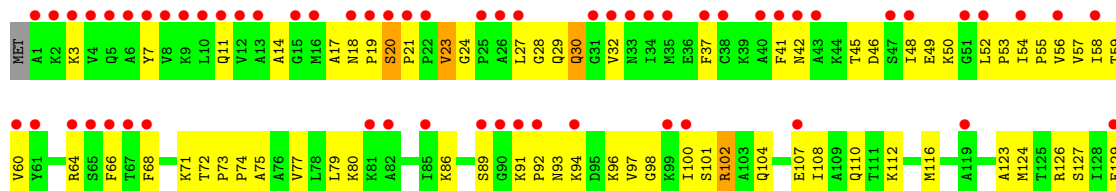
- Molecule 8: 50S ribosomal protein L9

Chain GH:



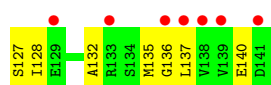
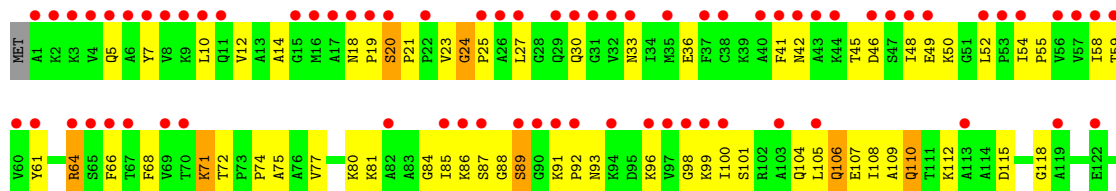
- Molecule 9: 50S ribosomal protein L11

Chain AI:

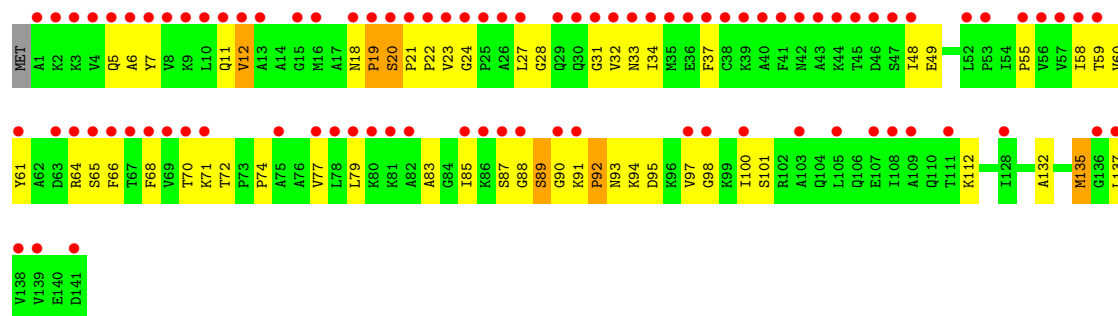


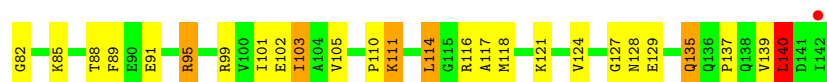
- Molecule 9: 50S ribosomal protein L11

Chain CI:



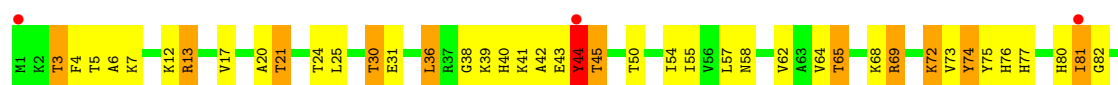
- Molecule 9: 50S ribosomal protein L11

Chain EI: 



- Molecule 10: 50S ribosomal protein L13

Chain GJ:



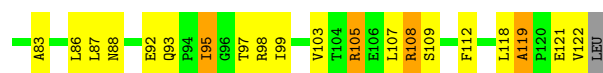
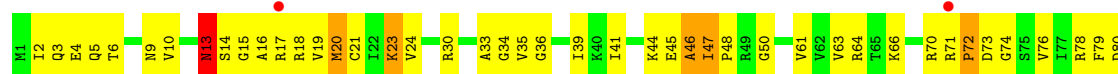
- Molecule 11: 50S ribosomal protein L14

Chain AK:



- Molecule 11: 50S ribosomal protein L14

Chain CK:



- Molecule 11: 50S ribosomal protein L14

Chain EK:



- Molecule 11: 50S ribosomal protein L14

Chain GK:





- Molecule 12: 50S ribosomal protein L15

Chain AL:



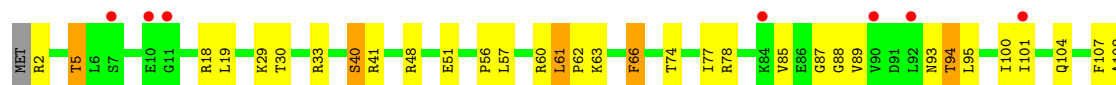
- Molecule 12: 50S ribosomal protein L15

Chain CL:



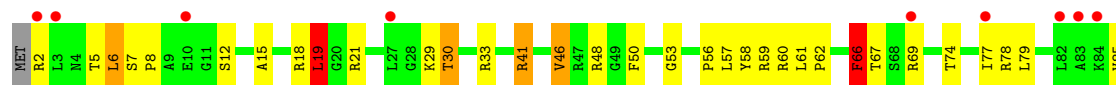
- Molecule 12: 50S ribosomal protein L15

Chain EL:



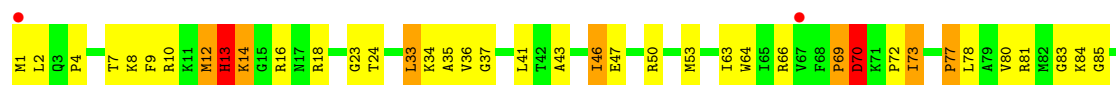
- Molecule 12: 50S ribosomal protein L15

Chain GL:



- Molecule 13: 50S ribosomal protein L16

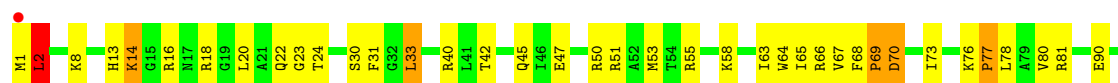
Chain AM:





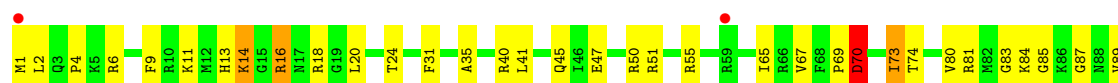
- Molecule 13: 50S ribosomal protein L16

Chain CM:



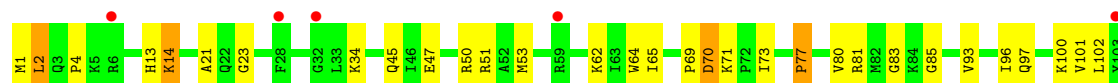
- Molecule 13: 50S ribosomal protein L16

Chain EM:



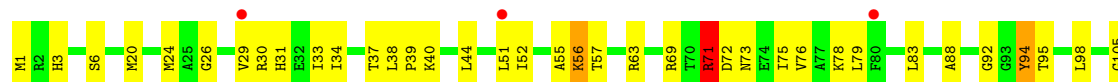
- Molecule 13: 50S ribosomal protein L16

Chain GM:



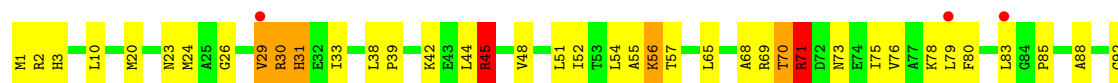
- Molecule 14: 50S ribosomal protein L17

Chain AN:



- Molecule 14: 50S ribosomal protein L17

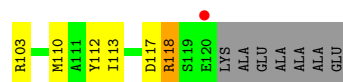
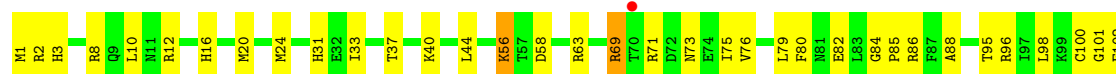
Chain CN:





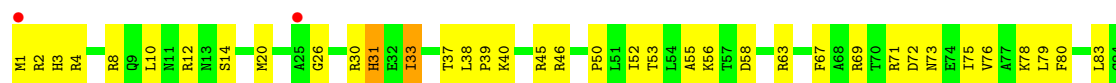
- Molecule 14: 50S ribosomal protein L17

Chain EN:



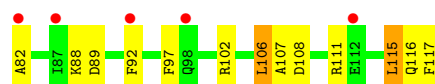
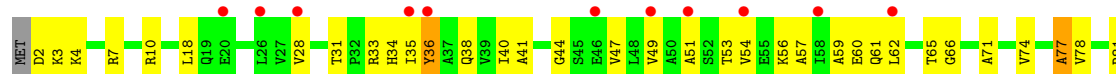
- Molecule 14: 50S ribosomal protein L17

Chain GN:



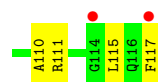
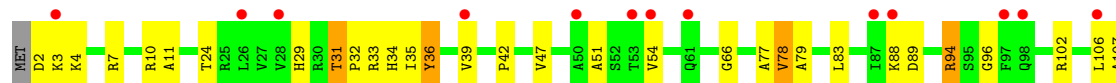
- Molecule 15: 50S ribosomal protein L18

Chain AO:



- Molecule 15: 50S ribosomal protein L18

Chain CO:

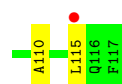


- Molecule 15: 50S ribosomal protein L18

Chain EO:







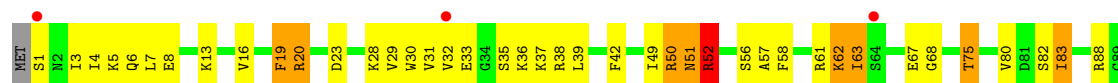
- Molecule 15: 50S ribosomal protein L18

Chain GO:



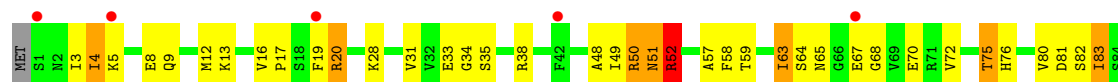
- Molecule 16: 50S ribosomal protein L19

Chain AP:



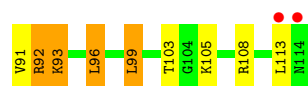
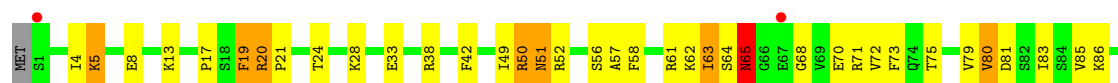
- Molecule 16: 50S ribosomal protein L19

Chain CP:



- Molecule 16: 50S ribosomal protein L19

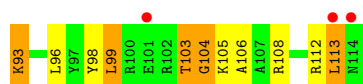
Chain EP:



- Molecule 16: 50S ribosomal protein L19

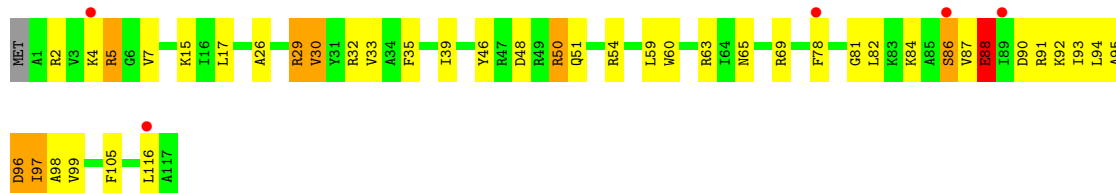
Chain GP:





- Molecule 17: 50S ribosomal protein L20

Chain AQ:



- Molecule 17: 50S ribosomal protein L20

Chain CQ:



- Molecule 17: 50S ribosomal protein L20

Chain EQ:



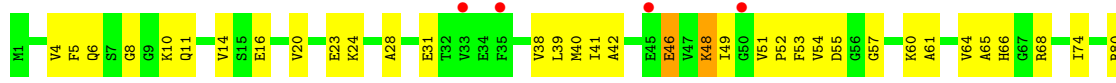
- Molecule 17: 50S ribosomal protein L20

Chain GQ:



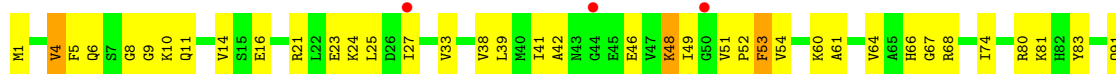
- Molecule 18: 50S ribosomal protein L21

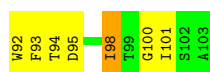
Chain AR:



- Molecule 18: 50S ribosomal protein L21

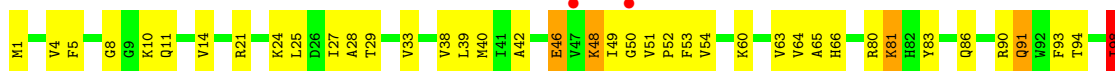
Chain CR:





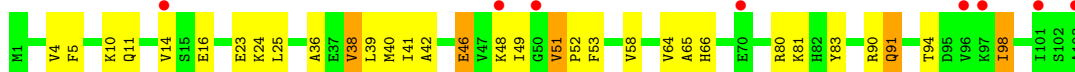
- Molecule 18: 50S ribosomal protein L21

Chain ER:



- Molecule 18: 50S ribosomal protein L21

Chain GR:



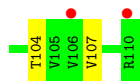
- Molecule 19: 50S ribosomal protein L22

Chain AS:



- Molecule 19: 50S ribosomal protein L22

Chain CS:



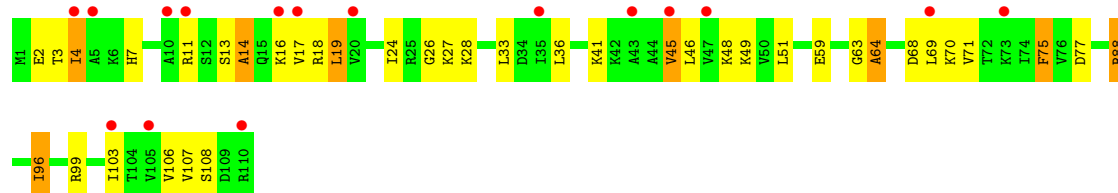
- Molecule 19: 50S ribosomal protein L22

Chain ES:



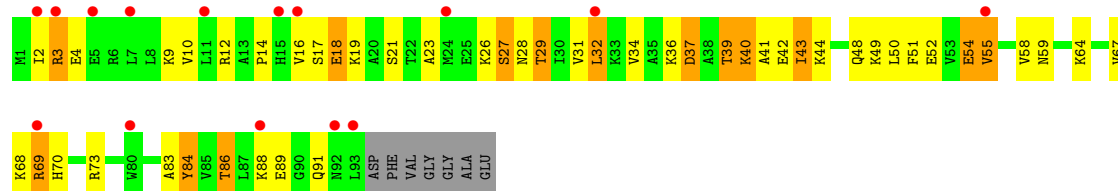
- Molecule 19: 50S ribosomal protein L22

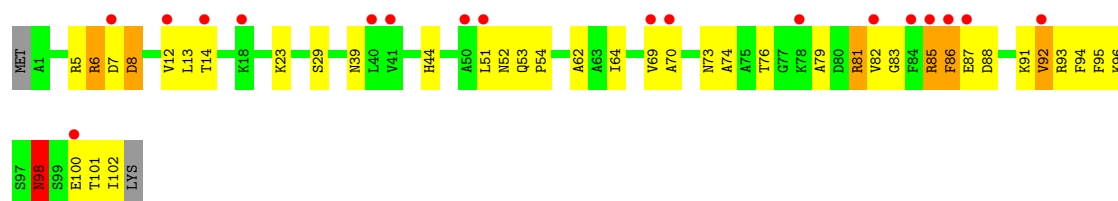
Chain GS:



- Molecule 20: 50S ribosomal protein L23

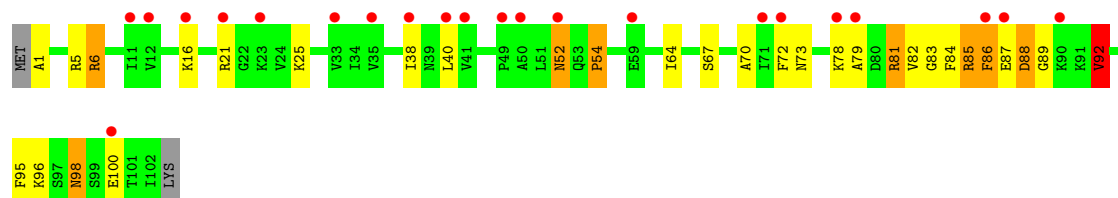
Chain AT:





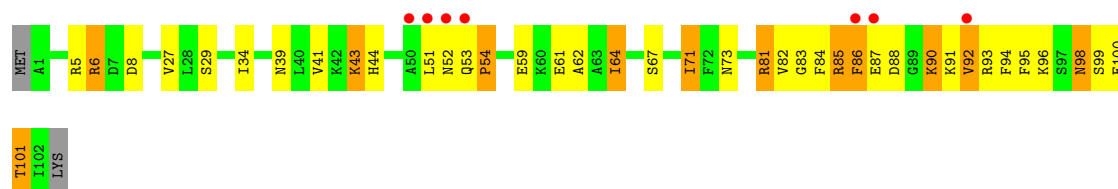
- Molecule 21: 50S ribosomal protein L24

Chain CU:



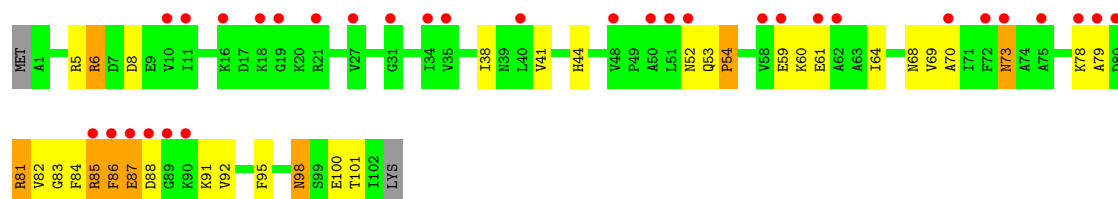
- Molecule 21: 50S ribosomal protein L24

Chain EU:



- Molecule 21: 50S ribosomal protein L24

Chain GU:



- Molecule 22: 50S ribosomal protein L25

Chain AV:



- Molecule 22: 50S ribosomal protein L25

Chain CV:



- Molecule 22: 50S ribosomal protein L25

Chain EV:



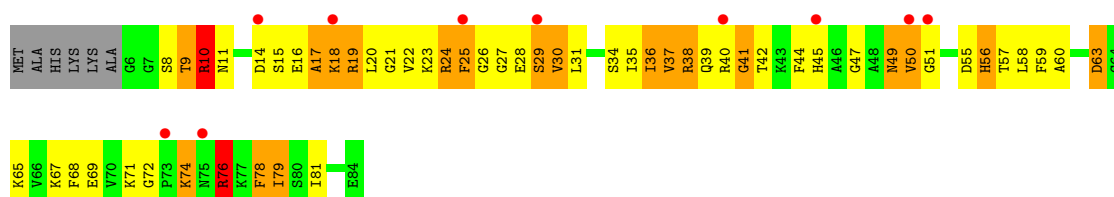
- Molecule 22: 50S ribosomal protein L25

Chain GV:



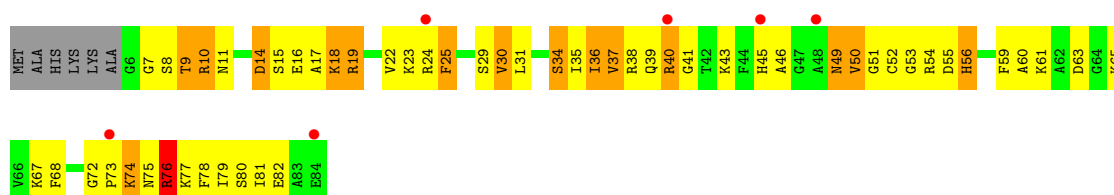
- Molecule 23: 50S ribosomal protein L27

Chain AW:



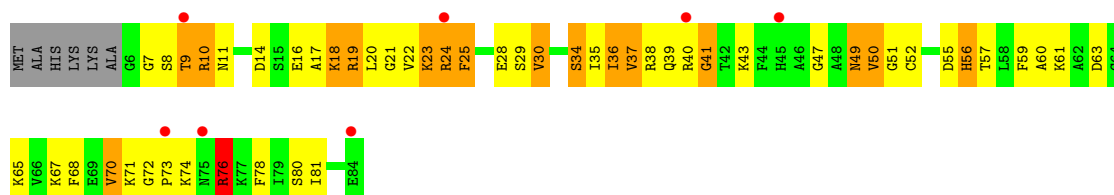
- Molecule 23: 50S ribosomal protein L27

Chain CW:



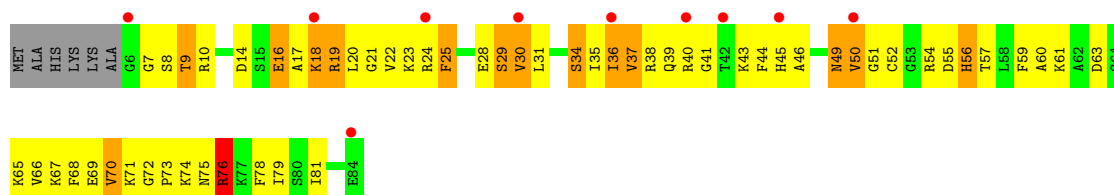
- Molecule 23: 50S ribosomal protein L27

Chain EW:



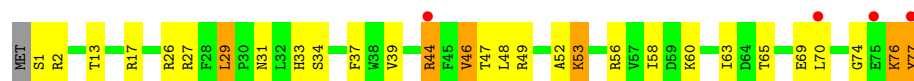
- Molecule 23: 50S ribosomal protein L27

Chain GW:



- Molecule 24: 50S ribosomal protein L28

Chain AX:



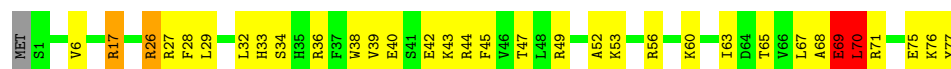
- Molecule 24: 50S ribosomal protein L28

Chain CX:



- Molecule 24: 50S ribosomal protein L28

Chain EX:



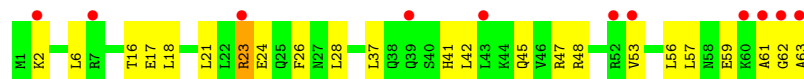
- Molecule 24: 50S ribosomal protein L28

Chain GX:



- Molecule 25: 50S ribosomal protein L29

Chain AY:



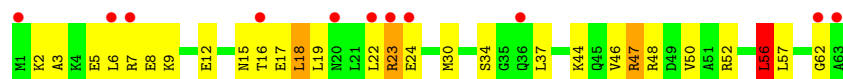
- Molecule 25: 50S ribosomal protein L29

Chain CY:



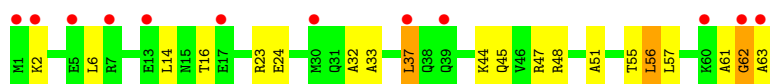
- Molecule 25: 50S ribosomal protein L29

Chain EY:



- Molecule 25: 50S ribosomal protein L29

Chain GY:



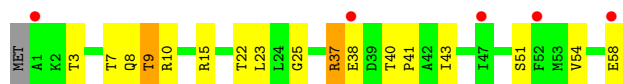
- Molecule 26: 50S ribosomal protein L30

Chain AZ:



- Molecule 26: 50S ribosomal protein L30

Chain CZ:



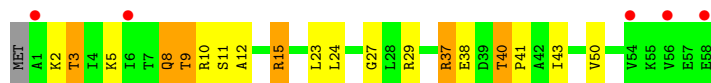
- Molecule 26: 50S ribosomal protein L30

Chain EZ:



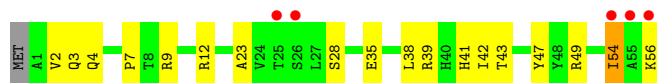
- Molecule 26: 50S ribosomal protein L30

Chain GZ:



- Molecule 27: 50S ribosomal protein L32

Chain A0:



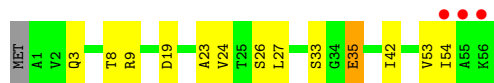
- Molecule 27: 50S ribosomal protein L32

Chain C0:



- Molecule 27: 50S ribosomal protein L32

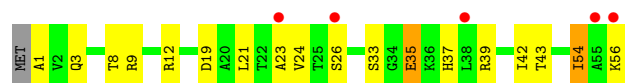
Chain E0:



- Molecule 27: 50S ribosomal protein L32



Chain G0:



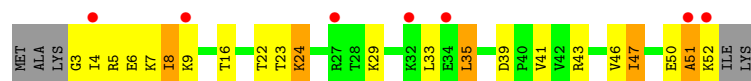
- Molecule 28: 50S ribosomal protein L33

Chain A1:



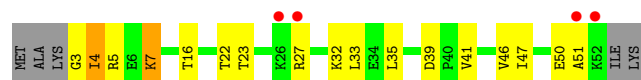
- Molecule 28: 50S ribosomal protein L33

Chain C1:



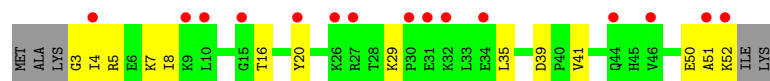
- Molecule 28: 50S ribosomal protein L33

Chain E1:



- Molecule 28: 50S ribosomal protein L33

Chain G1:



- Molecule 29: 50S ribosomal protein L34

Chain A2:



- Molecule 29: 50S ribosomal protein L34

Chain C2:



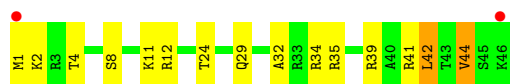
- Molecule 29: 50S ribosomal protein L34

Chain E2:



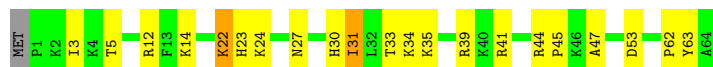
- Molecule 29: 50S ribosomal protein L34

Chain G2: 



- Molecule 30: 50S ribosomal protein L35

Chain A3: 



- Molecule 30: 50S ribosomal protein L35

Chain C3: 



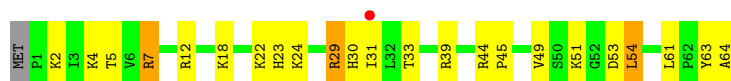
- Molecule 30: 50S ribosomal protein L35

Chain E3: 



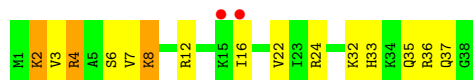
- Molecule 30: 50S ribosomal protein L35

Chain G3: 



- Molecule 31: 50S ribosomal protein L36

Chain A4: 



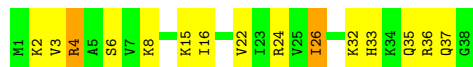
- Molecule 31: 50S ribosomal protein L36

Chain C4: 



- Molecule 31: 50S ribosomal protein L36

Chain E4: 



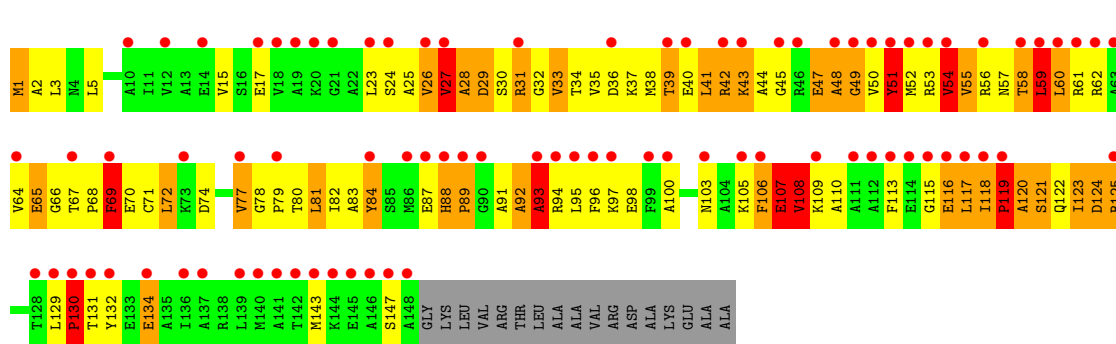
- Molecule 31: 50S ribosomal protein L36

Chain G4:



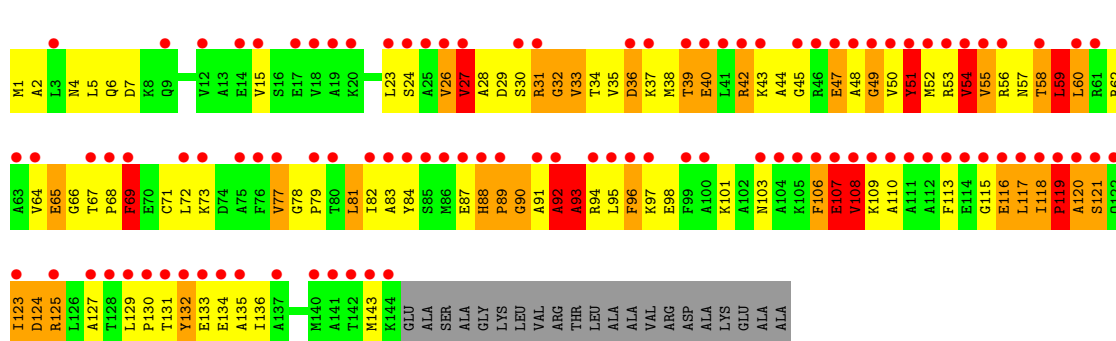
- Molecule 32: 50S ribosomal protein L10

Chain A5:



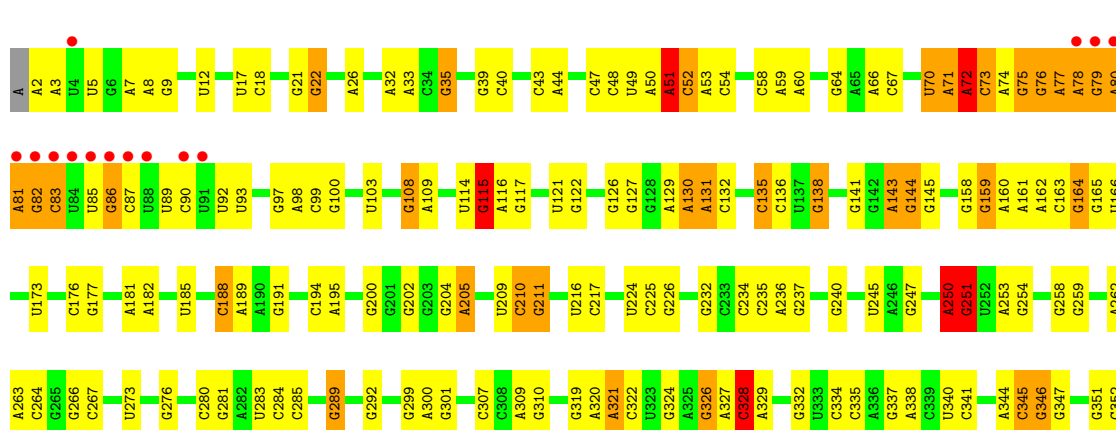
- Molecule 32: 50S ribosomal protein L10

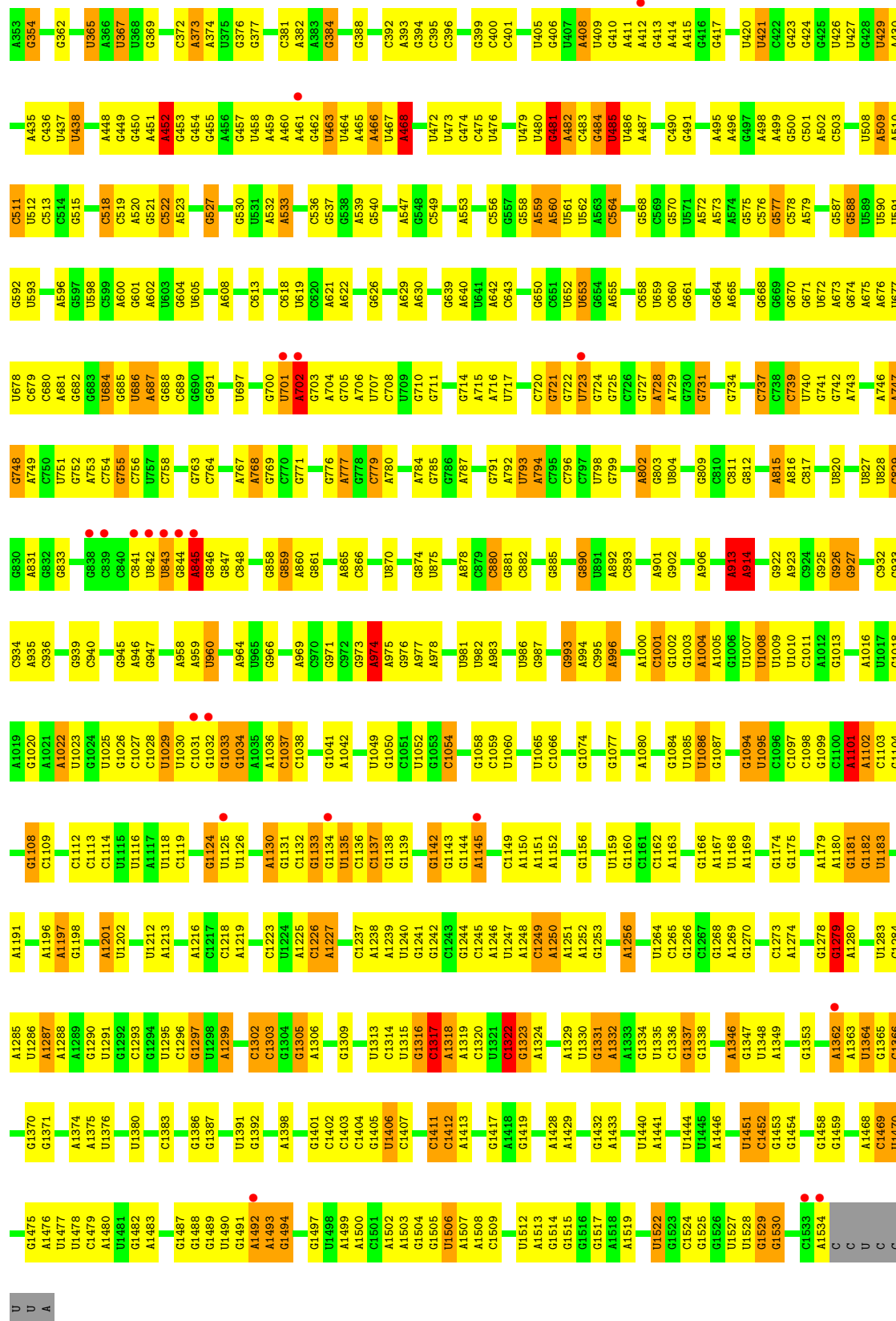
Chain E5:

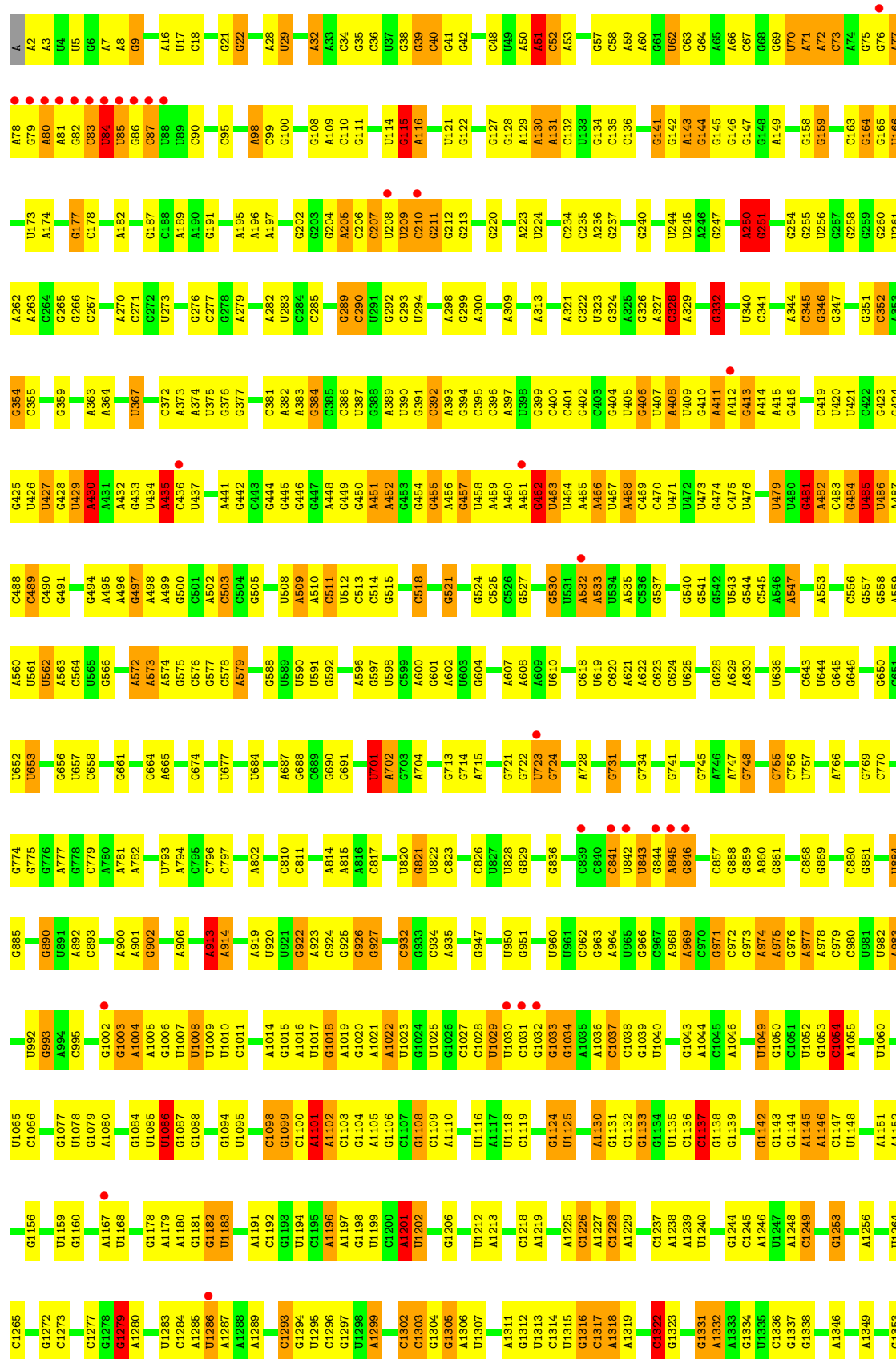


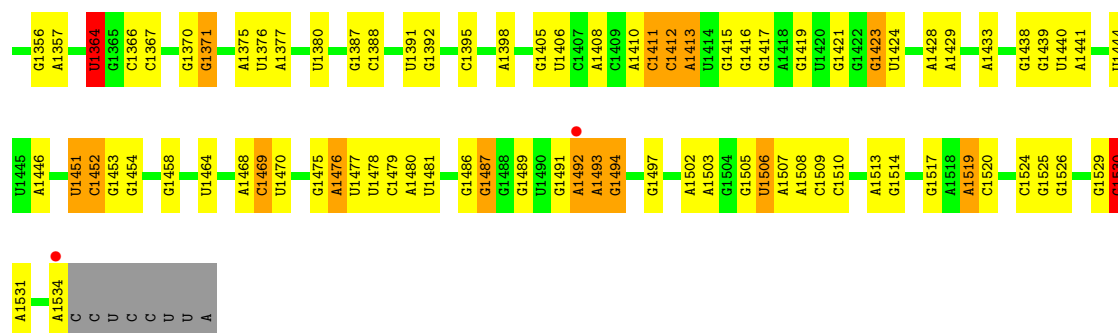
- Molecule 33: 16S rRNA

Chain BA:



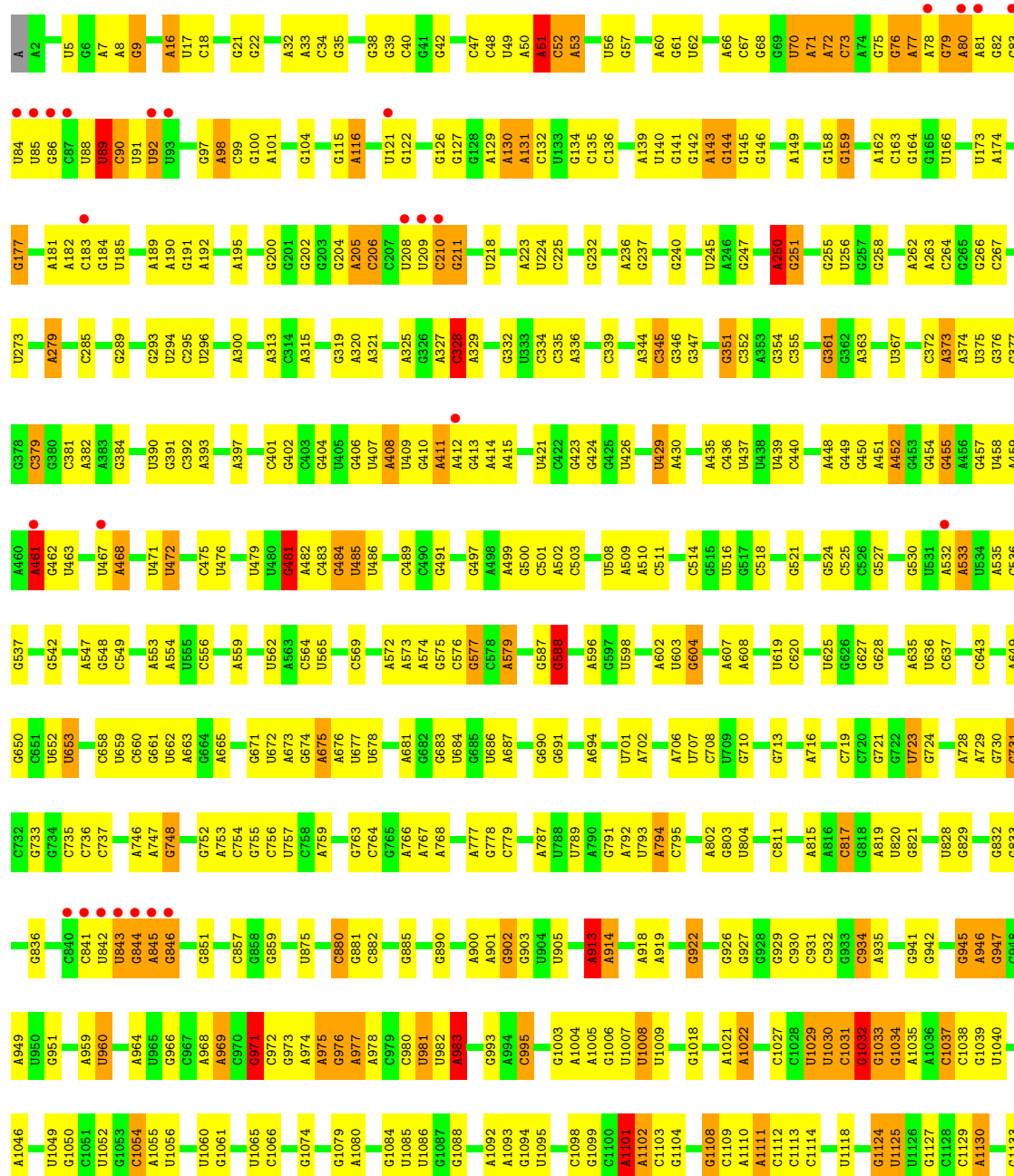


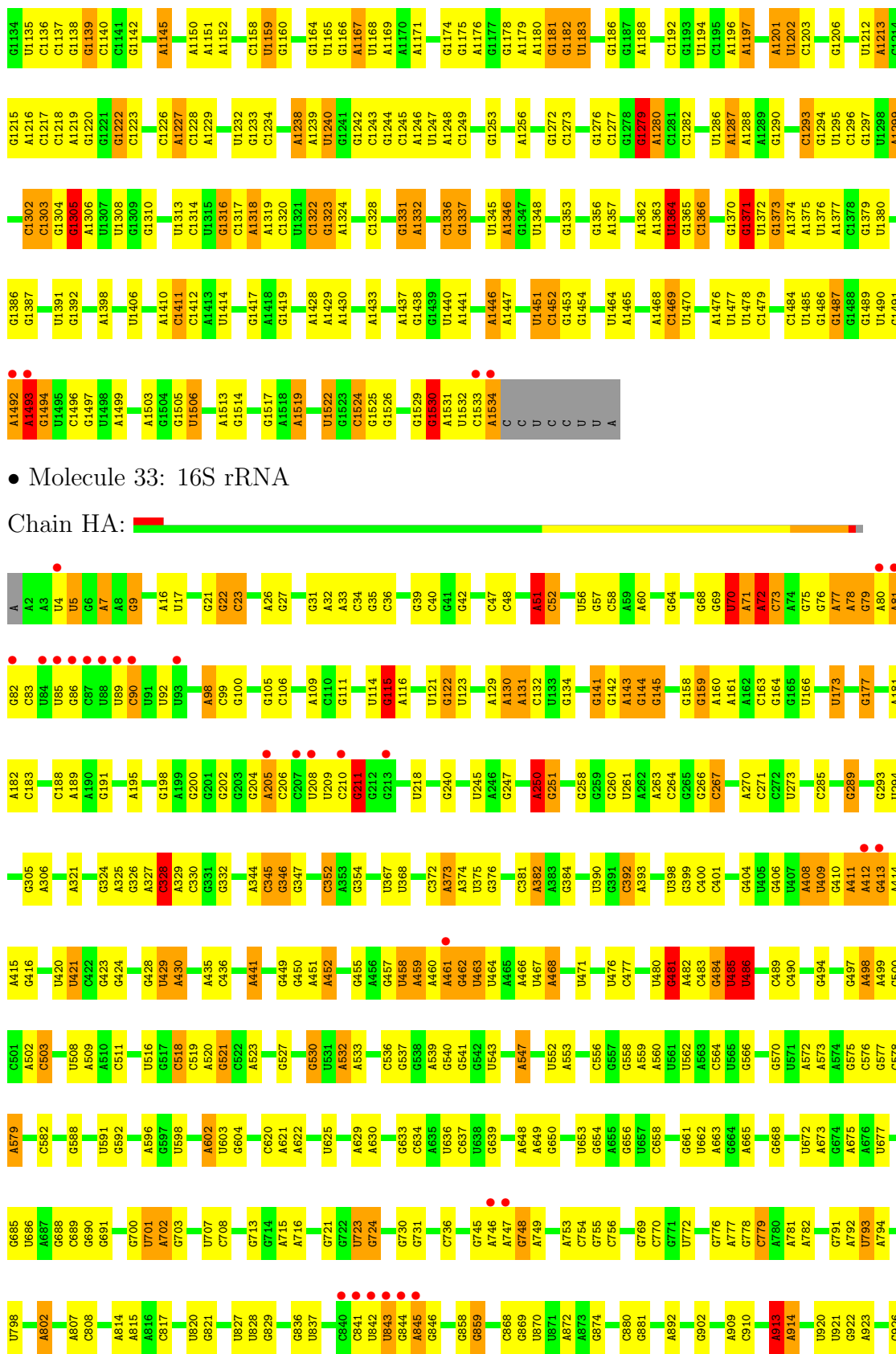




# Molecule 33: 16S rRNA

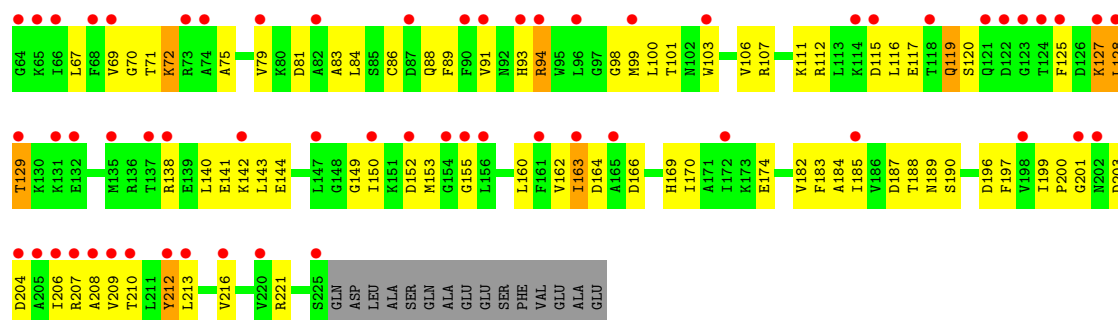
Chain FA:





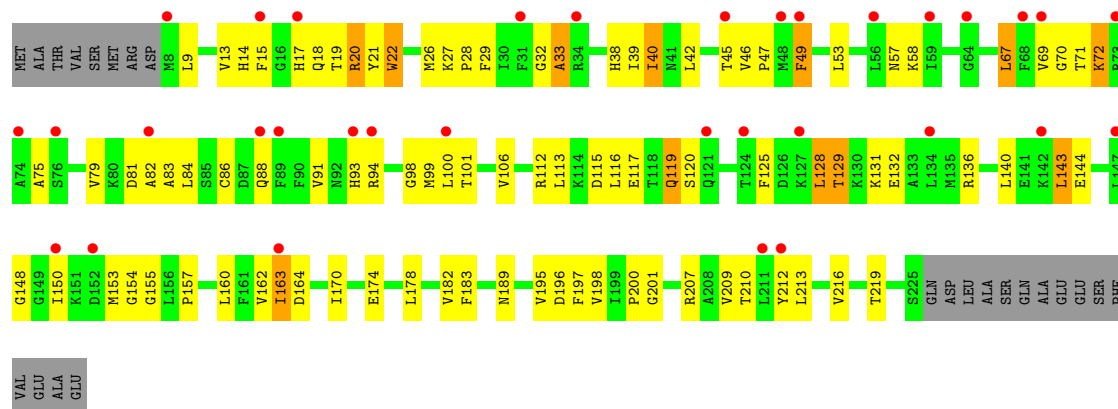






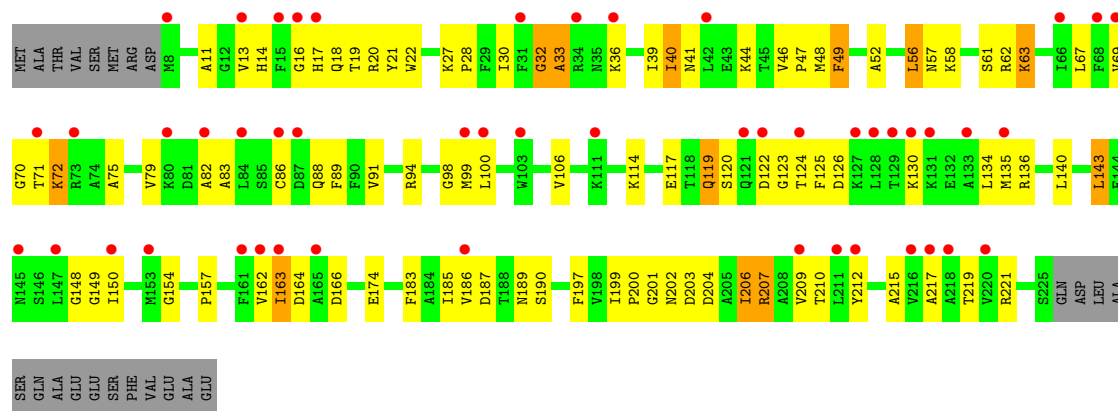
• Molecule 34: 30S ribosomal protein S2

Chain FB:



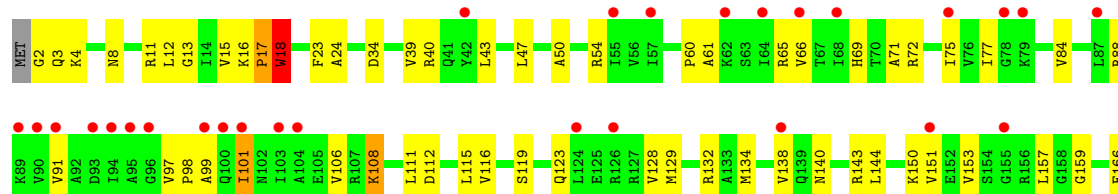
• Molecule 34: 30S ribosomal protein S2

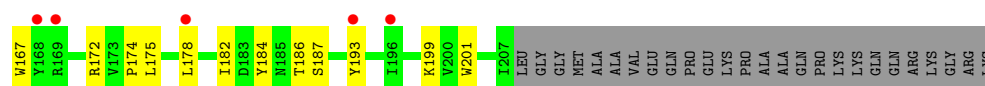
Chain HB:



• Molecule 35: 30S ribosomal protein S3

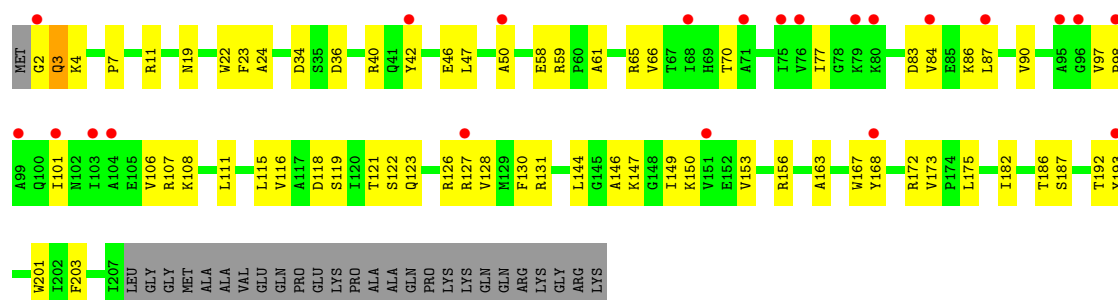
Chain BC:





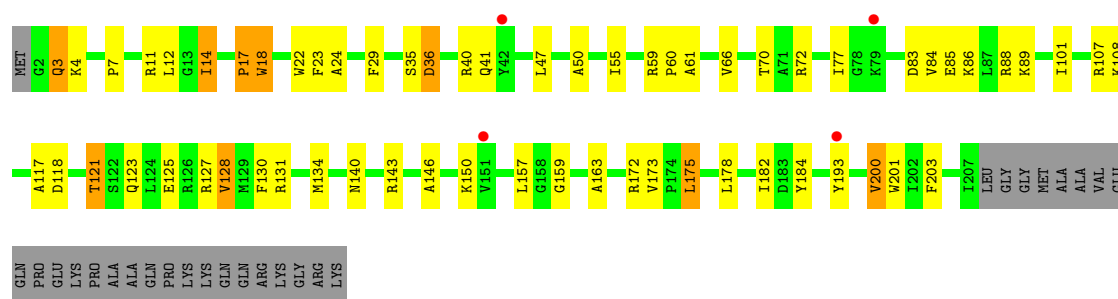
- Molecule 35: 30S ribosomal protein S3

Chain DC:



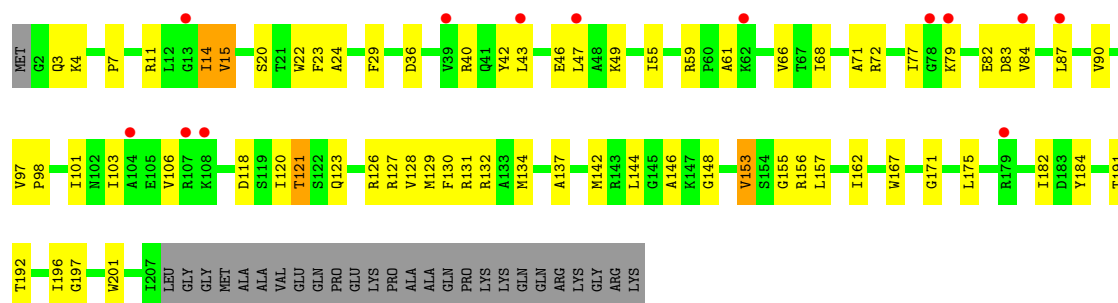
- Molecule 35: 30S ribosomal protein S3

Chain FC:



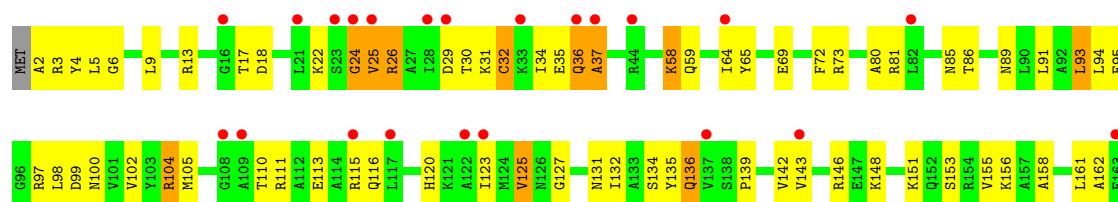
- Molecule 35: 30S ribosomal protein S3

Chain HC:



- Molecule 36: 30S ribosomal protein S4

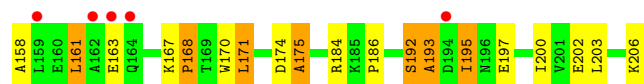
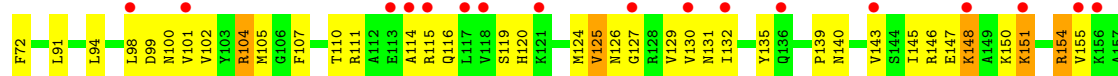
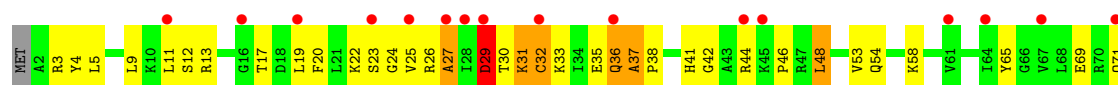
Chain BD:





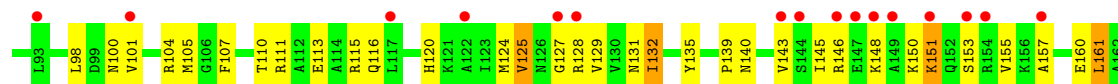
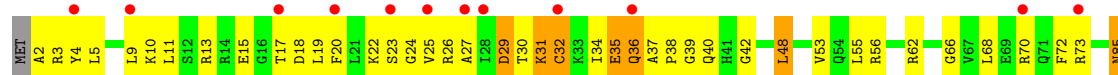
- Molecule 36: 30S ribosomal protein S4

Chain DD:



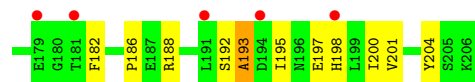
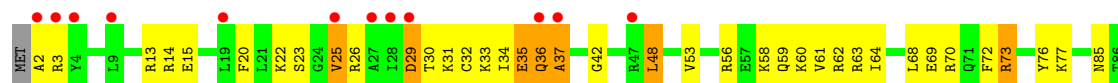
- Molecule 36: 30S ribosomal protein S4

Chain FD:



- Molecule 36: 30S ribosomal protein S4

Chain HD:



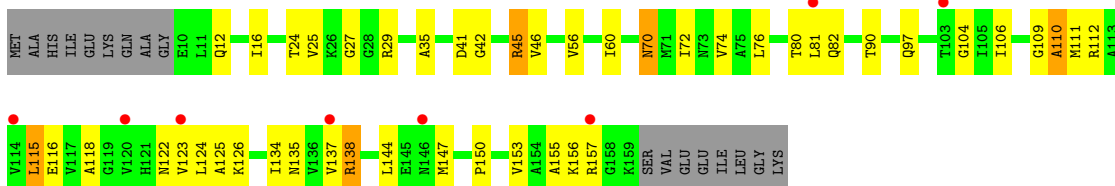
- Molecule 37: 30S ribosomal protein S5

Chain BE:

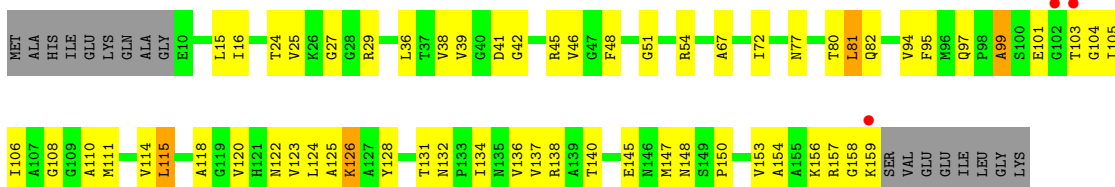




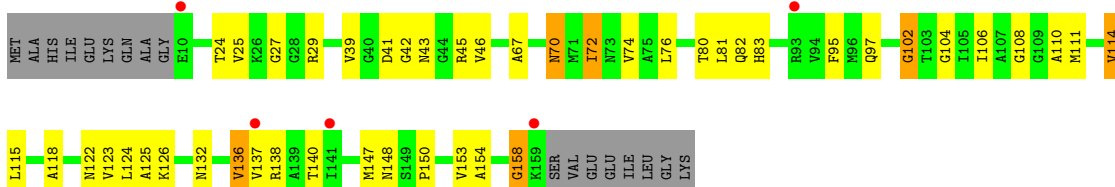
- Chain DE:



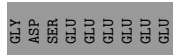
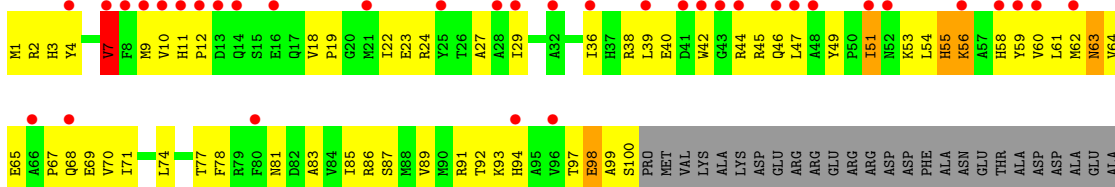
- Chain FE:



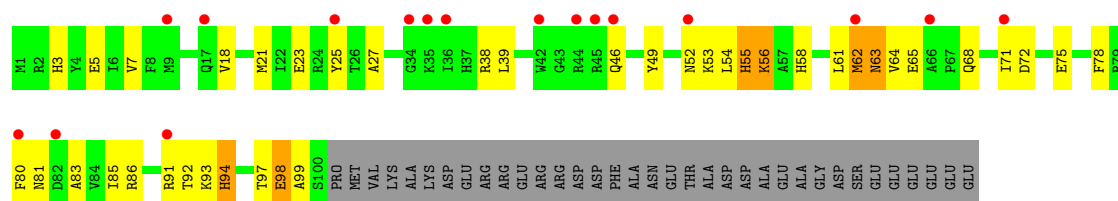
- Chain HE: 



- Chain BF:

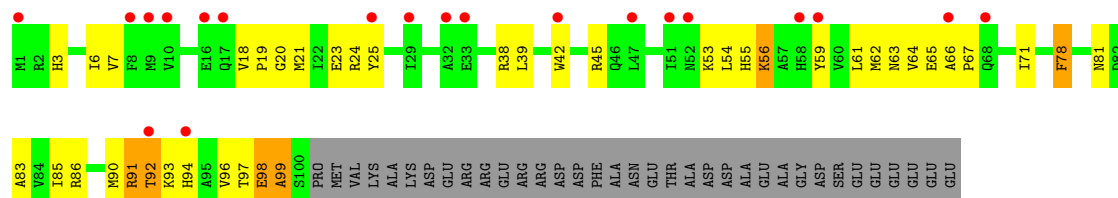


- Chain DF:



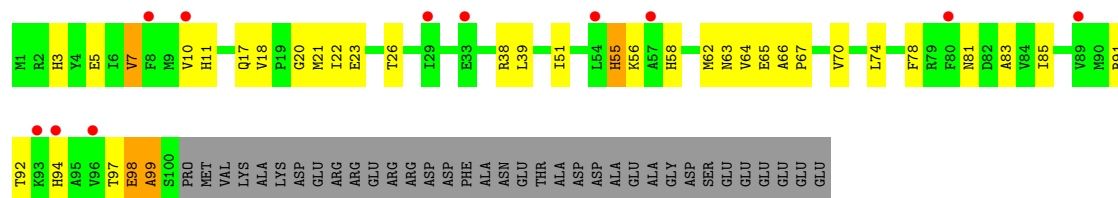
- Molecule 38: 30S ribosomal protein S6

Chain FF:



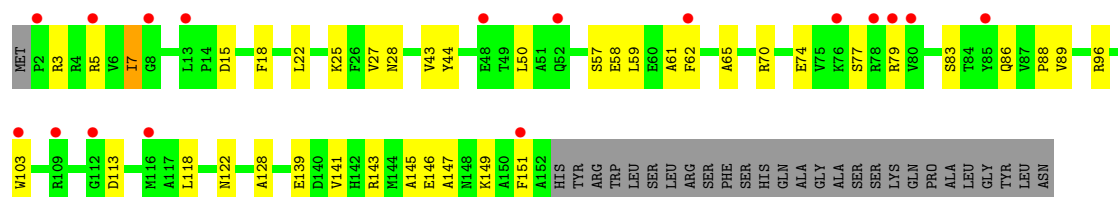
- Molecule 38: 30S ribosomal protein S6

Chain HF:



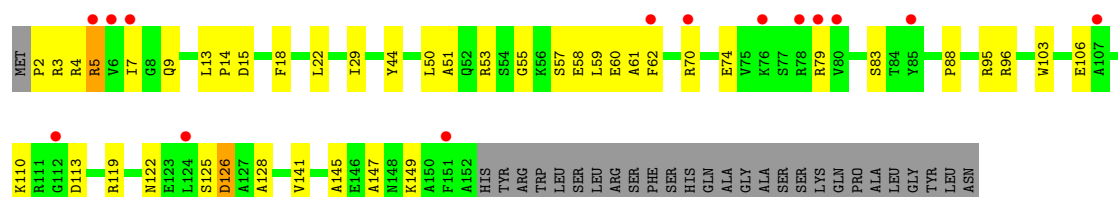
- Molecule 39: 30S ribosomal protein S7

Chain BG:



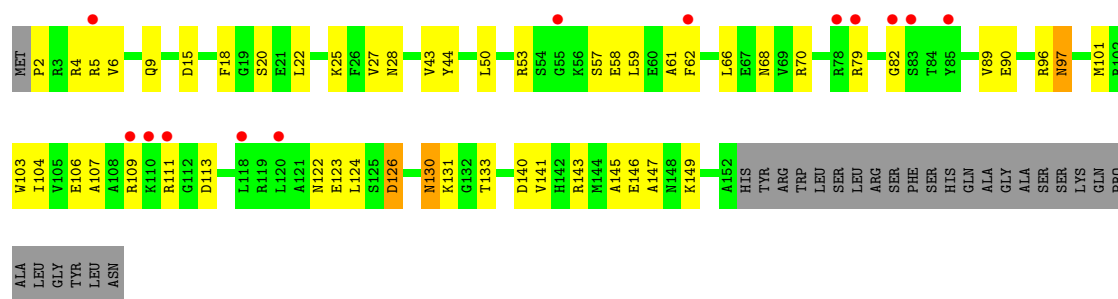
- Molecule 39: 30S ribosomal protein S7

Chain DG:



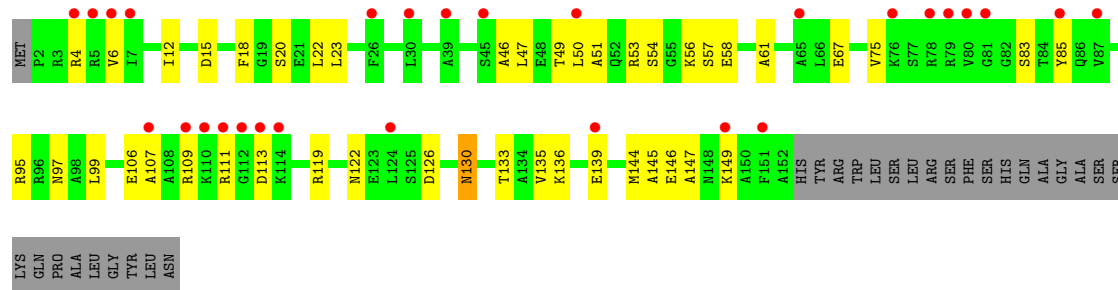
- Molecule 39: 30S ribosomal protein S7

Chain FG:



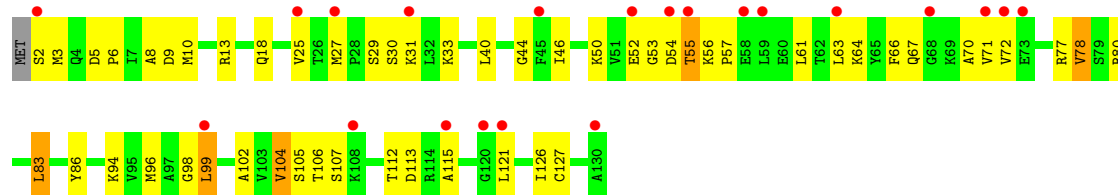
- Molecule 39: 30S ribosomal protein S7

Chain HG:



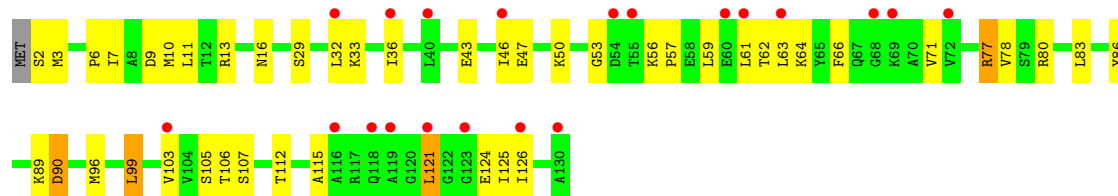
- Molecule 40: 30S ribosomal protein S8

Chain BH:



- Molecule 40: 30S ribosomal protein S8

Chain DH:

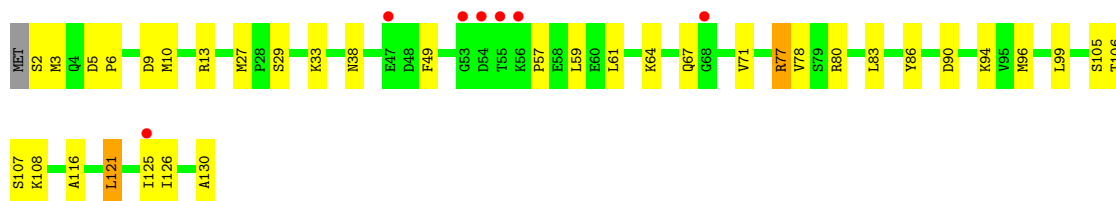


- Molecule 40: 30S ribosomal protein S8

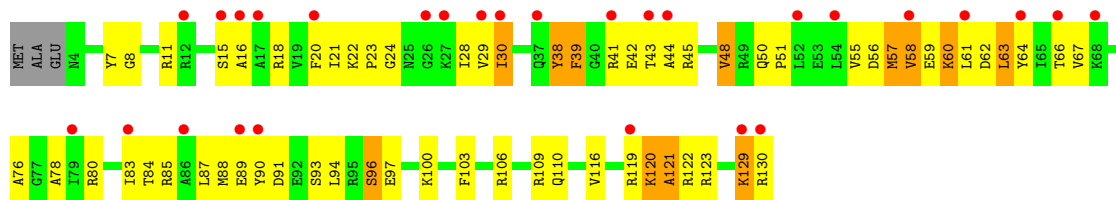
Chain FH:



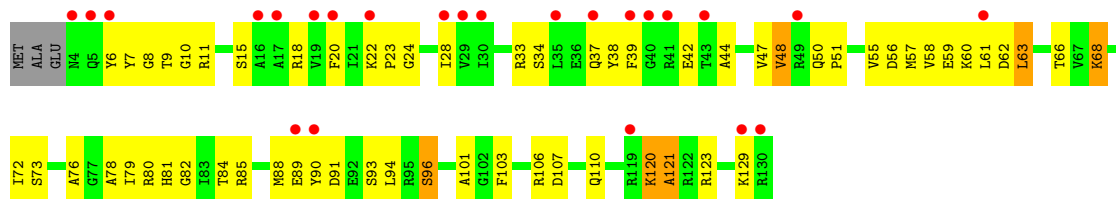
- Molecule 40: 30S ribosomal protein S8

Chain HH: 

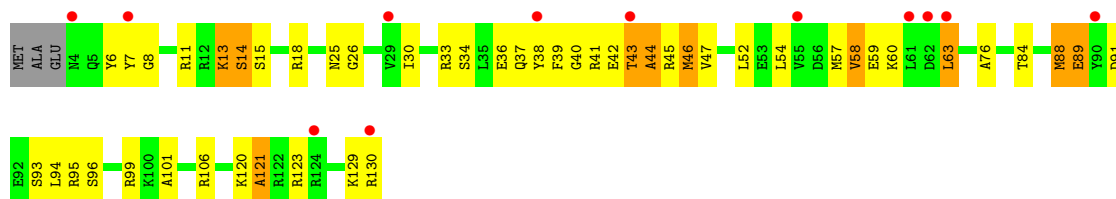
- Molecule 41: 30S ribosomal protein S9

Chain BI: 

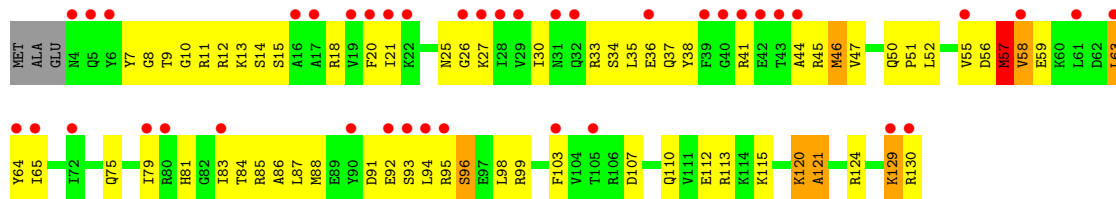
- Molecule 41: 30S ribosomal protein S9

Chain DI: 

- Molecule 41: 30S ribosomal protein S9

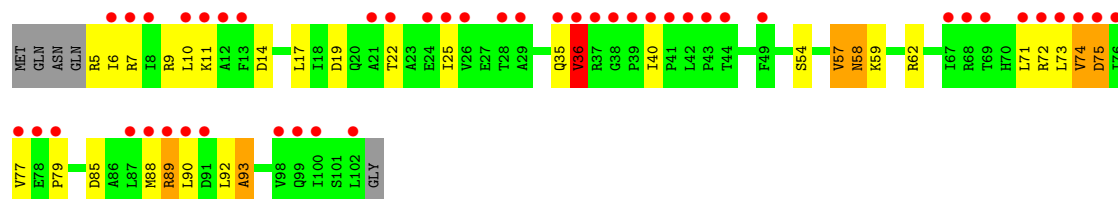
Chain FI: 

- Molecule 41: 30S ribosomal protein S9

Chain HI: 

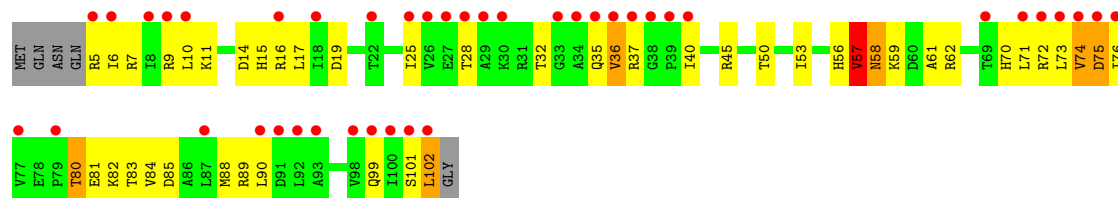
- Molecule 42: 30S ribosomal protein S10

Chain BJ:



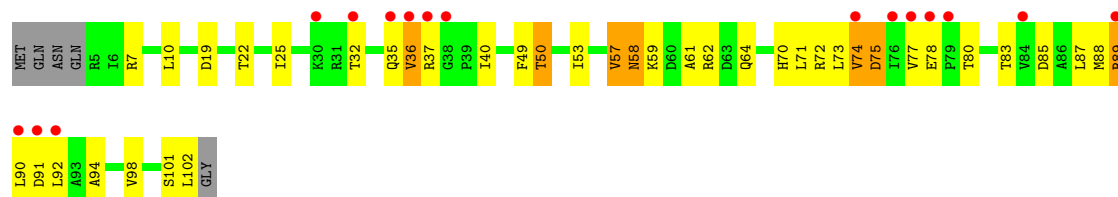
- Molecule 42: 30S ribosomal protein S10

Chain DJ:



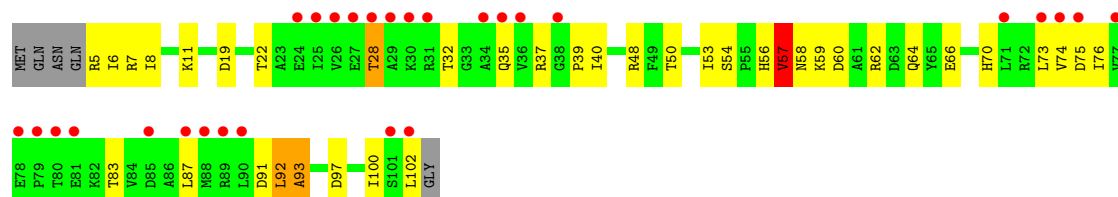
- Molecule 42: 30S ribosomal protein S10

Chain FJ:



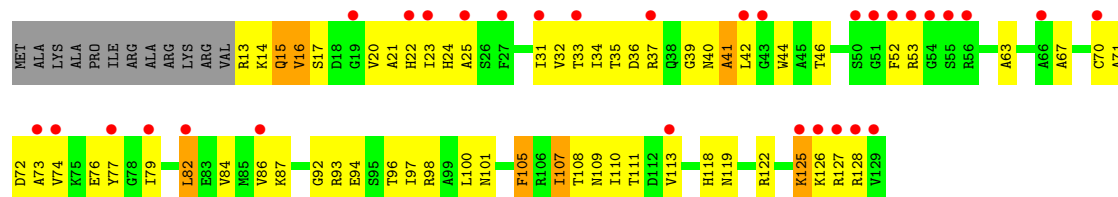
- Molecule 42: 30S ribosomal protein S10

Chain HJ:



- Molecule 43: 30S ribosomal protein S11

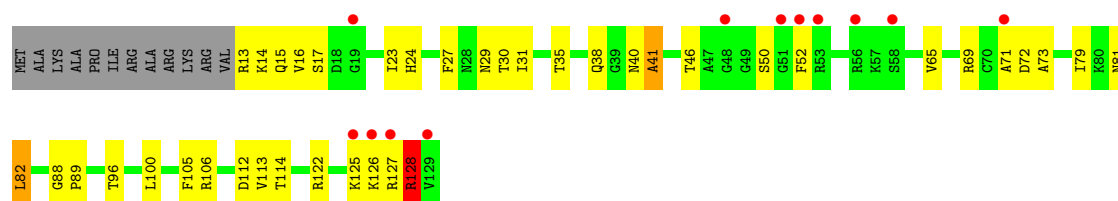
Chain BK:



- Molecule 43: 30S ribosomal protein S11

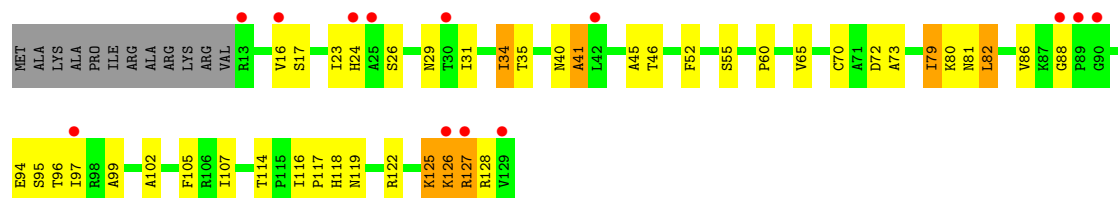
Chain DK:





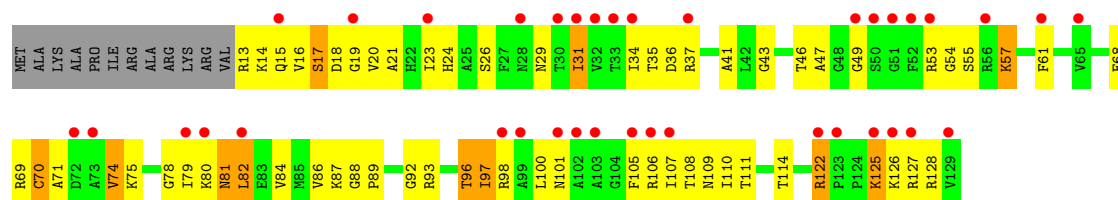
- Molecule 43: 30S ribosomal protein S11

Chain FK:



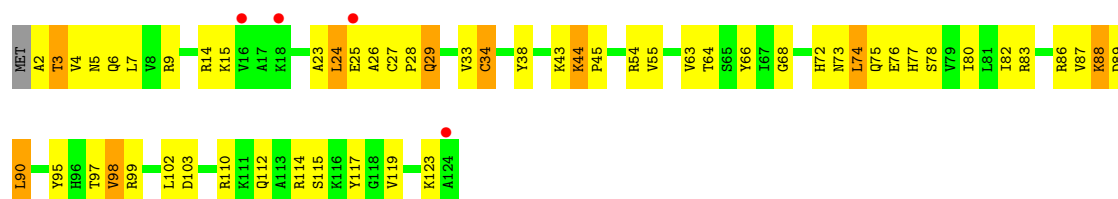
- Molecule 43: 30S ribosomal protein S11

Chain HK:



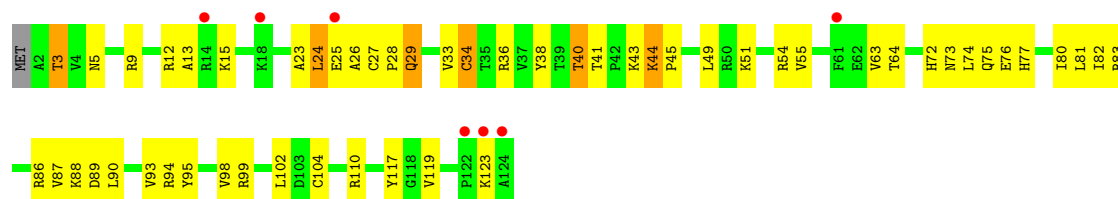
- Molecule 44: 30S ribosomal protein S12

Chain BL:



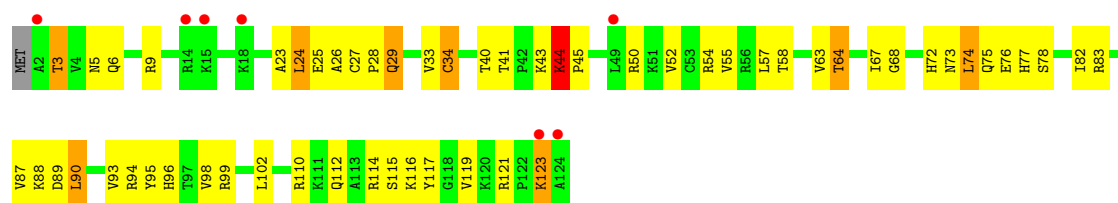
- Molecule 44: 30S ribosomal protein S12

Chain DL:



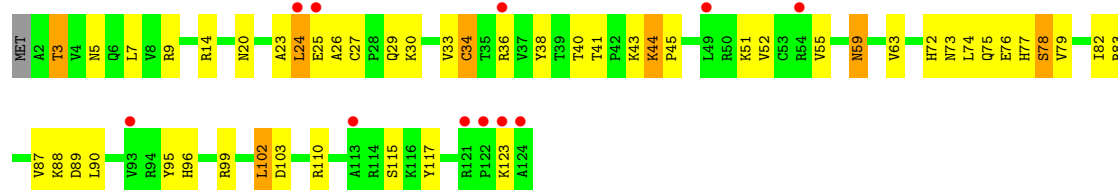
- Molecule 44: 30S ribosomal protein S12

Chain FL:



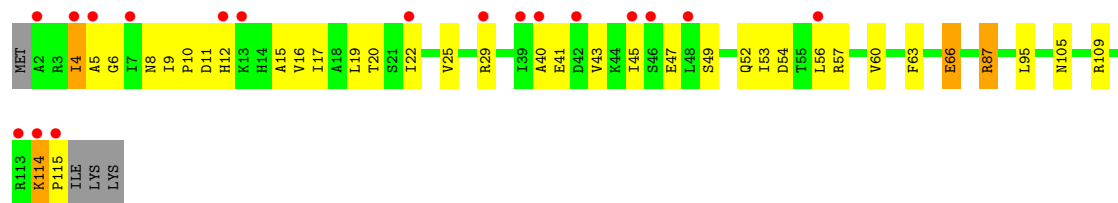
• Molecule 44: 30S ribosomal protein S12

Chain HL:



• Molecule 45: 30S ribosomal protein S13

Chain BM:



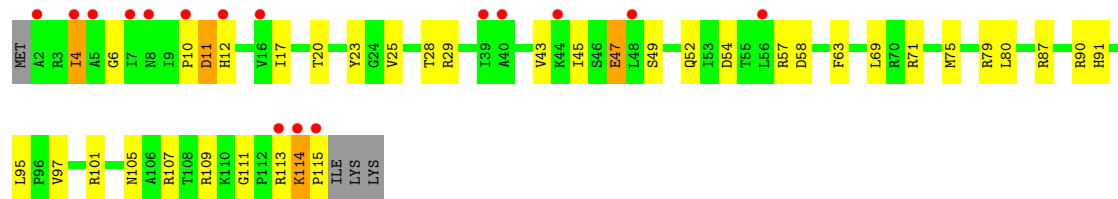
• Molecule 45: 30S ribosomal protein S13

Chain DM:



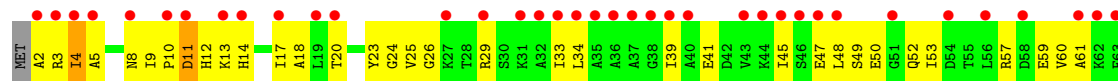
• Molecule 45: 30S ribosomal protein S13

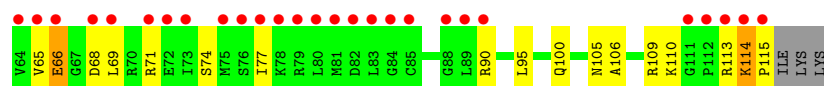
Chain FM:



• Molecule 45: 30S ribosomal protein S13

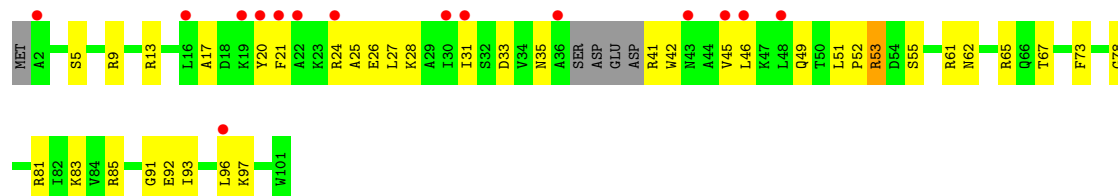
Chain HM:





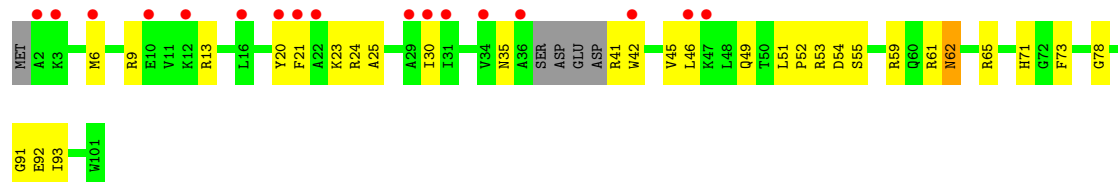
- Molecule 46: 30S ribosomal protein S14

Chain BN:



- Molecule 46: 30S ribosomal protein S14

Chain DN:



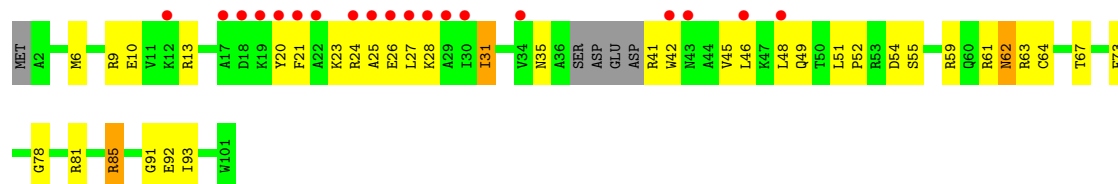
- Molecule 46: 30S ribosomal protein S14

Chain FN:



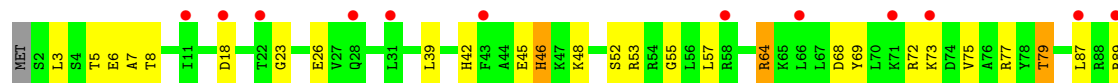
- Molecule 46: 30S ribosomal protein S14

Chain HN:



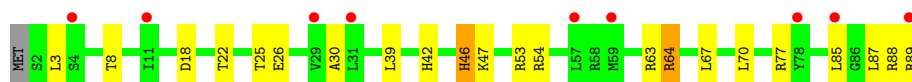
- Molecule 47: 30S ribosomal protein S15

Chain BO:



- Molecule 47: 30S ribosomal protein S15

Chain DO:



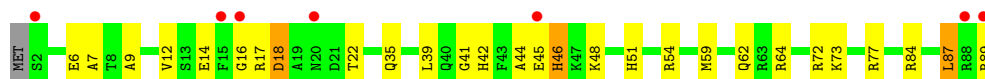
- Molecule 47: 30S ribosomal protein S15

Chain FO:



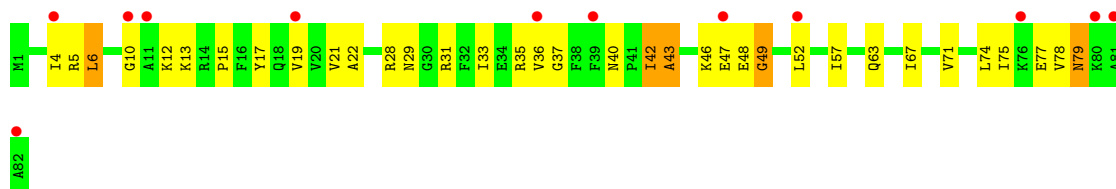
- Molecule 47: 30S ribosomal protein S15

Chain HO:



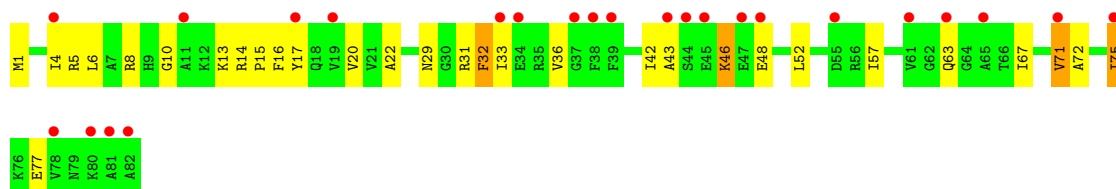
- Molecule 48: 30S ribosomal protein S16

Chain BP:



- Molecule 48: 30S ribosomal protein S16

Chain DP:



- Molecule 48: 30S ribosomal protein S16

Chain FP:



- Molecule 48: 30S ribosomal protein S16

Chain HP:



- Molecule 49: 30S ribosomal protein S17

Chain BQ:



- Molecule 49: 30S ribosomal protein S17

Chain DQ:



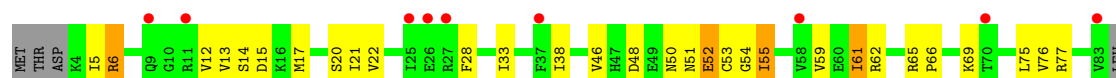
- Molecule 49: 30S ribosomal protein S17

Chain FQ:



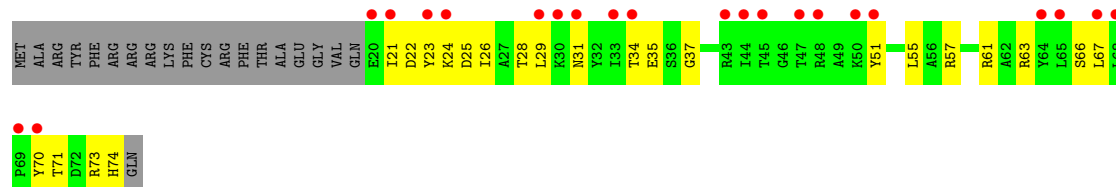
- Molecule 49: 30S ribosomal protein S17

Chain HQ:



- Molecule 50: 30S ribosomal protein S18

Chain BR:



- Molecule 50: 30S ribosomal protein S18

Chain DR:



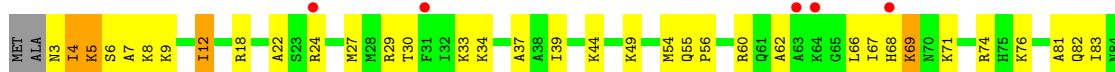
- Molecule 50: 30S ribosomal protein S18

Chain FR:



- Molecule 50: 30S ribosomal protein S18

Chain HR:





- Molecule 52: 30S ribosomal protein S20

Chain DT:



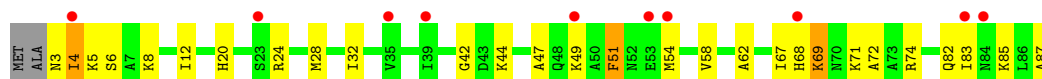
- Molecule 52: 30S ribosomal protein S20

Chain FT:



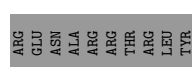
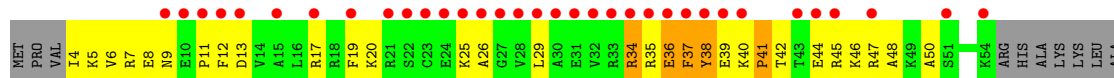
- Molecule 52: 30S ribosomal protein S20

Chain HT:



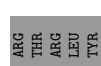
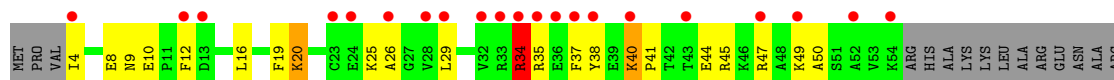
- Molecule 53: 30S ribosomal protein S21

Chain BU:



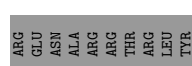
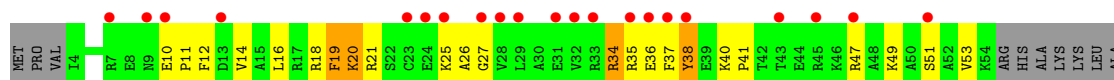
- Molecule 53: 30S ribosomal protein S21

Chain DU:

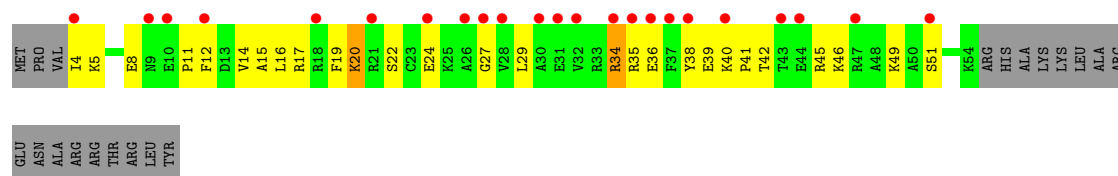


- Molecule 53: 30S ribosomal protein S21

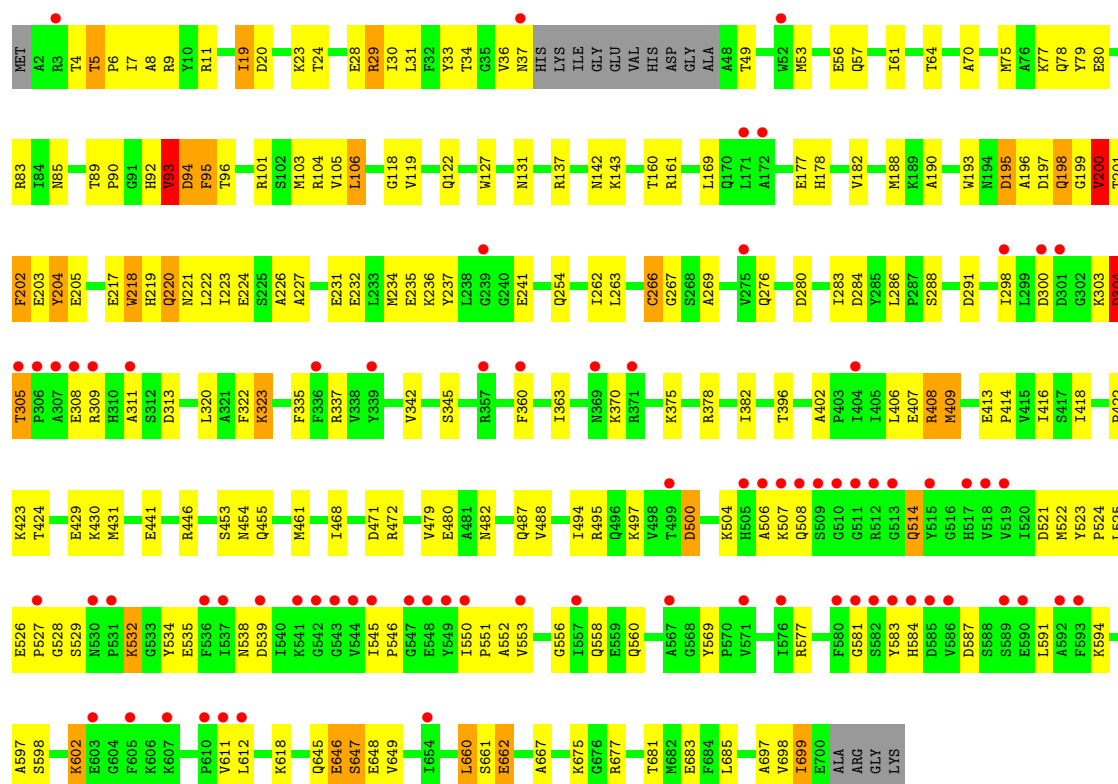
Chain FU:



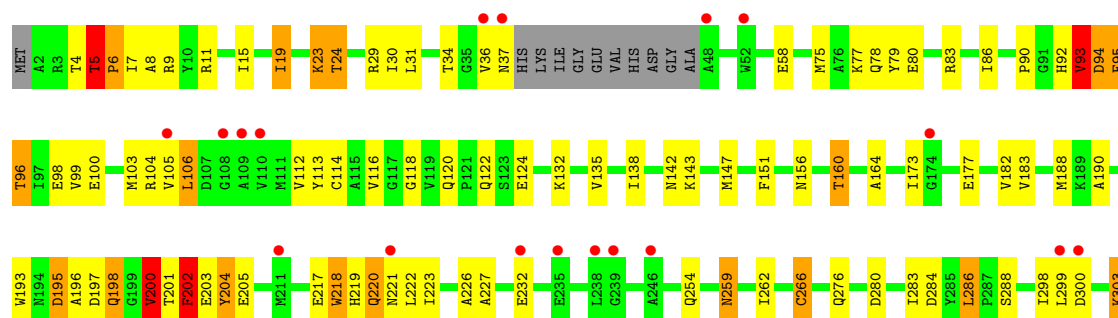
- Molecule 53: 30S ribosomal protein S21

Chain HU: 

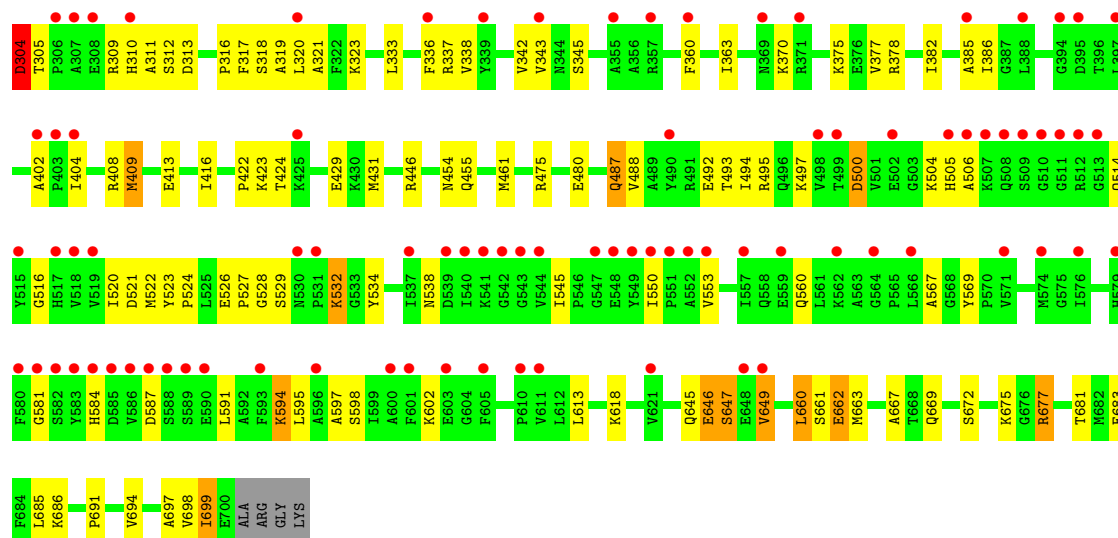
- Molecule 54: elongation factor G

Chain BV: 

- Molecule 54: elongation factor G

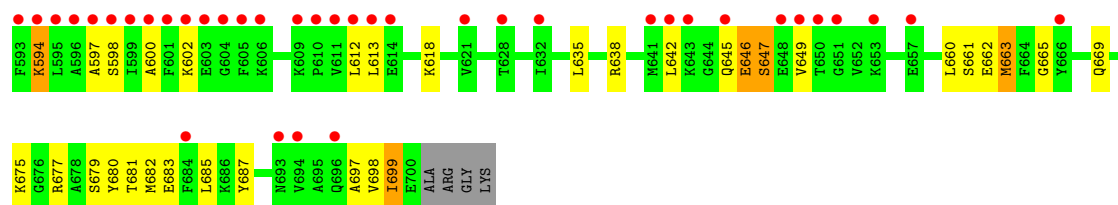
Chain DV: 





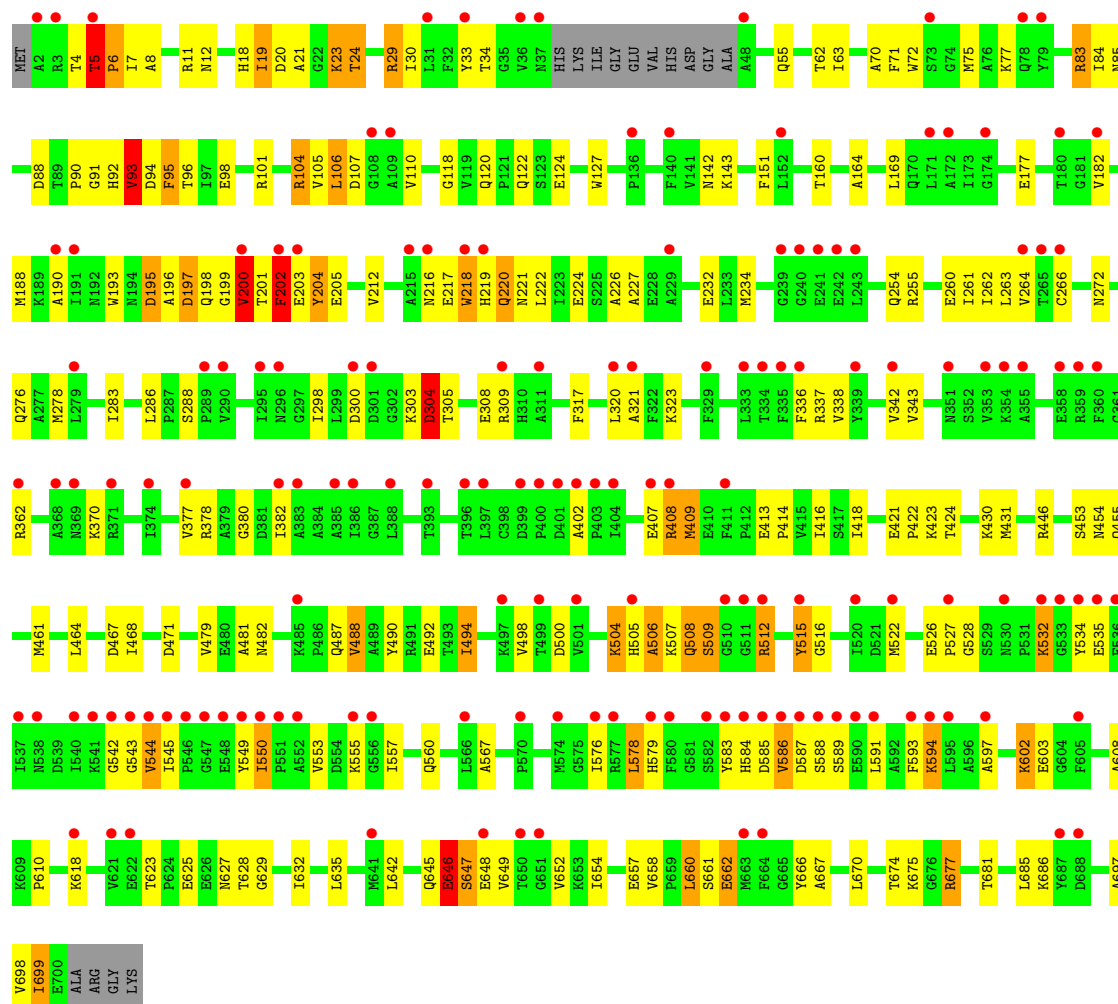
• Molecule 54: elongation factor G

Chain FV:



• Molecule 54: elongation factor G

Chain HV:



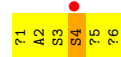
• Molecule 55: Viomycin

Chain BW:



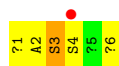
• Molecule 55: Viomycin

Chain DW:



- Molecule 55: Viomycin

Chain FW: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	361.14Å 360.51Å 429.73Å 90.00° 103.22° 90.00°	Depositor
Resolution (Å)	70.00 – 2.90 69.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-2.90) 77.4 (69.13-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.215 , 0.267 0.223 , 0.270	Depositor DCC
$R_{free}$ test set	3893 reflections (0.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 4.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 2019725 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	590573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.58 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.8072e-03.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DPP, MG, KBE, GCP, UAL, 5OH

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	0.74	9/68626 (0.0%)	1.28	446/107056 (0.4%)
1	CA	0.76	7/68626 (0.0%)	1.27	404/107056 (0.4%)
1	EA	0.90	29/68626 (0.0%)	1.41	729/107056 (0.7%)
1	GA	0.72	11/68626 (0.0%)	1.25	345/107056 (0.3%)
2	AB	0.67	0/2828	1.20	13/4410 (0.3%)
2	CB	0.61	0/2828	1.15	11/4410 (0.2%)
2	EB	0.75	1/2828 (0.0%)	1.38	18/4410 (0.4%)
2	GB	0.62	0/2828	1.09	2/4410 (0.0%)
3	AC	0.55	0/2121	0.83	3/2852 (0.1%)
3	CC	0.60	0/2121	0.81	0/2852
3	EC	0.62	0/2121	0.83	1/2852 (0.0%)
3	GC	0.59	0/2121	0.84	1/2852 (0.0%)
4	AD	0.60	0/1586	0.81	1/2134 (0.0%)
4	CD	0.55	0/1586	0.75	1/2134 (0.0%)
4	ED	0.63	0/1586	0.81	0/2134
4	GD	0.54	0/1586	0.78	1/2134 (0.0%)
5	AE	0.50	0/1571	0.76	1/2113 (0.0%)
5	CE	0.53	0/1571	0.71	0/2113
5	EE	0.59	0/1571	0.79	2/2113 (0.1%)
5	GE	0.49	0/1571	0.68	0/2113
6	AF	0.69	0/1434	0.89	0/1926
6	CF	0.52	0/1434	0.70	0/1926
6	EF	0.51	0/1434	0.73	0/1926
6	GF	0.58	0/1434	0.77	1/1926 (0.1%)
7	AG	0.54	0/1343	0.72	0/1816
7	CG	0.52	0/1343	0.73	0/1816
7	EG	0.53	0/1343	0.74	0/1816
7	GG	0.52	0/1343	0.72	0/1816
8	AH	0.54	0/389	0.71	0/523
8	CH	0.60	0/389	0.76	0/523
8	EH	0.57	0/389	0.73	0/523
8	GH	0.57	0/389	0.74	0/523

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	AI	0.58	0/1046	0.77	0/1410
9	CI	0.58	0/1046	0.74	0/1410
9	EI	0.61	0/1046	0.75	0/1410
9	GI	0.71	0/1046	0.84	0/1410
10	AJ	0.53	0/1152	0.77	0/1551
10	CJ	0.57	1/1152 (0.1%)	0.78	0/1551
10	EJ	0.70	1/1152 (0.1%)	0.82	1/1551 (0.1%)
10	GJ	0.55	1/1152 (0.1%)	0.71	0/1551
11	AK	0.62	0/947	0.79	0/1268
11	CK	0.63	0/947	0.78	0/1268
11	EK	0.59	0/947	0.83	0/1268
11	GK	0.55	0/947	0.80	0/1268
12	AL	0.53	0/1054	0.78	2/1403 (0.1%)
12	CL	0.53	0/1054	0.81	2/1403 (0.1%)
12	EL	0.61	0/1054	0.81	0/1403
12	GL	0.52	0/1054	0.78	0/1403
13	AM	0.61	1/1093 (0.1%)	0.81	1/1460 (0.1%)
13	CM	0.53	0/1093	0.75	0/1460
13	EM	0.62	0/1093	0.87	2/1460 (0.1%)
13	GM	0.52	0/1093	0.73	0/1460
14	AN	0.51	0/973	0.75	1/1301 (0.1%)
14	CN	0.46	0/973	0.77	4/1301 (0.3%)
14	EN	0.57	0/973	0.74	0/1301
14	GN	0.49	0/973	0.69	0/1301
15	AO	0.48	0/902	0.72	0/1209
15	CO	0.47	0/902	0.70	0/1209
15	EO	0.48	0/902	0.75	0/1209
15	GO	0.48	0/902	0.74	0/1209
16	AP	0.56	0/929	0.87	2/1242 (0.2%)
16	CP	0.56	0/929	0.85	2/1242 (0.2%)
16	EP	0.63	1/929 (0.1%)	0.89	1/1242 (0.1%)
16	GP	0.58	0/929	0.80	0/1242
17	AQ	0.56	0/960	0.75	1/1278 (0.1%)
17	CQ	0.60	0/960	0.78	1/1278 (0.1%)
17	EQ	0.70	0/960	0.88	2/1278 (0.2%)
17	GQ	0.53	0/960	0.74	0/1278
18	AR	0.59	0/829	0.75	0/1107
18	CR	0.59	0/829	0.75	0/1107
18	ER	0.68	2/829 (0.2%)	0.79	0/1107
18	GR	0.56	0/829	0.75	0/1107
19	AS	0.52	0/864	0.76	0/1156
19	CS	0.52	0/864	0.73	0/1156
19	ES	0.62	0/864	0.84	1/1156 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	GS	0.49	0/864	0.72	0/1156
20	AT	0.60	0/744	0.84	0/994
20	CT	0.56	0/744	0.89	0/994
20	ET	0.65	0/744	0.92	1/994 (0.1%)
20	GT	0.57	0/744	0.91	1/994 (0.1%)
21	AU	0.56	0/787	0.76	0/1051
21	CU	0.52	0/787	0.75	0/1051
21	EU	0.61	0/787	0.81	0/1051
21	GU	0.52	0/787	0.77	0/1051
22	AV	0.48	0/766	0.67	0/1025
22	CV	0.55	1/766 (0.1%)	0.67	0/1025
22	EV	0.57	0/766	0.72	0/1025
22	GV	0.47	0/766	0.65	0/1025
23	AW	0.63	0/603	0.93	1/797 (0.1%)
23	CW	0.70	0/603	0.94	1/797 (0.1%)
23	EW	0.78	0/603	0.97	1/797 (0.1%)
23	GW	0.66	0/603	0.92	0/797
24	AX	0.52	0/635	0.83	1/848 (0.1%)
24	CX	0.58	0/635	0.80	2/848 (0.2%)
24	EX	0.56	0/635	0.79	1/848 (0.1%)
24	GX	0.51	0/635	0.79	0/848
25	AY	0.47	0/510	0.75	0/677
25	CY	0.51	0/510	0.76	0/677
25	EY	0.54	0/510	0.85	1/677 (0.1%)
25	GY	0.55	0/510	0.79	1/677 (0.1%)
26	AZ	0.53	0/453	0.65	0/605
26	CZ	0.49	0/453	0.75	0/605
26	EZ	0.58	0/453	0.82	0/605
26	GZ	0.48	0/453	0.73	0/605
27	A0	0.50	0/450	0.77	0/599
27	C0	0.49	0/450	0.72	0/599
27	E0	0.68	1/450 (0.2%)	0.80	1/599 (0.2%)
27	G0	0.52	1/450 (0.2%)	0.69	0/599
28	A1	0.54	0/416	0.78	0/554
28	C1	0.51	0/416	0.76	0/554
28	E1	0.54	0/416	0.72	0/554
28	G1	0.54	0/416	0.73	0/554
29	A2	0.52	0/380	0.77	0/498
29	C2	0.56	0/380	0.73	0/498
29	E2	0.75	1/380 (0.3%)	0.84	1/498 (0.2%)
29	G2	0.59	0/380	0.75	0/498
30	A3	0.51	0/513	0.74	0/676
30	C3	0.54	0/513	0.68	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
30	E3	0.64	0/513	0.81	0/676
30	G3	0.50	0/513	0.70	0/676
31	A4	0.61	0/303	0.78	0/397
31	C4	0.60	0/303	0.81	0/397
31	E4	0.60	0/303	0.82	0/397
31	G4	0.53	0/303	0.77	0/397
32	A5	0.83	0/1131	1.34	28/1524 (1.8%)
32	E5	0.74	0/1106	1.34	26/1490 (1.7%)
33	BA	0.64	0/36834	1.15	99/57462 (0.2%)
33	DA	0.63	0/36834	1.13	95/57462 (0.2%)
33	FA	0.65	1/36834 (0.0%)	1.18	114/57462 (0.2%)
33	HA	0.64	0/36834	1.13	101/57462 (0.2%)
34	BB	0.53	0/1735	0.72	0/2338
34	DB	0.49	0/1735	0.70	0/2338
34	FB	0.54	0/1735	0.73	0/2338
34	HB	0.52	0/1735	0.72	0/2338
35	BC	0.47	0/1651	0.64	0/2225
35	DC	0.47	0/1651	0.61	0/2225
35	FC	0.50	0/1651	0.71	0/2225
35	HC	0.48	0/1651	0.67	0/2225
36	BD	0.52	0/1665	0.74	0/2227
36	DD	0.54	0/1665	0.76	0/2227
36	FD	0.49	0/1665	0.71	0/2227
36	HD	0.52	0/1665	0.73	0/2227
37	BE	0.56	1/1118 (0.1%)	0.77	0/1504
37	DE	0.50	0/1118	0.74	0/1504
37	FE	0.54	0/1118	0.78	0/1504
37	HE	0.52	0/1118	0.76	0/1504
38	BF	0.64	0/835	0.75	0/1128
38	DF	0.55	0/835	0.73	0/1128
38	FF	0.54	0/835	0.73	0/1128
38	HF	0.58	0/835	0.72	0/1128
39	BG	0.48	0/1195	0.66	0/1602
39	DG	0.47	0/1195	0.66	0/1602
39	FG	0.51	0/1195	0.70	0/1602
39	HG	0.51	0/1195	0.73	0/1602
40	BH	0.48	0/989	0.63	0/1326
40	DH	0.50	0/989	0.65	0/1326
40	FH	0.50	0/989	0.72	0/1326
40	HH	0.45	0/989	0.66	0/1326
41	BI	0.52	0/1034	0.77	0/1375
41	DI	0.49	0/1034	0.72	1/1375 (0.1%)
41	FI	0.52	0/1034	0.80	0/1375



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
41	HI	0.56	0/1034	0.76	1/1375 (0.1%)
42	BJ	0.53	0/796	0.73	1/1077 (0.1%)
42	DJ	0.55	0/796	0.75	0/1077
42	FJ	0.55	0/796	0.78	0/1077
42	HJ	0.54	0/796	0.77	0/1077
43	BK	0.59	0/893	0.81	0/1205
43	DK	0.51	0/893	0.80	1/1205 (0.1%)
43	FK	0.52	0/893	0.72	0/1205
43	HK	0.71	0/893	0.92	2/1205 (0.2%)
44	BL	0.55	0/969	0.78	0/1300
44	DL	0.54	0/969	0.79	0/1300
44	FL	0.51	0/969	0.75	1/1300 (0.1%)
44	HL	0.50	0/969	0.78	0/1300
45	BM	0.48	0/892	0.72	0/1193
45	DM	0.48	0/892	0.70	0/1193
45	FM	0.46	0/892	0.72	0/1193
45	HM	0.60	0/892	0.83	0/1193
46	BN	0.53	0/785	0.73	0/1043
46	DN	0.53	0/785	0.68	0/1043
46	FN	0.59	0/785	0.80	0/1043
46	HN	0.48	0/785	0.67	0/1043
47	BO	0.46	0/722	0.65	0/964
47	DO	0.47	0/722	0.64	0/964
47	FO	0.44	0/722	0.63	0/964
47	HO	0.50	0/722	0.68	0/964
48	BP	0.51	0/659	0.74	0/884
48	DP	0.52	0/659	0.72	0/884
48	FP	0.48	0/659	0.70	0/884
48	HP	0.51	0/659	0.67	0/884
49	BQ	0.51	0/657	0.73	0/881
49	DQ	0.50	0/657	0.74	0/881
49	FQ	0.49	0/657	0.66	0/881
49	HQ	0.51	0/657	0.75	0/881
50	BR	0.53	0/462	0.67	0/621
50	DR	0.50	0/462	0.71	0/621
50	FR	0.48	0/462	0.63	0/621
50	HR	0.53	0/462	0.77	1/621 (0.2%)
51	BS	0.47	0/652	0.78	0/877
51	DS	0.49	0/652	0.70	0/877
51	FS	0.48	0/652	0.72	0/877
51	HS	0.66	0/652	0.79	0/877
52	BT	0.50	0/671	0.65	0/888
52	DT	0.49	0/671	0.64	0/888

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
52	FT	0.48	0/671	0.68	0/888
52	HT	0.49	0/671	0.72	0/888
53	BU	0.67	0/430	0.75	0/570
53	DU	0.67	0/430	0.83	1/570 (0.2%)
53	FU	0.69	0/430	0.83	0/570
53	HU	0.78	0/430	0.82	0/570
54	BV	0.48	0/5418	0.68	1/7329 (0.0%)
54	DV	0.46	0/5418	0.66	1/7329 (0.0%)
54	FV	0.57	0/5418	0.68	1/7329 (0.0%)
54	HV	0.50	0/5418	0.70	1/7329 (0.0%)
55	BW	2.44	1/11 (9.1%)	1.38	0/13
55	DW	2.31	1/11 (9.1%)	1.57	0/13
55	FW	2.44	1/11 (9.1%)	2.53	1/13 (7.7%)
All	All	0.68	73/635346 (0.0%)	1.13	2493/946873 (0.3%)

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
3	CC	0	1
3	EC	0	1
3	GC	0	1
4	CD	0	2
4	ED	0	1
4	GD	0	1
32	A5	0	2
41	FI	0	1
44	BL	0	1
44	DL	0	1
44	FL	0	1
44	HL	0	1
54	BV	0	2
54	DV	0	2
54	FV	0	2
54	HV	0	3
All	All	0	23

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EA	984	A	N9-C4	-10.08	1.31	1.37
1	EA	528	A	N9-C4	-9.15	1.32	1.37
37	BE	94	VAL	CB-CG2	9.12	1.72	1.52
13	AM	13	HIS	CG-CD2	8.66	1.50	1.35
10	EJ	44	TYR	CD1-CE1	-7.92	1.27	1.39

The worst 5 of 2493 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EA	834	G	N1-C6-O6	16.23	129.64	119.90
1	EA	984	A	C2-N3-C4	-15.83	102.68	110.60
1	EA	974	G	C4-C5-N7	15.17	116.87	110.80
1	AA	2544	G	N1-C6-O6	14.98	128.89	119.90
1	AA	2053	G	N1-C6-O6	14.67	128.70	119.90

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	A5	130	PRO	Peptide
32	A5	134	GLU	Peptide
44	BL	23	ALA	Peptide
54	BV	218	TRP	Peptide
54	BV	304	ASP	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	61274	0	30818	1057	0
1	CA	61274	0	30819	919	0
1	EA	61274	0	30819	835	0
1	GA	61274	0	30819	917	3
2	AB	2529	0	1281	36	0
2	CB	2529	0	1281	34	0
2	EB	2529	0	1281	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	GB	2529	0	1281	37	0
3	AC	2082	0	2157	67	0
3	CC	2082	0	2157	68	0
3	EC	2082	0	2157	65	0
3	GC	2082	0	2157	57	0
4	AD	1565	0	1616	78	0
4	CD	1565	0	1616	75	0
4	ED	1565	0	1616	72	0
4	GD	1565	0	1616	77	0
5	AE	1552	0	1619	63	0
5	CE	1552	0	1619	34	0
5	EE	1552	0	1619	42	0
5	GE	1552	0	1619	56	0
6	AF	1410	0	1447	133	0
6	CF	1410	0	1447	53	0
6	EF	1410	0	1447	60	0
6	GF	1410	0	1447	92	1
7	AG	1323	0	1374	65	0
7	CG	1323	0	1374	65	0
7	EG	1323	0	1374	48	0
7	GG	1323	0	1374	58	0
8	AH	384	0	405	12	0
8	CH	384	0	405	18	0
8	EH	384	0	405	15	0
8	GH	384	0	405	11	0
9	AI	1032	0	1088	70	0
9	CI	1032	0	1088	62	0
9	EI	1032	0	1088	48	0
9	GI	1032	0	1088	82	0
10	AJ	1129	0	1162	49	0
10	CJ	1129	0	1162	58	0
10	EJ	1129	0	1162	76	0
10	GJ	1129	0	1162	57	0
11	AK	938	0	1012	40	0
11	CK	938	0	1012	57	0
11	EK	938	0	1012	49	0
11	GK	938	0	1012	42	0
12	AL	1045	0	1117	51	0
12	CL	1045	0	1117	38	0
12	EL	1045	0	1117	35	0
12	GL	1045	0	1117	50	0
13	AM	1074	0	1157	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	CM	1074	0	1157	33	0
13	EM	1074	0	1157	29	0
13	GM	1074	0	1157	24	0
14	AN	960	0	1000	35	0
14	CN	960	0	1000	44	0
14	EN	960	0	1000	33	0
14	GN	960	0	1000	36	0
15	AO	892	0	923	41	0
15	CO	892	0	923	32	0
15	EO	892	0	923	21	0
15	GO	892	0	923	29	0
16	AP	917	0	965	63	0
16	CP	917	0	965	58	0
16	EP	917	0	965	52	0
16	GP	917	0	965	49	0
17	AQ	947	0	1022	53	0
17	CQ	947	0	1022	56	0
17	EQ	947	0	1022	58	0
17	GQ	947	0	1022	56	0
18	AR	816	0	839	41	0
18	CR	816	0	839	49	0
18	ER	816	0	839	46	0
18	GR	816	0	839	34	0
19	AS	857	0	922	21	0
19	CS	857	0	922	27	0
19	ES	857	0	922	26	0
19	GS	857	0	922	30	0
20	AT	738	0	807	51	0
20	CT	738	0	807	54	0
20	ET	738	0	807	34	0
20	GT	738	0	807	47	0
21	AU	779	0	834	31	0
21	CU	779	0	834	19	0
21	EU	779	0	834	28	0
21	GU	779	0	834	27	1
22	AV	753	0	780	10	0
22	CV	753	0	780	16	0
22	EV	753	0	780	16	0
22	GV	753	0	780	25	0
23	AW	596	0	610	83	0
23	CW	596	0	610	78	0
23	EW	596	0	610	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	GW	596	0	610	85	0
24	AX	625	0	655	21	0
24	CX	625	0	655	20	0
24	EX	625	0	655	26	0
24	GX	625	0	655	24	0
25	AY	509	0	543	12	0
25	CY	509	0	543	16	0
25	EY	509	0	543	17	0
25	GY	509	0	543	11	0
26	AZ	449	0	491	6	0
26	CZ	449	0	491	11	0
26	EZ	449	0	491	15	0
26	GZ	449	0	491	14	0
27	A0	444	0	461	20	0
27	C0	444	0	461	15	0
27	E0	444	0	461	6	0
27	G0	444	0	461	12	0
28	A1	409	0	440	18	0
28	C1	409	0	440	23	0
28	E1	409	0	440	14	0
28	G1	409	0	440	13	0
29	A2	377	0	418	12	0
29	C2	377	0	418	9	0
29	E2	377	0	418	15	0
29	G2	377	0	418	8	0
30	A3	504	0	574	20	0
30	C3	504	0	574	16	0
30	E3	504	0	574	14	0
30	G3	504	0	574	21	0
31	A4	302	0	340	14	0
31	C4	302	0	340	17	0
31	E4	302	0	340	14	0
31	G4	302	0	340	13	0
32	A5	1117	0	1155	135	0
32	E5	1092	0	1134	122	0
33	BA	32895	0	16553	571	0
33	DA	32895	0	16553	534	0
33	FA	32895	0	16553	435	3
33	HA	32895	0	16553	430	0
34	BB	1704	0	1732	67	0
34	DB	1704	0	1732	87	0
34	FB	1704	0	1732	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	HB	1704	0	1732	72	0
35	BC	1624	0	1696	52	0
35	DC	1624	0	1696	40	0
35	FC	1624	0	1696	38	0
35	HC	1624	0	1696	50	0
36	BD	1643	0	1707	80	0
36	DD	1643	0	1707	83	0
36	FD	1643	0	1707	73	0
36	HD	1643	0	1707	72	0
37	BE	1105	0	1148	61	0
37	DE	1105	0	1148	33	0
37	FE	1105	0	1148	50	0
37	HE	1105	0	1148	37	0
38	BF	817	0	808	51	0
38	DF	817	0	808	28	0
38	FF	817	0	808	28	0
38	HF	817	0	808	25	0
39	BG	1181	0	1238	25	0
39	DG	1181	0	1238	31	0
39	FG	1181	0	1238	35	0
39	HG	1181	0	1238	38	0
40	BH	979	0	1031	50	0
40	DH	979	0	1031	28	0
40	FH	979	0	1031	34	0
40	HH	979	0	1031	28	0
41	BI	1022	0	1070	58	0
41	DI	1022	0	1070	53	0
41	FI	1022	0	1070	44	0
41	HI	1022	0	1070	59	0
42	BJ	786	0	828	26	0
42	DJ	786	0	828	34	0
42	FJ	786	0	828	43	0
42	HJ	786	0	828	34	0
43	BK	877	0	887	75	0
43	DK	877	0	887	45	0
43	FK	877	0	887	38	0
43	HK	877	0	887	75	0
44	BL	955	0	1016	55	0
44	DL	955	0	1016	52	0
44	FL	955	0	1016	51	0
44	HL	955	0	1016	39	0
45	BM	883	0	941	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	DM	883	0	941	25	0
45	FM	883	0	941	34	0
45	HM	883	0	941	53	0
46	BN	774	0	824	32	0
46	DN	774	0	824	21	0
46	FN	774	0	824	30	0
46	HN	774	0	824	29	0
47	BO	714	0	734	18	0
47	DO	714	0	734	13	0
47	FO	714	0	734	17	0
47	HO	714	0	734	21	0
48	BP	649	0	666	29	0
48	DP	649	0	666	25	0
48	FP	649	0	666	18	0
48	HP	649	0	666	19	0
49	BQ	648	0	691	19	0
49	DQ	648	0	691	21	0
49	FQ	648	0	691	16	0
49	HQ	648	0	691	21	0
50	BR	455	0	478	19	0
50	DR	455	0	478	16	0
50	FR	455	0	478	16	0
50	HR	455	0	478	15	0
51	BS	637	0	665	23	0
51	DS	637	0	665	17	0
51	FS	637	0	665	30	0
51	HS	637	0	665	21	0
52	BT	665	0	714	30	0
52	DT	665	0	714	26	0
52	FT	665	0	714	30	0
52	HT	665	0	714	19	0
53	BU	425	0	449	40	0
53	DU	425	0	449	28	0
53	FU	425	0	449	24	0
53	HU	425	0	449	36	0
54	BV	5319	0	5228	105	0
54	DV	5319	0	5228	113	0
54	FV	5319	0	5229	111	0
54	HV	5319	0	5227	145	0
55	BW	48	0	41	7	0
55	DW	48	0	41	8	0
55	FW	48	0	39	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	A3	1	0	0	0	0
56	AA	130	0	0	0	0
56	AB	4	0	0	0	0
56	AC	3	0	0	0	0
56	AD	1	0	0	0	0
56	AE	1	0	0	0	0
56	AT	1	0	0	0	0
56	BA	40	0	0	0	0
56	BE	1	0	0	0	0
56	BL	1	0	0	0	0
56	BU	1	0	0	0	0
56	BV	1	0	0	0	0
56	C4	1	0	0	0	0
56	CA	134	0	0	0	0
56	CB	4	0	0	0	0
56	CD	1	0	0	0	0
56	CE	1	0	0	0	0
56	DA	42	0	0	0	0
56	DU	1	0	0	0	0
56	DV	1	0	0	0	0
56	EA	133	0	0	0	0
56	EB	4	0	0	0	0
56	EC	1	0	0	0	0
56	ED	2	0	0	0	0
56	EQ	1	0	0	0	0
56	FA	41	0	0	0	0
56	FE	1	0	0	0	0
56	FU	1	0	0	0	0
56	FV	1	0	0	0	0
56	GA	134	0	0	0	0
56	GB	4	0	0	0	0
56	GC	1	0	0	0	0
56	GL	1	0	0	0	0
56	GS	1	0	0	0	0
56	HA	40	0	0	0	0
56	HC	1	0	0	0	0
56	HE	1	0	0	0	0
56	HT	1	0	0	0	0
56	HV	1	0	0	0	0
57	A4	1	0	0	0	0
57	C4	1	0	0	0	0
57	E4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	G4	1	0	0	0	0
58	BV	32	0	14	2	0
58	DV	32	0	14	1	0
58	FV	32	0	14	5	0
58	HV	32	0	14	1	0
59	A0	1	0	0	0	0
59	A3	1	0	0	0	0
59	A4	2	0	0	0	0
59	AA	608	0	0	111	0
59	AB	19	0	0	1	0
59	AC	10	0	0	0	0
59	AD	3	0	0	0	0
59	AE	1	0	0	0	0
59	AJ	1	0	0	1	0
59	AL	7	0	0	1	0
59	AN	4	0	0	0	0
59	AP	1	0	0	0	0
59	AQ	1	0	0	0	0
59	AS	1	0	0	0	0
59	AU	1	0	0	0	0
59	BA	197	0	0	36	0
59	BC	1	0	0	0	0
59	BD	1	0	0	0	0
59	BI	1	0	0	0	0
59	BK	1	0	0	0	0
59	BN	3	0	0	0	0
59	BT	2	0	0	0	0
59	BU	1	0	0	0	0
59	BV	1	0	0	1	0
59	C2	1	0	0	0	0
59	C3	1	0	0	0	0
59	C4	2	0	0	0	0
59	CA	604	0	0	104	0
59	CB	20	0	0	2	0
59	CC	11	0	0	4	0
59	CD	3	0	0	0	0
59	CE	1	0	0	0	0
59	CF	1	0	0	0	0
59	CJ	3	0	0	2	0
59	CL	6	0	0	1	0
59	CN	4	0	0	0	0
59	CS	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	CT	2	0	0	0	0
59	DA	193	0	0	32	0
59	DC	1	0	0	0	0
59	DE	2	0	0	0	0
59	DG	1	0	0	0	0
59	DK	1	0	0	0	0
59	DL	1	0	0	0	0
59	DN	6	0	0	0	0
59	DQ	1	0	0	0	0
59	DT	1	0	0	1	0
59	DU	1	0	0	0	0
59	DV	1	0	0	1	0
59	E0	2	0	0	0	0
59	E3	2	0	0	0	0
59	E4	1	0	0	0	0
59	EA	617	0	0	88	0
59	EB	20	0	0	1	0
59	EC	8	0	0	0	0
59	ED	1	0	0	0	0
59	EL	4	0	0	0	0
59	EN	2	0	0	0	0
59	ER	1	0	0	0	0
59	ET	1	0	0	0	0
59	EU	1	0	0	0	0
59	FA	198	0	0	21	0
59	FE	1	0	0	0	0
59	FK	1	0	0	0	0
59	FN	3	0	0	0	0
59	FQ	1	0	0	0	0
59	FT	4	0	0	1	0
59	FV	1	0	0	1	0
59	G2	2	0	0	0	0
59	G3	1	0	0	0	0
59	G4	1	0	0	0	0
59	GA	607	0	0	87	0
59	GB	19	0	0	1	0
59	GC	9	0	0	2	0
59	GD	4	0	0	0	0
59	GE	2	0	0	0	0
59	GL	4	0	0	1	0
59	GN	3	0	0	0	0
59	GQ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	GR	2	0	0	0	0
59	GS	1	0	0	0	0
59	GT	1	0	0	0	0
59	GU	2	0	0	0	0
59	GV	1	0	0	1	0
59	HA	197	0	0	33	0
59	HD	1	0	0	0	0
59	HE	3	0	0	0	0
59	HN	5	0	0	0	0
59	HT	1	0	0	0	0
59	HU	1	0	0	0	0
59	HV	1	0	0	1	0
All	All	590573	0	402393	12569	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

The worst 5 of 12569 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
32:A5:117:LEU:CD2	32:A5:120:ALA:HA	1.56	1.35
32:A5:24:SER:CB	32:A5:116:GLU:HG2	1.59	1.32
32:A5:24:SER:O	32:A5:116:GLU:HB3	1.37	1.24
32:E5:117:LEU:CD2	32:E5:120:ALA:HA	1.70	1.20
32:E5:24:SER:CB	32:E5:116:GLU:HG2	1.75	1.16

All (4) 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	Distance(Å)	Clash(Å)
33:FA:1029:U:O3'	1:GA:1508:A:N6[1_565]	2.13	0.07
33:FA:1029:U:OP2	1:GA:1509:A:N6[1_565]	2.16	0.04
33:FA:1029:U:O2'	1:GA:1508:A:N6[1_565]	2.16	0.04
6:GF:20:ASN:ND2	21:GU:52:ASN:OD1[2_556]	2.18	0.02

## 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	
3	AC	269/273 (98%)	220 (82%)	34 (13%)	15 (6%)	3	8
3	CC	269/273 (98%)	218 (81%)	35 (13%)	16 (6%)	2	7
3	EC	269/273 (98%)	219 (81%)	36 (13%)	14 (5%)	3	10
3	GC	269/273 (98%)	225 (84%)	30 (11%)	14 (5%)	3	10
4	AD	207/209 (99%)	161 (78%)	33 (16%)	13 (6%)	2	6
4	CD	207/209 (99%)	160 (77%)	33 (16%)	14 (7%)	2	5
4	ED	207/209 (99%)	155 (75%)	34 (16%)	18 (9%)	1	3
4	GD	207/209 (99%)	158 (76%)	34 (16%)	15 (7%)	2	4
5	AE	199/201 (99%)	163 (82%)	24 (12%)	12 (6%)	2	7
5	CE	199/201 (99%)	161 (81%)	26 (13%)	12 (6%)	2	7
5	EE	199/201 (99%)	162 (81%)	25 (13%)	12 (6%)	2	7
5	GE	199/201 (99%)	162 (81%)	25 (13%)	12 (6%)	2	7
6	AF	175/179 (98%)	128 (73%)	41 (23%)	6 (3%)	6	23
6	CF	175/179 (98%)	132 (75%)	37 (21%)	6 (3%)	6	23
6	EF	175/179 (98%)	139 (79%)	29 (17%)	7 (4%)	5	17
6	GF	175/179 (98%)	132 (75%)	40 (23%)	3 (2%)	14	45
7	AG	174/177 (98%)	124 (71%)	33 (19%)	17 (10%)	1	2
7	CG	174/177 (98%)	123 (71%)	37 (21%)	14 (8%)	1	3
7	EG	174/177 (98%)	120 (69%)	43 (25%)	11 (6%)	2	6
7	GG	174/177 (98%)	118 (68%)	41 (24%)	15 (9%)	1	3
8	AH	48/50 (96%)	24 (50%)	19 (40%)	5 (10%)	1	2
8	CH	48/50 (96%)	23 (48%)	19 (40%)	6 (12%)	1	1
8	EH	48/50 (96%)	24 (50%)	19 (40%)	5 (10%)	1	2
8	GH	48/50 (96%)	24 (50%)	21 (44%)	3 (6%)	2	6
9	AI	139/142 (98%)	87 (63%)	45 (32%)	7 (5%)	3	11
9	CI	139/142 (98%)	92 (66%)	37 (27%)	10 (7%)	2	4
9	EI	139/142 (98%)	90 (65%)	42 (30%)	7 (5%)	3	11
9	GI	139/142 (98%)	89 (64%)	38 (27%)	12 (9%)	1	3
10	AJ	140/142 (99%)	114 (81%)	18 (13%)	8 (6%)	3	8
10	CJ	140/142 (99%)	113 (81%)	19 (14%)	8 (6%)	3	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	EJ	140/142 (99%)	113 (81%)	19 (14%)	8 (6%)	3	8
10	GJ	140/142 (99%)	114 (81%)	17 (12%)	9 (6%)	2	6
11	AK	120/123 (98%)	93 (78%)	17 (14%)	10 (8%)	1	3
11	CK	120/123 (98%)	91 (76%)	21 (18%)	8 (7%)	2	5
11	EK	120/123 (98%)	92 (77%)	17 (14%)	11 (9%)	1	2
11	GK	120/123 (98%)	92 (77%)	19 (16%)	9 (8%)	2	4
12	AL	141/144 (98%)	107 (76%)	26 (18%)	8 (6%)	3	8
12	CL	141/144 (98%)	107 (76%)	27 (19%)	7 (5%)	3	11
12	EL	141/144 (98%)	108 (77%)	26 (18%)	7 (5%)	3	11
12	GL	141/144 (98%)	109 (77%)	25 (18%)	7 (5%)	3	11
13	AM	134/136 (98%)	105 (78%)	22 (16%)	7 (5%)	3	10
13	CM	134/136 (98%)	111 (83%)	16 (12%)	7 (5%)	3	10
13	EM	134/136 (98%)	110 (82%)	18 (13%)	6 (4%)	4	14
13	GM	134/136 (98%)	112 (84%)	16 (12%)	6 (4%)	4	14
14	AN	118/127 (93%)	101 (86%)	15 (13%)	2 (2%)	14	45
14	CN	118/127 (93%)	98 (83%)	17 (14%)	3 (2%)	9	32
14	EN	118/127 (93%)	101 (86%)	14 (12%)	3 (2%)	9	32
14	GN	118/127 (93%)	98 (83%)	19 (16%)	1 (1%)	27	68
15	AO	114/117 (97%)	99 (87%)	14 (12%)	1 (1%)	25	66
15	CO	114/117 (97%)	96 (84%)	17 (15%)	1 (1%)	25	66
15	EO	114/117 (97%)	96 (84%)	18 (16%)	0	100	100
15	GO	114/117 (97%)	97 (85%)	13 (11%)	4 (4%)	6	23
16	AP	112/115 (97%)	83 (74%)	22 (20%)	7 (6%)	2	6
16	CP	112/115 (97%)	81 (72%)	22 (20%)	9 (8%)	1	3
16	EP	112/115 (97%)	83 (74%)	22 (20%)	7 (6%)	2	6
16	GP	112/115 (97%)	79 (70%)	21 (19%)	12 (11%)	1	2
17	AQ	115/118 (98%)	101 (88%)	9 (8%)	5 (4%)	4	15
17	CQ	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	6	23
17	EQ	115/118 (98%)	102 (89%)	8 (7%)	5 (4%)	4	15
17	GQ	115/118 (98%)	103 (90%)	7 (6%)	5 (4%)	4	15
18	AR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	7	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	7	27
18	ER	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	7	27
18	GR	101/103 (98%)	84 (83%)	13 (13%)	4 (4%)	5	17
19	AS	108/110 (98%)	93 (86%)	10 (9%)	5 (5%)	4	14
19	CS	108/110 (98%)	96 (89%)	8 (7%)	4 (4%)	5	20
19	ES	108/110 (98%)	91 (84%)	12 (11%)	5 (5%)	4	14
19	GS	108/110 (98%)	92 (85%)	11 (10%)	5 (5%)	4	14
20	AT	91/100 (91%)	59 (65%)	24 (26%)	8 (9%)	1	3
20	CT	91/100 (91%)	60 (66%)	23 (25%)	8 (9%)	1	3
20	ET	91/100 (91%)	59 (65%)	25 (28%)	7 (8%)	1	3
20	GT	91/100 (91%)	60 (66%)	22 (24%)	9 (10%)	1	2
21	AU	100/104 (96%)	73 (73%)	18 (18%)	9 (9%)	1	2
21	CU	100/104 (96%)	74 (74%)	16 (16%)	10 (10%)	1	2
21	EU	100/104 (96%)	74 (74%)	13 (13%)	13 (13%)	0	1
21	GU	100/104 (96%)	73 (73%)	18 (18%)	9 (9%)	1	2
22	AV	92/94 (98%)	82 (89%)	9 (10%)	1 (1%)	21	60
22	CV	92/94 (98%)	79 (86%)	12 (13%)	1 (1%)	21	60
22	EV	92/94 (98%)	82 (89%)	9 (10%)	1 (1%)	21	60
22	GV	92/94 (98%)	83 (90%)	8 (9%)	1 (1%)	21	60
23	AW	77/85 (91%)	41 (53%)	19 (25%)	17 (22%)	0	0
23	CW	77/85 (91%)	42 (54%)	21 (27%)	14 (18%)	0	0
23	EW	77/85 (91%)	42 (54%)	19 (25%)	16 (21%)	0	0
23	GW	77/85 (91%)	42 (54%)	21 (27%)	14 (18%)	0	0
24	AX	75/78 (96%)	65 (87%)	7 (9%)	3 (4%)	5	17
24	CX	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	5	17
24	EX	75/78 (96%)	64 (85%)	9 (12%)	2 (3%)	8	30
24	GX	75/78 (96%)	65 (87%)	9 (12%)	1 (1%)	18	54
25	AY	61/63 (97%)	40 (66%)	19 (31%)	2 (3%)	6	24
25	CY	61/63 (97%)	43 (70%)	17 (28%)	1 (2%)	14	47
25	EY	61/63 (97%)	38 (62%)	19 (31%)	4 (7%)	2	5
25	GY	61/63 (97%)	42 (69%)	17 (28%)	2 (3%)	6	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	AZ	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	5	22
26	CZ	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	5	22
26	EZ	56/59 (95%)	48 (86%)	6 (11%)	2 (4%)	5	22
26	GZ	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	5	22
27	A0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	3	8
27	C0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	3	8
27	E0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	3	8
27	G0	54/57 (95%)	45 (83%)	6 (11%)	3 (6%)	3	8
28	A1	48/55 (87%)	40 (83%)	5 (10%)	3 (6%)	2	6
28	C1	48/55 (87%)	40 (83%)	6 (12%)	2 (4%)	4	16
28	E1	48/55 (87%)	42 (88%)	5 (10%)	1 (2%)	11	39
28	G1	48/55 (87%)	41 (85%)	5 (10%)	2 (4%)	4	16
29	A2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	10	36
29	C2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	10	36
29	E2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	10	36
29	G2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	10	36
30	A3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	6	25
30	C3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	6	25
30	E3	62/65 (95%)	55 (89%)	5 (8%)	2 (3%)	6	25
30	G3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	6	25
31	A4	36/38 (95%)	31 (86%)	2 (6%)	3 (8%)	1	3
31	C4	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	3	8
31	E4	36/38 (95%)	31 (86%)	2 (6%)	3 (8%)	1	3
31	G4	36/38 (95%)	30 (83%)	4 (11%)	2 (6%)	3	8
32	A5	146/165 (88%)	80 (55%)	44 (30%)	22 (15%)	0	1
32	E5	142/165 (86%)	80 (56%)	39 (28%)	23 (16%)	0	0
34	BB	216/241 (90%)	147 (68%)	57 (26%)	12 (6%)	3	8
34	DB	216/241 (90%)	145 (67%)	59 (27%)	12 (6%)	3	8
34	FB	216/241 (90%)	146 (68%)	60 (28%)	10 (5%)	4	14
34	HB	216/241 (90%)	149 (69%)	55 (26%)	12 (6%)	3	8
35	BC	204/233 (88%)	180 (88%)	16 (8%)	8 (4%)	5	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	DC	204/233 (88%)	177 (87%)	23 (11%)	4 (2%)	11	40
35	FC	204/233 (88%)	181 (89%)	17 (8%)	6 (3%)	7	28
35	HC	204/233 (88%)	183 (90%)	16 (8%)	5 (2%)	9	32
36	BD	203/206 (98%)	157 (77%)	34 (17%)	12 (6%)	2	7
36	DD	203/206 (98%)	157 (77%)	30 (15%)	16 (8%)	1	3
36	FD	203/206 (98%)	155 (76%)	34 (17%)	14 (7%)	2	4
36	HD	203/206 (98%)	159 (78%)	35 (17%)	9 (4%)	4	15
37	BE	148/167 (89%)	124 (84%)	19 (13%)	5 (3%)	6	23
37	DE	148/167 (89%)	125 (84%)	18 (12%)	5 (3%)	6	23
37	FE	148/167 (89%)	122 (82%)	22 (15%)	4 (3%)	8	30
37	HE	148/167 (89%)	122 (82%)	22 (15%)	4 (3%)	8	30
38	BF	98/135 (73%)	73 (74%)	20 (20%)	5 (5%)	3	10
38	DF	98/135 (73%)	71 (72%)	20 (20%)	7 (7%)	2	4
38	FF	98/135 (73%)	72 (74%)	16 (16%)	10 (10%)	1	2
38	HF	98/135 (73%)	75 (76%)	18 (18%)	5 (5%)	3	10
39	BG	149/179 (83%)	126 (85%)	23 (15%)	0	100	100
39	DG	149/179 (83%)	123 (83%)	25 (17%)	1 (1%)	30	72
39	FG	149/179 (83%)	126 (85%)	23 (15%)	0	100	100
39	HG	149/179 (83%)	122 (82%)	25 (17%)	2 (1%)	18	54
40	BH	127/130 (98%)	108 (85%)	18 (14%)	1 (1%)	27	68
40	DH	127/130 (98%)	110 (87%)	15 (12%)	2 (2%)	14	47
40	FH	127/130 (98%)	113 (89%)	12 (9%)	2 (2%)	14	47
40	HH	127/130 (98%)	111 (87%)	16 (13%)	0	100	100
41	BI	125/130 (96%)	96 (77%)	21 (17%)	8 (6%)	2	6
41	DI	125/130 (96%)	99 (79%)	19 (15%)	7 (6%)	3	8
41	FI	125/130 (96%)	97 (78%)	22 (18%)	6 (5%)	4	12
41	HI	125/130 (96%)	98 (78%)	21 (17%)	6 (5%)	4	12
42	BJ	96/103 (93%)	73 (76%)	16 (17%)	7 (7%)	2	4
42	DJ	96/103 (93%)	72 (75%)	18 (19%)	6 (6%)	2	6
42	FJ	96/103 (93%)	73 (76%)	17 (18%)	6 (6%)	2	6
42	HJ	96/103 (93%)	73 (76%)	19 (20%)	4 (4%)	4	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BK	115/129 (89%)	92 (80%)	17 (15%)	6 (5%)	3	10
43	DK	115/129 (89%)	90 (78%)	23 (20%)	2 (2%)	14	45
43	FK	115/129 (89%)	92 (80%)	20 (17%)	3 (3%)	8	32
43	HK	115/129 (89%)	87 (76%)	24 (21%)	4 (4%)	6	23
44	BL	121/124 (98%)	95 (78%)	17 (14%)	9 (7%)	2	4
44	DL	121/124 (98%)	95 (78%)	18 (15%)	8 (7%)	2	5
44	FL	121/124 (98%)	96 (79%)	17 (14%)	8 (7%)	2	5
44	HL	121/124 (98%)	97 (80%)	15 (12%)	9 (7%)	2	4
45	BM	112/118 (95%)	98 (88%)	8 (7%)	6 (5%)	3	9
45	DM	112/118 (95%)	99 (88%)	7 (6%)	6 (5%)	3	9
45	FM	112/118 (95%)	98 (88%)	9 (8%)	5 (4%)	4	14
45	HM	112/118 (95%)	91 (81%)	14 (12%)	7 (6%)	2	6
46	BN	92/101 (91%)	71 (77%)	18 (20%)	3 (3%)	6	24
46	DN	92/101 (91%)	71 (77%)	19 (21%)	2 (2%)	10	37
46	FN	92/101 (91%)	69 (75%)	20 (22%)	3 (3%)	6	24
46	HN	92/101 (91%)	70 (76%)	20 (22%)	2 (2%)	10	37
47	BO	86/89 (97%)	72 (84%)	12 (14%)	2 (2%)	10	36
47	DO	86/89 (97%)	73 (85%)	11 (13%)	2 (2%)	10	36
47	FO	86/89 (97%)	72 (84%)	12 (14%)	2 (2%)	10	36
47	HO	86/89 (97%)	70 (81%)	14 (16%)	2 (2%)	10	36
48	BP	80/82 (98%)	60 (75%)	16 (20%)	4 (5%)	3	11
48	DP	80/82 (98%)	62 (78%)	16 (20%)	2 (2%)	9	32
48	FP	80/82 (98%)	65 (81%)	13 (16%)	2 (2%)	9	32
48	HP	80/82 (98%)	61 (76%)	15 (19%)	4 (5%)	3	11
49	BQ	78/84 (93%)	54 (69%)	19 (24%)	5 (6%)	2	6
49	DQ	78/84 (93%)	56 (72%)	16 (20%)	6 (8%)	1	3
49	FQ	78/84 (93%)	57 (73%)	18 (23%)	3 (4%)	5	19
49	HQ	78/84 (93%)	57 (73%)	16 (20%)	5 (6%)	2	6
50	BR	53/75 (71%)	41 (77%)	12 (23%)	0	100	100
50	DR	53/75 (71%)	43 (81%)	10 (19%)	0	100	100
50	FR	53/75 (71%)	40 (76%)	13 (24%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	HR	53/75 (71%)	43 (81%)	10 (19%)	0	100	100
51	BS	77/92 (84%)	69 (90%)	7 (9%)	1 (1%)	18	54
51	DS	77/92 (84%)	70 (91%)	6 (8%)	1 (1%)	18	54
51	FS	77/92 (84%)	67 (87%)	6 (8%)	4 (5%)	3	10
51	HS	77/92 (84%)	68 (88%)	9 (12%)	0	100	100
52	BT	83/87 (95%)	66 (80%)	15 (18%)	2 (2%)	9	35
52	DT	83/87 (95%)	69 (83%)	11 (13%)	3 (4%)	5	22
52	FT	83/87 (95%)	66 (80%)	15 (18%)	2 (2%)	9	35
52	HT	83/87 (95%)	68 (82%)	14 (17%)	1 (1%)	19	57
53	BU	49/71 (69%)	25 (51%)	20 (41%)	4 (8%)	1	3
53	DU	49/71 (69%)	27 (55%)	20 (41%)	2 (4%)	4	17
53	FU	49/71 (69%)	28 (57%)	19 (39%)	2 (4%)	4	17
53	HU	49/71 (69%)	24 (49%)	22 (45%)	3 (6%)	2	7
54	BV	685/704 (97%)	559 (82%)	90 (13%)	36 (5%)	3	9
54	DV	685/704 (97%)	558 (82%)	92 (13%)	35 (5%)	3	10
54	FV	685/704 (97%)	556 (81%)	91 (13%)	38 (6%)	3	8
54	HV	685/704 (97%)	556 (81%)	91 (13%)	38 (6%)	3	8
55	BW	2/6 (33%)	0	0	2 (100%)	0	0
55	DW	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
55	FW	2/6 (33%)	2 (100%)	0	0	100	100
All	All	25122/26708 (94%)	19751 (79%)	4073 (16%)	1298 (5%)	3	10

5 of 1298 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	70	LYS
3	AC	104	LEU
3	AC	121	ALA
3	AC	140	VAL
3	AC	256	THR

### 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	
3	AC	216/218 (99%)	203 (94%)	13 (6%)	27	63
3	CC	216/218 (99%)	201 (93%)	15 (7%)	22	54
3	EC	216/218 (99%)	200 (93%)	16 (7%)	20	50
3	GC	216/218 (99%)	198 (92%)	18 (8%)	16	43
4	AD	164/164 (100%)	153 (93%)	11 (7%)	23	56
4	CD	164/164 (100%)	156 (95%)	8 (5%)	35	73
4	ED	164/164 (100%)	155 (94%)	9 (6%)	30	68
4	GD	164/164 (100%)	156 (95%)	8 (5%)	35	73
5	AE	165/165 (100%)	154 (93%)	11 (7%)	23	56
5	CE	165/165 (100%)	158 (96%)	7 (4%)	40	79
5	EE	165/165 (100%)	153 (93%)	12 (7%)	20	51
5	GE	165/165 (100%)	160 (97%)	5 (3%)	53	89
6	AF	148/150 (99%)	140 (95%)	8 (5%)	31	69
6	CF	148/150 (99%)	139 (94%)	9 (6%)	26	62
6	EF	148/150 (99%)	138 (93%)	10 (7%)	22	55
6	GF	148/150 (99%)	144 (97%)	4 (3%)	57	90
7	AG	137/138 (99%)	126 (92%)	11 (8%)	17	45
7	CG	137/138 (99%)	126 (92%)	11 (8%)	17	45
7	EG	137/138 (99%)	125 (91%)	12 (9%)	14	40
7	GG	137/138 (99%)	130 (95%)	7 (5%)	33	72
8	AH	40/40 (100%)	38 (95%)	2 (5%)	34	73
8	CH	40/40 (100%)	39 (98%)	1 (2%)	60	91
8	EH	40/40 (100%)	36 (90%)	4 (10%)	11	32
8	GH	40/40 (100%)	36 (90%)	4 (10%)	11	32
9	AI	109/110 (99%)	105 (96%)	4 (4%)	45	84
9	CI	109/110 (99%)	108 (99%)	1 (1%)	87	97
9	EI	109/110 (99%)	108 (99%)	1 (1%)	87	97
9	GI	109/110 (99%)	108 (99%)	1 (1%)	87	97
10	AJ	116/116 (100%)	97 (84%)	19 (16%)	3	10
10	CJ	116/116 (100%)	102 (88%)	14 (12%)	7	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	EJ	116/116 (100%)	96 (83%)	20 (17%)	3	8
10	GJ	116/116 (100%)	103 (89%)	13 (11%)	9	25
11	AK	103/104 (99%)	93 (90%)	10 (10%)	12	35
11	CK	103/104 (99%)	94 (91%)	9 (9%)	15	41
11	EK	103/104 (99%)	95 (92%)	8 (8%)	18	46
11	GK	103/104 (99%)	96 (93%)	7 (7%)	22	55
12	AL	102/103 (99%)	96 (94%)	6 (6%)	28	64
12	CL	102/103 (99%)	96 (94%)	6 (6%)	28	64
12	EL	102/103 (99%)	97 (95%)	5 (5%)	35	73
12	GL	102/103 (99%)	94 (92%)	8 (8%)	18	46
13	AM	109/109 (100%)	94 (86%)	15 (14%)	5	14
13	CM	109/109 (100%)	96 (88%)	13 (12%)	8	21
13	EM	109/109 (100%)	100 (92%)	9 (8%)	16	43
13	GM	109/109 (100%)	102 (94%)	7 (6%)	25	59
14	AN	100/103 (97%)	94 (94%)	6 (6%)	27	63
14	CN	100/103 (97%)	93 (93%)	7 (7%)	21	53
14	EN	100/103 (97%)	98 (98%)	2 (2%)	68	92
14	GN	100/103 (97%)	96 (96%)	4 (4%)	42	81
15	AO	86/87 (99%)	81 (94%)	5 (6%)	28	65
15	CO	86/87 (99%)	80 (93%)	6 (7%)	21	53
15	EO	86/87 (99%)	79 (92%)	7 (8%)	17	45
15	GO	86/87 (99%)	83 (96%)	3 (4%)	48	85
16	AP	99/100 (99%)	85 (86%)	14 (14%)	5	14
16	CP	99/100 (99%)	88 (89%)	11 (11%)	9	26
16	EP	99/100 (99%)	91 (92%)	8 (8%)	17	45
16	GP	99/100 (99%)	88 (89%)	11 (11%)	9	26
17	AQ	89/90 (99%)	83 (93%)	6 (7%)	23	56
17	CQ	89/90 (99%)	82 (92%)	7 (8%)	18	46
17	EQ	89/90 (99%)	80 (90%)	9 (10%)	11	32
17	GQ	89/90 (99%)	86 (97%)	3 (3%)	49	86
18	AR	84/84 (100%)	79 (94%)	5 (6%)	27	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	CR	84/84 (100%)	78 (93%)	6 (7%)	21	52
18	ER	84/84 (100%)	77 (92%)	7 (8%)	16	43
18	GR	84/84 (100%)	80 (95%)	4 (5%)	35	74
19	AS	93/93 (100%)	85 (91%)	8 (9%)	15	41
19	CS	93/93 (100%)	86 (92%)	7 (8%)	19	49
19	ES	93/93 (100%)	84 (90%)	9 (10%)	12	35
19	GS	93/93 (100%)	86 (92%)	7 (8%)	19	49
20	AT	80/84 (95%)	71 (89%)	9 (11%)	9	25
20	CT	80/84 (95%)	77 (96%)	3 (4%)	44	83
20	ET	80/84 (95%)	73 (91%)	7 (9%)	14	40
20	GT	80/84 (95%)	76 (95%)	4 (5%)	34	73
21	AU	83/85 (98%)	79 (95%)	4 (5%)	35	74
21	CU	83/85 (98%)	80 (96%)	3 (4%)	47	85
21	EU	83/85 (98%)	76 (92%)	7 (8%)	16	42
21	GU	83/85 (98%)	80 (96%)	3 (4%)	47	85
22	AV	78/78 (100%)	73 (94%)	5 (6%)	25	59
22	CV	78/78 (100%)	75 (96%)	3 (4%)	44	83
22	EV	78/78 (100%)	76 (97%)	2 (3%)	59	90
22	GV	78/78 (100%)	75 (96%)	3 (4%)	44	83
23	AW	59/63 (94%)	49 (83%)	10 (17%)	3	9
23	CW	59/63 (94%)	51 (86%)	8 (14%)	5	15
23	EW	59/63 (94%)	52 (88%)	7 (12%)	8	21
23	GW	59/63 (94%)	53 (90%)	6 (10%)	11	31
24	AX	67/68 (98%)	61 (91%)	6 (9%)	14	39
24	CX	67/68 (98%)	60 (90%)	7 (10%)	10	29
24	EX	67/68 (98%)	60 (90%)	7 (10%)	10	29
24	GX	67/68 (98%)	61 (91%)	6 (9%)	14	39
25	AY	55/55 (100%)	49 (89%)	6 (11%)	9	26
25	CY	55/55 (100%)	53 (96%)	2 (4%)	47	85
25	EY	55/55 (100%)	49 (89%)	6 (11%)	9	26
25	GY	55/55 (100%)	51 (93%)	4 (7%)	20	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	AZ	48/49 (98%)	44 (92%)	4 (8%)	16	43
26	CZ	48/49 (98%)	43 (90%)	5 (10%)	10	29
26	EZ	48/49 (98%)	44 (92%)	4 (8%)	16	43
26	GZ	48/49 (98%)	43 (90%)	5 (10%)	10	29
27	A0	47/48 (98%)	47 (100%)	0	100	100
27	C0	47/48 (98%)	45 (96%)	2 (4%)	40	78
27	E0	47/48 (98%)	45 (96%)	2 (4%)	40	78
27	G0	47/48 (98%)	47 (100%)	0	100	100
28	A1	45/49 (92%)	42 (93%)	3 (7%)	23	56
28	C1	45/49 (92%)	41 (91%)	4 (9%)	14	40
28	E1	45/49 (92%)	43 (96%)	2 (4%)	39	77
28	G1	45/49 (92%)	44 (98%)	1 (2%)	64	92
29	A2	38/38 (100%)	37 (97%)	1 (3%)	59	90
29	C2	38/38 (100%)	35 (92%)	3 (8%)	18	46
29	E2	38/38 (100%)	33 (87%)	5 (13%)	6	16
29	G2	38/38 (100%)	34 (90%)	4 (10%)	10	29
30	A3	51/52 (98%)	49 (96%)	2 (4%)	43	82
30	C3	51/52 (98%)	50 (98%)	1 (2%)	68	92
30	E3	51/52 (98%)	47 (92%)	4 (8%)	18	46
30	G3	51/52 (98%)	47 (92%)	4 (8%)	18	46
31	A4	34/34 (100%)	32 (94%)	2 (6%)	28	64
31	C4	34/34 (100%)	32 (94%)	2 (6%)	28	64
31	E4	34/34 (100%)	32 (94%)	2 (6%)	28	64
31	G4	34/34 (100%)	31 (91%)	3 (9%)	14	40
32	A5	112/123 (91%)	95 (85%)	17 (15%)	4	12
32	E5	110/123 (89%)	96 (87%)	14 (13%)	6	18
34	BB	180/199 (90%)	171 (95%)	9 (5%)	34	73
34	DB	180/199 (90%)	171 (95%)	9 (5%)	34	73
34	FB	180/199 (90%)	172 (96%)	8 (4%)	39	77
34	HB	180/199 (90%)	170 (94%)	10 (6%)	30	66
35	BC	170/190 (90%)	167 (98%)	3 (2%)	71	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	DC	170/190 (90%)	166 (98%)	4 (2%)	61	91
35	FC	170/190 (90%)	158 (93%)	12 (7%)	21	52
35	HC	170/190 (90%)	164 (96%)	6 (4%)	48	85
36	BD	172/173 (99%)	163 (95%)	9 (5%)	32	71
36	DD	172/173 (99%)	162 (94%)	10 (6%)	28	65
36	FD	172/173 (99%)	162 (94%)	10 (6%)	28	65
36	HD	172/173 (99%)	163 (95%)	9 (5%)	32	71
37	BE	113/126 (90%)	107 (95%)	6 (5%)	32	70
37	DE	113/126 (90%)	110 (97%)	3 (3%)	57	90
37	FE	113/126 (90%)	104 (92%)	9 (8%)	17	45
37	HE	113/126 (90%)	106 (94%)	7 (6%)	26	61
38	BF	87/116 (75%)	83 (95%)	4 (5%)	37	76
38	DF	87/116 (75%)	85 (98%)	2 (2%)	63	92
38	FF	87/116 (75%)	84 (97%)	3 (3%)	49	86
38	HF	87/116 (75%)	85 (98%)	2 (2%)	63	92
39	BG	124/147 (84%)	122 (98%)	2 (2%)	75	95
39	DG	124/147 (84%)	121 (98%)	3 (2%)	61	91
39	FG	124/147 (84%)	120 (97%)	4 (3%)	51	88
39	HG	124/147 (84%)	123 (99%)	1 (1%)	89	97
40	BH	104/105 (99%)	98 (94%)	6 (6%)	28	65
40	DH	104/105 (99%)	97 (93%)	7 (7%)	23	56
40	FH	104/105 (99%)	97 (93%)	7 (7%)	23	56
40	HH	104/105 (99%)	98 (94%)	6 (6%)	28	65
41	BI	105/107 (98%)	96 (91%)	9 (9%)	15	41
41	DI	105/107 (98%)	102 (97%)	3 (3%)	55	89
41	FI	105/107 (98%)	98 (93%)	7 (7%)	23	56
41	HI	105/107 (98%)	99 (94%)	6 (6%)	29	66
42	BJ	86/90 (96%)	85 (99%)	1 (1%)	82	96
42	DJ	86/90 (96%)	80 (93%)	6 (7%)	21	53
42	FJ	86/90 (96%)	84 (98%)	2 (2%)	63	92
42	HJ	86/90 (96%)	83 (96%)	3 (4%)	48	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BK	90/99 (91%)	87 (97%)	3 (3%)	50	87
43	DK	90/99 (91%)	88 (98%)	2 (2%)	64	92
43	FK	90/99 (91%)	85 (94%)	5 (6%)	30	66
43	HK	90/99 (91%)	82 (91%)	8 (9%)	14	40
44	BL	103/104 (99%)	100 (97%)	3 (3%)	55	89
44	DL	103/104 (99%)	101 (98%)	2 (2%)	69	93
44	FL	103/104 (99%)	97 (94%)	6 (6%)	28	65
44	HL	103/104 (99%)	94 (91%)	9 (9%)	15	41
45	BM	92/96 (96%)	89 (97%)	3 (3%)	50	87
45	DM	92/96 (96%)	92 (100%)	0	100	100
45	FM	92/96 (96%)	92 (100%)	0	100	100
45	HM	92/96 (96%)	92 (100%)	0	100	100
46	BN	79/84 (94%)	79 (100%)	0	100	100
46	DN	79/84 (94%)	78 (99%)	1 (1%)	80	96
46	FN	79/84 (94%)	75 (95%)	4 (5%)	33	72
46	HN	79/84 (94%)	77 (98%)	2 (2%)	60	91
47	BO	76/77 (99%)	72 (95%)	4 (5%)	32	70
47	DO	76/77 (99%)	74 (97%)	2 (3%)	59	90
47	FO	76/77 (99%)	74 (97%)	2 (3%)	59	90
47	HO	76/77 (99%)	74 (97%)	2 (3%)	59	90
48	BP	65/65 (100%)	63 (97%)	2 (3%)	52	88
48	DP	65/65 (100%)	60 (92%)	5 (8%)	18	47
48	FP	65/65 (100%)	64 (98%)	1 (2%)	76	95
48	HP	65/65 (100%)	63 (97%)	2 (3%)	52	88
49	BQ	74/78 (95%)	70 (95%)	4 (5%)	31	69
49	DQ	74/78 (95%)	72 (97%)	2 (3%)	57	90
49	FQ	74/78 (95%)	73 (99%)	1 (1%)	78	96
49	HQ	74/78 (95%)	69 (93%)	5 (7%)	22	55
50	BR	48/65 (74%)	48 (100%)	0	100	100
50	DR	48/65 (74%)	48 (100%)	0	100	100
50	FR	48/65 (74%)	46 (96%)	2 (4%)	40	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	HR	48/65 (74%)	48 (100%)	0	100	100
51	BS	70/79 (89%)	69 (99%)	1 (1%)	78	96
51	DS	70/79 (89%)	67 (96%)	3 (4%)	40	78
51	FS	70/79 (89%)	64 (91%)	6 (9%)	15	41
51	HS	70/79 (89%)	67 (96%)	3 (4%)	40	78
52	BT	65/66 (98%)	60 (92%)	5 (8%)	18	47
52	DT	65/66 (98%)	58 (89%)	7 (11%)	9	27
52	FT	65/66 (98%)	60 (92%)	5 (8%)	18	47
52	HT	65/66 (98%)	60 (92%)	5 (8%)	18	47
53	BU	44/61 (72%)	42 (96%)	2 (4%)	38	77
53	DU	44/61 (72%)	41 (93%)	3 (7%)	22	55
53	FU	44/61 (72%)	41 (93%)	3 (7%)	22	55
53	HU	44/61 (72%)	42 (96%)	2 (4%)	38	77
54	BV	557/578 (96%)	503 (90%)	54 (10%)	12	35
54	DV	557/578 (96%)	508 (91%)	49 (9%)	14	40
54	FV	557/578 (96%)	508 (91%)	49 (9%)	14	40
54	HV	557/578 (96%)	507 (91%)	50 (9%)	14	39
55	BW	2/2 (100%)	1 (50%)	1 (50%)	0	0
55	DW	2/2 (100%)	1 (50%)	1 (50%)	0	0
55	FW	2/2 (100%)	2 (100%)	0	100	100
All	All	20824/21780 (96%)	19507 (94%)	1317 (6%)	25	60

5 of 1317 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	DQ	48	ASP
10	EJ	95	ARG
40	HH	94	LYS
54	DV	77	LYS
3	EC	176	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
7	EG	115	GLN
34	FB	57	ASN
51	HS	52	HIS
9	EI	33	ASN
22	EV	80	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2850/2904 (98%)	472 (16%)	48 (1%)
1	CA	2850/2904 (98%)	470 (16%)	50 (1%)
1	EA	2850/2904 (98%)	471 (16%)	45 (1%)
1	GA	2850/2904 (98%)	471 (16%)	51 (1%)
2	AB	117/120 (97%)	17 (14%)	0
2	CB	117/120 (97%)	18 (15%)	1 (0%)
2	EB	117/120 (97%)	17 (14%)	0
2	GB	117/120 (97%)	19 (16%)	0
33	BA	1532/1542 (99%)	272 (17%)	18 (1%)
33	DA	1532/1542 (99%)	269 (17%)	18 (1%)
33	FA	1532/1542 (99%)	265 (17%)	17 (1%)
33	HA	1532/1542 (99%)	273 (17%)	18 (1%)
All	All	17996/18264 (98%)	3034 (16%)	266 (1%)

5 of 3034 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	A
1	AA	12	U
1	AA	15	G
1	AA	34	U
1	AA	35	G

5 of 266 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	DA	250	A
1	EA	764	A
1	GA	2756	U
33	DA	499	A
1	EA	119	A

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
55	KBE	BW	1	55	8,8,9	6.06	2 (25%)	6,8,10	0.92	0
55	DPP	BW	2	55	5,5,6	7.85	1 (20%)	3,5,7	2.83	1 (33%)
55	UAL	BW	5	55	7,8,9	5.18	4 (57%)	6,9,11	2.07	1 (16%)
55	5OH	BW	6	55	12,12,13	5.58	3 (25%)	13,16,18	2.22	4 (30%)
55	KBE	DW	1	55	8,8,9	6.27	2 (25%)	6,8,10	1.03	0
55	DPP	DW	2	55	5,5,6	7.70	1 (20%)	3,5,7	1.51	1 (33%)
55	UAL	DW	5	55	7,8,9	4.88	4 (57%)	6,9,11	1.79	1 (16%)
55	5OH	DW	6	55	12,12,13	5.48	4 (33%)	13,16,18	1.32	2 (15%)
55	KBE	FW	1	55	8,8,9	5.93	2 (25%)	6,8,10	0.82	0
55	DPP	FW	2	55	5,5,6	8.31	1 (20%)	3,5,7	1.34	1 (33%)
55	UAL	FW	5	55	7,8,9	4.86	4 (57%)	6,9,11	1.92	2 (33%)
55	5OH	FW	6	55	12,12,13	5.94	4 (33%)	13,16,18	1.46	4 (30%)

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
55	KBE	BW	1	55	-	0/6/7/8	0/0/0/0
55	DPP	BW	2	55	-	0/2/4/6	0/0/0/0
55	UAL	BW	5	55	-	0/3/7/9	0/0/0/0
55	5OH	BW	6	55	-	0/2/18/20	0/1/1/1
55	KBE	DW	1	55	-	0/6/7/8	0/0/0/0
55	DPP	DW	2	55	-	0/2/4/6	0/0/0/0
55	UAL	DW	5	55	-	0/3/7/9	0/0/0/0
55	5OH	DW	6	55	-	0/2/18/20	0/1/1/1
55	KBE	FW	1	55	-	0/6/7/8	0/0/0/0
55	DPP	FW	2	55	-	0/2/4/6	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	UAL	FW	5	55	-	0/3/7/9	0/0/0/0
55	5OH	FW	6	55	-	0/2/18/20	0/1/1/1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	FW	2	DPP	O-C	18.46	1.24	1.11
55	DW	1	KBE	O-C	17.48	1.23	1.11
55	BW	2	DPP	O-C	17.44	1.23	1.11
55	DW	2	DPP	O-C	17.14	1.23	1.11
55	FW	6	5OH	O-C	16.99	1.23	1.11

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BW	2	DPP	C-CA-N	-4.66	109.18	113.83
55	BW	5	UAL	CA-CB-N1	-4.27	112.65	124.09
55	BW	6	5OH	C-CA-N	-3.87	105.65	111.94
55	FW	5	UAL	CA-CB-N1	-3.81	113.88	124.09
55	BW	6	5OH	CR-CB-NP	3.75	114.17	108.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 748 ligands modelled in this entry, 744 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	GCP	BV	801	56	34,34,34	2.48	9 (26%)	52,54,54	2.28	12 (23%)
58	GCP	DV	801	56	34,34,34	2.62	8 (23%)	52,54,54	2.21	12 (23%)
58	GCP	FV	801	56	34,34,34	1.65	9 (26%)	52,54,54	2.84	9 (17%)
58	GCP	HV	801	56	34,34,34	2.55	9 (26%)	52,54,54	2.35	9 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GCP	BV	801	56	-	0/20/38/38	0/3/3/3
58	GCP	DV	801	56	-	0/20/38/38	0/3/3/3
58	GCP	FV	801	56	-	0/20/38/38	0/3/3/3
58	GCP	HV	801	56	-	0/20/38/38	0/3/3/3

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	DV	801	GCP	C2-N2	8.89	1.45	1.32
58	HV	801	GCP	C2-N2	8.62	1.45	1.32
58	BV	801	GCP	C2-N2	8.60	1.45	1.32
58	DV	801	GCP	C2'-C1'	-6.36	1.44	1.53
58	BV	801	GCP	C2'-C1'	-5.87	1.45	1.53

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	FV	801	GCP	C6-C5-N7	14.71	136.12	134.14
58	BV	801	GCP	C4'-O4'-C1'	-8.69	100.17	109.72
58	HV	801	GCP	C6-C5-N7	-8.47	133.00	134.14
58	DV	801	GCP	C4'-O4'-C1'	-7.51	101.47	109.72
58	FV	801	GCP	C5-C4-N3	-6.53	118.55	126.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	2854/2904 (98%)	-0.06	72 (2%) 54 64	4, 28, 65, 87	0
1	CA	2854/2904 (98%)	-0.08	69 (2%) 56 65	3, 25, 63, 88	0
1	EA	2854/2904 (98%)	-0.08	51 (1%) 65 74	1, 14, 60, 92	0
1	GA	2854/2904 (98%)	-0.05	80 (2%) 50 59	5, 29, 68, 89	0
2	AB	118/120 (98%)	-0.33	0 100 100	18, 48, 62, 72	0
2	CB	118/120 (98%)	-0.49	0 100 100	18, 41, 54, 72	0
2	EB	118/120 (98%)	-0.38	0 100 100	3, 25, 45, 56	0
2	GB	118/120 (98%)	-0.38	1 (0%) 83 89	23, 44, 61, 78	0
3	AC	271/273 (99%)	-0.09	2 (0%) 84 90	5, 26, 40, 60	0
3	CC	271/273 (99%)	-0.20	1 (0%) 90 94	2, 18, 34, 44	0
3	EC	271/273 (99%)	-0.28	1 (0%) 90 94	1, 15, 32, 57	0
3	GC	271/273 (99%)	-0.26	0 100 100	3, 17, 30, 42	0
4	AD	209/209 (100%)	-0.09	3 (1%) 72 80	6, 27, 47, 60	0
4	CD	209/209 (100%)	0.00	6 (2%) 49 58	3, 31, 52, 61	0
4	ED	209/209 (100%)	-0.15	5 (2%) 56 65	1, 20, 43, 56	0
4	GD	209/209 (100%)	0.15	7 (3%) 44 53	4, 36, 54, 62	0
5	AE	201/201 (100%)	0.26	11 (5%) 24 29	7, 33, 55, 63	0
5	CE	201/201 (100%)	0.20	12 (5%) 21 25	4, 33, 54, 60	0
5	EE	201/201 (100%)	-0.03	4 (1%) 62 71	2, 19, 45, 69	0
5	GE	201/201 (100%)	0.39	14 (6%) 16 19	7, 41, 56, 67	0
6	AF	177/179 (98%)	2.72	99 (55%) 0 0	45, 61, 71, 79	0
6	CF	177/179 (98%)	0.79	25 (14%) 3 5	32, 49, 63, 67	0
6	EF	177/179 (98%)	0.70	21 (11%) 5 7	19, 42, 61, 68	0
6	GF	177/179 (98%)	2.20	79 (44%) 1 0	36, 61, 72, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
7	AG	176/177 (99%)	0.53	18 (10%) 7 9	20, 42, 60, 69	0
7	CG	176/177 (99%)	0.75	32 (18%) 2 3	23, 46, 61, 69	0
7	EG	176/177 (99%)	0.25	16 (9%) 9 12	19, 37, 55, 63	0
7	GG	176/177 (99%)	0.82	33 (18%) 2 2	32, 48, 63, 68	0
8	AH	50/50 (100%)	1.36	10 (20%) 2 2	28, 51, 67, 77	0
8	CH	50/50 (100%)	1.70	19 (38%) 1 0	39, 56, 68, 74	0
8	EH	50/50 (100%)	1.60	16 (32%) 1 1	24, 49, 69, 79	0
8	GH	50/50 (100%)	1.56	19 (38%) 1 0	26, 46, 64, 69	0
9	AI	141/142 (99%)	2.39	65 (46%) 1 0	44, 64, 75, 82	0
9	CI	141/142 (99%)	2.79	79 (56%) 0 0	49, 63, 73, 76	0
9	EI	141/142 (99%)	3.24	90 (63%) 0 0	48, 65, 77, 82	0
9	GI	141/142 (99%)	4.43	114 (80%) 0 0	49, 68, 77, 81	0
10	AJ	142/142 (100%)	-0.06	4 (2%) 50 59	12, 29, 41, 60	0
10	CJ	142/142 (100%)	0.03	3 (2%) 60 69	13, 29, 42, 58	0
10	EJ	142/142 (100%)	-0.15	1 (0%) 84 90	3, 13, 30, 47	0
10	GJ	142/142 (100%)	0.20	7 (4%) 28 34	15, 32, 47, 61	0
11	AK	122/123 (99%)	-0.14	4 (3%) 44 53	5, 19, 34, 54	0
11	CK	122/123 (99%)	-0.10	2 (1%) 68 78	9, 22, 39, 56	0
11	EK	122/123 (99%)	-0.04	4 (3%) 44 53	4, 18, 37, 49	0
11	GK	122/123 (99%)	0.22	2 (1%) 68 78	13, 27, 42, 59	0
12	AL	143/144 (99%)	0.37	7 (4%) 28 34	10, 30, 48, 58	0
12	CL	143/144 (99%)	0.15	4 (2%) 50 59	3, 29, 47, 62	0
12	EL	143/144 (99%)	0.19	8 (5%) 24 28	1, 18, 39, 54	0
12	GL	143/144 (99%)	0.67	23 (16%) 2 3	10, 35, 53, 67	0
13	AM	136/136 (100%)	0.06	3 (2%) 59 67	8, 19, 37, 55	0
13	CM	136/136 (100%)	-0.01	1 (0%) 84 90	8, 21, 38, 56	0
13	EM	136/136 (100%)	-0.19	2 (1%) 70 79	1, 11, 29, 60	0
13	GM	136/136 (100%)	0.29	8 (5%) 22 25	11, 28, 45, 58	0
14	AN	120/127 (94%)	0.20	5 (4%) 35 41	14, 29, 41, 62	0
14	CN	120/127 (94%)	0.08	4 (3%) 44 53	18, 31, 43, 62	0
14	EN	120/127 (94%)	-0.01	2 (1%) 67 76	6, 19, 32, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
14	GN	120/127 (94%)	0.14	3 (2%) 54 64	19, 31, 43, 72	0
15	AO	116/117 (99%)	0.77	16 (13%) 4 5	28, 47, 56, 62	0
15	CO	116/117 (99%)	0.51	15 (12%) 4 6	28, 42, 55, 61	0
15	EO	116/117 (99%)	0.19	8 (6%) 17 20	16, 30, 43, 55	0
15	GO	116/117 (99%)	0.66	17 (14%) 3 5	28, 40, 58, 63	0
16	AP	114/115 (99%)	0.13	3 (2%) 53 63	13, 31, 47, 62	0
16	CP	114/115 (99%)	0.15	5 (4%) 33 40	17, 35, 49, 62	0
16	EP	114/115 (99%)	-0.16	4 (3%) 42 50	6, 24, 43, 66	0
16	GP	114/115 (99%)	0.28	5 (4%) 33 40	14, 35, 50, 59	0
17	AQ	117/118 (99%)	0.07	5 (4%) 34 40	10, 26, 43, 56	0
17	CQ	117/118 (99%)	0.02	3 (2%) 53 63	6, 24, 39, 60	0
17	EQ	117/118 (99%)	-0.18	1 (0%) 81 88	2, 9, 25, 46	0
17	GQ	117/118 (99%)	0.16	4 (3%) 43 51	19, 29, 42, 56	0
18	AR	103/103 (100%)	0.26	5 (4%) 28 34	10, 37, 52, 60	0
18	CR	103/103 (100%)	0.15	3 (2%) 49 58	9, 34, 49, 63	0
18	ER	103/103 (100%)	-0.17	2 (1%) 64 72	2, 21, 41, 52	0
18	GR	103/103 (100%)	0.61	8 (7%) 13 16	13, 40, 53, 63	0
19	AS	110/110 (100%)	0.29	5 (4%) 32 39	13, 28, 45, 62	0
19	CS	110/110 (100%)	0.21	4 (3%) 41 48	7, 27, 45, 65	0
19	ES	110/110 (100%)	-0.03	2 (1%) 65 74	2, 12, 36, 49	0
19	GS	110/110 (100%)	0.65	16 (14%) 3 5	12, 31, 50, 69	0
20	AT	93/100 (93%)	0.82	15 (16%) 2 3	18, 37, 58, 63	0
20	CT	93/100 (93%)	0.57	13 (13%) 3 5	14, 37, 57, 67	0
20	ET	93/100 (93%)	0.53	10 (10%) 6 8	6, 24, 53, 61	0
20	GT	93/100 (93%)	0.87	21 (22%) 1 2	19, 36, 57, 62	0
21	AU	102/104 (98%)	0.88	18 (17%) 2 3	24, 40, 56, 64	0
21	CU	102/104 (98%)	1.04	22 (21%) 1 2	24, 41, 61, 73	0
21	EU	102/104 (98%)	0.51	7 (6%) 17 20	13, 28, 51, 65	0
21	GU	102/104 (98%)	1.54	32 (31%) 1 1	32, 46, 63, 75	0
22	AV	94/94 (100%)	-0.03	2 (2%) 60 69	23, 38, 48, 57	0
22	CV	94/94 (100%)	0.02	2 (2%) 60 69	25, 39, 52, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
22	EV	94/94 (100%)	-0.26	0 100 100	9, 22, 40, 45	0
22	GV	94/94 (100%)	0.36	7 (7%) 14 17	29, 42, 55, 60	0
23	AW	79/85 (92%)	0.68	10 (12%) 4 6	17, 35, 52, 61	0
23	CW	79/85 (92%)	0.51	6 (7%) 14 17	15, 29, 51, 65	0
23	EW	79/85 (92%)	0.42	7 (8%) 10 12	5, 17, 44, 50	0
23	GW	79/85 (92%)	0.63	10 (12%) 4 6	15, 33, 55, 63	0
24	AX	77/78 (98%)	0.57	4 (5%) 26 32	16, 31, 47, 57	0
24	CX	77/78 (98%)	0.20	2 (2%) 53 63	8, 22, 46, 49	0
24	EX	77/78 (98%)	0.17	0 100 100	4, 18, 40, 50	0
24	GX	77/78 (98%)	0.19	2 (2%) 53 63	14, 25, 46, 56	0
25	AY	63/63 (100%)	1.06	11 (17%) 2 3	30, 47, 61, 65	0
25	CY	63/63 (100%)	0.85	10 (15%) 3 4	27, 44, 58, 67	0
25	EY	63/63 (100%)	0.87	11 (17%) 2 3	13, 33, 51, 70	0
25	GY	63/63 (100%)	1.26	12 (19%) 2 2	29, 45, 60, 68	0
26	AZ	58/59 (98%)	0.61	3 (5%) 26 32	15, 31, 55, 71	0
26	CZ	58/59 (98%)	0.43	5 (8%) 11 13	17, 30, 53, 65	0
26	EZ	58/59 (98%)	-0.11	1 (1%) 67 76	2, 10, 35, 59	0
26	GZ	58/59 (98%)	0.41	5 (8%) 11 13	20, 32, 51, 53	0
27	A0	56/57 (98%)	0.42	5 (8%) 10 12	11, 33, 54, 62	0
27	C0	56/57 (98%)	0.23	3 (5%) 25 30	8, 35, 50, 60	0
27	E0	56/57 (98%)	0.12	3 (5%) 25 30	3, 25, 48, 56	0
27	G0	56/57 (98%)	0.30	5 (8%) 10 12	15, 35, 58, 67	0
28	A1	50/55 (90%)	1.21	11 (22%) 1 2	27, 38, 51, 61	0
28	C1	50/55 (90%)	1.07	7 (14%) 3 5	21, 35, 48, 59	0
28	E1	50/55 (90%)	0.65	4 (8%) 12 15	11, 26, 44, 47	0
28	G1	50/55 (90%)	1.37	15 (30%) 1 1	25, 38, 55, 61	0
29	A2	46/46 (100%)	0.26	2 (4%) 34 40	9, 22, 34, 55	0
29	C2	46/46 (100%)	0.11	2 (4%) 34 40	7, 14, 30, 54	0
29	E2	46/46 (100%)	-0.16	1 (2%) 59 67	2, 7, 15, 53	0
29	G2	46/46 (100%)	0.21	2 (4%) 34 40	8, 17, 28, 51	0
30	A3	64/65 (98%)	0.09	0 100 100	12, 22, 37, 40	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
30	C3	64/65 (98%)	0.03	1 (1%) 68 78	10, 18, 27, 35	0
30	E3	64/65 (98%)	-0.07	1 (1%) 68 78	2, 8, 14, 27	0
30	G3	64/65 (98%)	0.26	1 (1%) 68 78	13, 22, 37, 48	0
31	A4	38/38 (100%)	0.23	2 (5%) 25 31	13, 22, 36, 38	0
31	C4	38/38 (100%)	0.28	1 (2%) 53 63	14, 27, 39, 46	0
31	E4	38/38 (100%)	0.01	0 100 100	5, 16, 35, 38	0
31	G4	38/38 (100%)	0.61	4 (10%) 7 9	22, 33, 44, 49	0
32	A5	148/165 (89%)	3.24	85 (57%) 0 0	36, 54, 65, 74	0
32	E5	144/165 (87%)	3.61	103 (71%) 0 0	35, 61, 72, 82	0
33	BA	1533/1542 (99%)	-0.07	35 (2%) 57 66	11, 42, 70, 91	0
33	DA	1533/1542 (99%)	-0.09	33 (2%) 59 67	12, 43, 69, 85	0
33	FA	1533/1542 (99%)	-0.14	30 (1%) 62 71	8, 33, 61, 85	0
33	HA	1533/1542 (99%)	0.01	60 (3%) 37 45	15, 41, 72, 90	0
34	BB	218/241 (90%)	1.52	75 (34%) 1 1	41, 58, 69, 79	0
34	DB	218/241 (90%)	1.71	84 (38%) 1 0	40, 57, 69, 79	0
34	FB	218/241 (90%)	0.77	33 (15%) 3 4	26, 49, 63, 69	0
34	HB	218/241 (90%)	1.15	49 (22%) 1 2	33, 51, 67, 73	0
35	BC	206/233 (88%)	0.73	33 (16%) 3 3	30, 50, 60, 69	0
35	DC	206/233 (88%)	0.48	22 (10%) 6 8	35, 50, 60, 67	0
35	FC	206/233 (88%)	-0.02	4 (1%) 64 72	13, 30, 46, 58	0
35	HC	206/233 (88%)	0.35	13 (6%) 19 23	21, 40, 56, 66	0
36	BD	205/206 (99%)	0.51	24 (11%) 5 7	23, 39, 57, 64	0
36	DD	205/206 (99%)	1.00	38 (18%) 2 3	26, 47, 60, 65	0
36	FD	205/206 (99%)	0.83	36 (17%) 2 3	27, 44, 60, 73	0
36	HD	205/206 (99%)	0.79	28 (13%) 4 5	25, 47, 61, 79	0
37	BE	150/167 (89%)	0.33	14 (9%) 9 11	17, 48, 63, 76	0
37	DE	150/167 (89%)	0.23	8 (5%) 25 31	25, 45, 62, 71	0
37	FE	150/167 (89%)	-0.03	3 (2%) 62 71	18, 34, 50, 65	0
37	HE	150/167 (89%)	0.08	5 (3%) 44 53	21, 37, 54, 67	0
38	BF	100/135 (74%)	1.64	36 (36%) 1 1	50, 62, 70, 74	0
38	DF	100/135 (74%)	0.65	17 (17%) 2 3	32, 49, 62, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
38	FF	100/135 (74%)	0.86	20 (20%) 2 2	32, 51, 63, 66	0
38	HF	100/135 (74%)	0.76	11 (11%) 6 8	31, 51, 64, 71	0
39	BG	151/179 (84%)	0.52	17 (11%) 6 7	28, 49, 60, 66	0
39	DG	151/179 (84%)	0.50	14 (9%) 9 11	32, 46, 58, 63	0
39	FG	151/179 (84%)	0.41	13 (8%) 11 13	23, 39, 55, 63	0
39	HG	151/179 (84%)	0.97	28 (18%) 2 3	32, 48, 62, 68	0
40	BH	129/130 (99%)	0.86	21 (16%) 2 3	40, 51, 62, 70	0
40	DH	129/130 (99%)	0.73	20 (15%) 3 4	28, 47, 59, 73	0
40	FH	129/130 (99%)	0.05	4 (3%) 47 55	20, 32, 47, 66	0
40	HH	129/130 (99%)	0.36	7 (5%) 25 30	23, 35, 51, 69	0
41	BI	127/130 (97%)	1.20	28 (22%) 1 2	24, 52, 65, 70	0
41	DI	127/130 (97%)	1.03	24 (18%) 2 2	31, 52, 64, 74	0
41	FI	127/130 (97%)	0.54	12 (9%) 9 11	14, 43, 60, 69	0
41	HI	127/130 (97%)	1.57	41 (32%) 1 1	29, 55, 70, 75	0
42	BJ	98/103 (95%)	2.23	46 (46%) 1 0	30, 55, 68, 72	0
42	DJ	98/103 (95%)	1.97	41 (41%) 1 0	35, 57, 70, 74	0
42	FJ	98/103 (95%)	0.70	16 (16%) 2 3	14, 32, 59, 65	0
42	HJ	98/103 (95%)	1.54	28 (28%) 1 1	30, 51, 69, 78	0
43	BK	117/129 (90%)	1.54	31 (26%) 1 1	33, 56, 66, 80	0
43	DK	117/129 (90%)	0.36	12 (10%) 7 9	26, 41, 56, 60	0
43	FK	117/129 (90%)	0.50	13 (11%) 6 8	18, 42, 59, 64	0
43	HK	117/129 (90%)	1.62	37 (31%) 1 1	23, 50, 70, 74	0
44	BL	123/124 (99%)	-0.04	4 (3%) 44 53	15, 24, 43, 74	0
44	DL	123/124 (99%)	0.13	7 (5%) 23 28	20, 34, 48, 61	0
44	FL	123/124 (99%)	0.07	7 (5%) 23 28	9, 28, 44, 67	0
44	HL	123/124 (99%)	0.35	11 (8%) 10 12	21, 37, 55, 63	0
45	BM	114/118 (96%)	0.74	18 (15%) 3 4	28, 49, 64, 74	0
45	DM	114/118 (96%)	0.54	12 (10%) 7 9	36, 50, 63, 67	0
45	FM	114/118 (96%)	0.66	16 (14%) 3 5	19, 45, 63, 68	0
45	HM	114/118 (96%)	2.72	64 (56%) 0 0	42, 63, 72, 75	0
46	BN	96/101 (95%)	0.75	15 (15%) 3 4	32, 46, 60, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
46	DN	96/101 (95%)	0.77	17 (17%) 2 3	30, 49, 62, 65	0
46	FN	96/101 (95%)	0.08	3 (3%) 47 55	11, 24, 53, 60	0
46	HN	96/101 (95%)	0.74	19 (19%) 2 2	27, 47, 64, 70	0
47	BO	88/89 (98%)	0.76	12 (13%) 4 5	35, 50, 61, 64	0
47	DO	88/89 (98%)	0.52	9 (10%) 7 9	31, 45, 56, 61	0
47	FO	88/89 (98%)	0.35	2 (2%) 57 66	23, 37, 49, 56	0
47	HO	88/89 (98%)	0.36	7 (7%) 12 15	22, 39, 53, 70	0
48	BP	82/82 (100%)	0.93	12 (14%) 3 5	24, 35, 61, 68	0
48	DP	82/82 (100%)	1.44	24 (29%) 1 1	28, 43, 62, 79	0
48	FP	82/82 (100%)	0.38	6 (7%) 15 18	21, 34, 62, 77	0
48	HP	82/82 (100%)	0.93	12 (14%) 3 5	22, 39, 62, 71	0
49	BQ	80/84 (95%)	0.93	11 (13%) 4 5	30, 45, 55, 63	0
49	DQ	80/84 (95%)	0.83	11 (13%) 4 5	29, 44, 57, 68	0
49	FQ	80/84 (95%)	0.39	3 (3%) 38 45	22, 38, 54, 63	0
49	HQ	80/84 (95%)	0.59	9 (11%) 6 7	27, 41, 51, 57	0
50	BR	55/75 (73%)	1.97	22 (40%) 1 0	46, 55, 66, 69	0
50	DR	55/75 (73%)	0.93	10 (18%) 2 3	35, 44, 60, 66	0
50	FR	55/75 (73%)	0.59	6 (10%) 6 8	35, 44, 53, 61	0
50	HR	55/75 (73%)	0.64	6 (10%) 6 8	26, 40, 55, 64	0
51	BS	79/92 (85%)	0.42	7 (8%) 10 12	30, 44, 59, 64	0
51	DS	79/92 (85%)	0.78	12 (15%) 3 4	36, 49, 63, 67	0
51	FS	79/92 (85%)	-0.01	5 (6%) 19 23	22, 32, 52, 63	0
51	HS	79/92 (85%)	2.97	51 (64%) 0 0	43, 58, 70, 74	0
52	BT	85/87 (97%)	0.74	7 (8%) 12 15	25, 40, 50, 59	0
52	DT	85/87 (97%)	0.82	10 (11%) 5 7	30, 40, 55, 73	0
52	FT	85/87 (97%)	0.45	8 (9%) 9 11	24, 36, 50, 63	0
52	HT	85/87 (97%)	0.94	10 (11%) 5 7	23, 38, 53, 56	0
53	BU	51/71 (71%)	3.93	34 (66%) 0 0	53, 62, 71, 82	0
53	DU	51/71 (71%)	1.87	21 (41%) 1 0	40, 54, 69, 74	0
53	FU	51/71 (71%)	1.84	21 (41%) 1 0	40, 53, 65, 69	0
53	HU	51/71 (71%)	2.62	23 (45%) 1 0	40, 57, 67, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
54	BV	689/704 (97%)	0.48	75 (10%) 6 8	18, 46, 66, 76	0
54	DV	689/704 (97%)	0.66	104 (15%) 3 4	27, 50, 68, 77	0
54	FV	689/704 (97%)	2.89	376 (54%) 0 0	33, 66, 76, 82	0
54	HV	689/704 (97%)	1.14	155 (22%) 1 2	32, 56, 70, 80	0
55	BW	2/6 (33%)	2.82	1 (50%) 0 0	41, 41, 41, 43	2 (100%)
55	DW	2/6 (33%)	2.98	1 (50%) 0 0	40, 40, 40, 44	2 (100%)
55	FW	2/6 (33%)	2.87	1 (50%) 0 0	41, 41, 41, 42	2 (100%)
All	All	43562/44972 (96%)	0.39	4249 (9%) 8 10	1, 37, 66, 92	6 (0%)

The worst 5 of 4249 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	GI	8	VAL	21.6
26	AZ	1	ALA	20.6
48	DP	81	ALA	19.9
32	A5	112	ALA	19.2
43	BK	19	GLY	18.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
55	KBE	BW	1	9/10	0.62	6.14	37,39,42,44	9
55	DPP	FW	2	6/7	0.98	5.69	37,42,43,43	6
55	KBE	FW	1	9/10	0.56	4.99	28,36,40,42	9
55	KBE	DW	1	9/10	0.37	4.62	32,33,40,41	9
55	5OH	FW	6	12/13	0.72	3.85	37,42,45,46	12
55	UAL	FW	5	9/10	0.62	2.81	35,37,39,41	9
55	UAL	BW	5	9/10	0.60	2.14	32,40,42,42	9
55	DPP	BW	2	6/7	0.51	1.91	34,36,39,40	6
55	5OH	BW	6	12/13	0.48	1.51	36,37,41,43	12
55	5OH	DW	6	12/13	0.46	1.32	33,41,43,48	12
55	DPP	DW	2	6/7	0.43	1.28	32,34,37,44	6

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	UAL	DW	5	9/10	0.43	0.92	35,39,42,46	9

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	EA	3011	1/1	0.85	62.54	17,17,17,17	0
56	MG	EA	3055	1/1	0.44	57.91	14,14,14,14	0
56	MG	DA	1629	1/1	0.43	54.82	54,54,54,54	0
56	MG	EA	3087	1/1	0.67	46.81	30,30,30,30	0
56	MG	CA	3114	1/1	0.53	41.68	25,25,25,25	0
56	MG	AA	3055	1/1	0.17	39.00	18,18,18,18	0
56	MG	HA	1613	1/1	0.65	37.83	41,41,41,41	0
56	MG	AA	3059	1/1	0.57	36.88	12,12,12,12	0
56	MG	FA	1636	1/1	0.58	36.80	38,38,38,38	0
56	MG	CA	3118	1/1	0.30	35.50	29,29,29,29	0
56	MG	GA	3059	1/1	0.49	32.45	44,44,44,44	0
56	MG	CA	3011	1/1	0.37	30.08	23,23,23,23	0
56	MG	AA	3060	1/1	0.43	28.55	25,25,25,25	0
56	MG	GA	3073	1/1	0.49	27.75	20,20,20,20	0
56	MG	AC	303	1/1	0.97	26.36	34,34,34,34	0
56	MG	CA	3097	1/1	0.75	24.78	22,22,22,22	0
56	MG	GA	3094	1/1	0.48	23.59	22,22,22,22	0
56	MG	EQ	201	1/1	0.60	22.24	31,31,31,31	0
56	MG	DA	1602	1/1	0.40	21.28	31,31,31,31	0
56	MG	EA	3015	1/1	0.49	20.06	1,1,1,1	0
56	MG	EA	3042	1/1	0.19	19.42	2,2,2,2	0
56	MG	BA	1606	1/1	0.43	18.84	39,39,39,39	0
56	MG	AA	3123	1/1	0.17	17.71	14,14,14,14	0
56	MG	GA	3037	1/1	0.21	17.44	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	GA	3133	1/1	0.21	16.26	4,4,4,4	0
56	MG	HA	1611	1/1	0.23	15.83	20,20,20,20	0
56	MG	FE	201	1/1	0.71	14.91	52,52,52,52	0
56	MG	AA	3098	1/1	0.21	14.73	5,5,5,5	0
56	MG	GS	201	1/1	0.48	13.33	33,33,33,33	0
56	MG	EA	3099	1/1	0.29	13.22	2,2,2,2	0
56	MG	FA	1609	1/1	0.33	11.78	16,16,16,16	0
56	MG	EA	3020	1/1	0.25	11.66	4,4,4,4	0
56	MG	GA	3123	1/1	0.22	11.64	11,11,11,11	0
56	MG	GA	3087	1/1	0.19	10.82	19,19,19,19	0
56	MG	EA	3069	1/1	0.44	10.80	4,4,4,4	0
56	MG	FA	1610	1/1	0.18	10.38	35,35,35,35	0
56	MG	DA	1628	1/1	0.35	9.92	37,37,37,37	0
56	MG	EA	3060	1/1	0.30	9.62	3,3,3,3	0
56	MG	BA	1607	1/1	0.26	9.32	8,8,8,8	0
56	MG	HA	1621	1/1	0.32	9.18	29,29,29,29	0
56	MG	CA	3051	1/1	0.28	9.07	7,7,7,7	0
56	MG	BA	1635	1/1	0.22	9.03	29,29,29,29	0
56	MG	FA	1624	1/1	0.19	8.94	18,18,18,18	0
56	MG	HA	1610	1/1	0.27	8.86	13,13,13,13	0
56	MG	DA	1636	1/1	0.24	8.82	41,41,41,41	0
56	MG	GA	3100	1/1	0.20	8.73	19,19,19,19	0
56	MG	GA	3068	1/1	0.22	8.52	15,15,15,15	0
56	MG	BA	1614	1/1	0.33	8.18	26,26,26,26	0
56	MG	AA	3117	1/1	0.25	8.09	7,7,7,7	0
56	MG	FA	1639	1/1	0.26	7.93	25,25,25,25	0
56	MG	AA	3102	1/1	0.24	7.79	0,0,0,0	0
56	MG	EA	3120	1/1	0.22	7.71	0,0,0,0	0
56	MG	GA	3118	1/1	0.27	7.70	9,9,9,9	0
56	MG	AA	3028	1/1	0.26	7.68	2,2,2,2	0
56	MG	AA	3109	1/1	0.23	7.61	6,6,6,6	0
56	MG	GA	3102	1/1	0.30	7.40	40,40,40,40	0
56	MG	GA	3060	1/1	0.38	7.38	23,23,23,23	0
56	MG	EA	3067	1/1	0.25	7.27	4,4,4,4	0
56	MG	CA	3085	1/1	0.25	7.16	28,28,28,28	0
56	MG	AC	301	1/1	0.42	7.07	10,10,10,10	0
56	MG	DA	1640	1/1	0.19	7.01	21,21,21,21	0
56	MG	FA	1612	1/1	0.28	7.00	17,17,17,17	0
56	MG	GA	3063	1/1	0.26	6.99	3,3,3,3	0
56	MG	AA	3005	1/1	0.18	6.95	23,23,23,23	0
56	MG	EA	3123	1/1	0.30	6.81	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3091	1/1	0.21	6.76	40,40,40,40	0
56	MG	GA	3070	1/1	0.20	6.71	13,13,13,13	0
56	MG	EA	3121	1/1	0.23	6.66	1,1,1,1	0
56	MG	GA	3103	1/1	0.24	6.52	12,12,12,12	0
56	MG	HA	1604	1/1	0.19	6.40	27,27,27,27	0
56	MG	FA	1623	1/1	0.21	6.25	7,7,7,7	0
56	MG	BA	1612	1/1	0.22	6.22	5,5,5,5	0
56	MG	HA	1612	1/1	0.18	6.18	8,8,8,8	0
56	MG	GA	3067	1/1	0.20	6.15	16,16,16,16	0
56	MG	GA	3044	1/1	0.21	6.13	23,23,23,23	0
56	MG	GA	3115	1/1	0.23	6.05	23,23,23,23	0
56	MG	GA	3081	1/1	0.20	5.99	16,16,16,16	0
56	MG	FA	1628	1/1	0.20	5.99	19,19,19,19	0
56	MG	HT	101	1/1	0.46	5.96	41,41,41,41	0
56	MG	HA	1626	1/1	0.30	5.93	32,32,32,32	0
56	MG	GA	3034	1/1	0.19	5.89	16,16,16,16	0
56	MG	CA	3073	1/1	0.25	5.83	5,5,5,5	0
56	MG	AA	3083	1/1	0.27	5.79	33,33,33,33	0
56	MG	GB	1202	1/1	0.16	5.70	36,36,36,36	0
56	MG	CA	3040	1/1	0.20	5.57	12,12,12,12	0
56	MG	EA	3049	1/1	0.23	5.53	8,8,8,8	0
56	MG	CA	3079	1/1	0.23	5.53	12,12,12,12	0
56	MG	EA	3073	1/1	0.19	5.48	0,0,0,0	0
56	MG	GA	3039	1/1	0.18	5.40	15,15,15,15	0
56	MG	GA	3040	1/1	0.23	5.27	16,16,16,16	0
56	MG	GA	3080	1/1	0.22	5.26	5,5,5,5	0
56	MG	HA	1625	1/1	0.28	5.23	22,22,22,22	0
56	MG	CA	3096	1/1	0.22	5.13	10,10,10,10	0
56	MG	GA	3084	1/1	0.27	5.13	25,25,25,25	0
56	MG	AA	3018	1/1	0.19	5.09	12,12,12,12	0
56	MG	FA	1621	1/1	0.19	5.03	10,10,10,10	0
56	MG	HA	1601	1/1	0.15	5.01	38,38,38,38	0
56	MG	GA	3131	1/1	0.20	4.93	41,41,41,41	0
56	MG	AA	3010	1/1	0.23	4.88	13,13,13,13	0
56	MG	AA	3009	1/1	0.23	4.85	12,12,12,12	0
56	MG	BA	1637	1/1	0.27	4.84	29,29,29,29	0
56	MG	CA	3005	1/1	0.20	4.84	31,31,31,31	0
56	MG	CA	3121	1/1	0.22	4.84	3,3,3,3	0
56	MG	GA	3014	1/1	0.27	4.78	8,8,8,8	0
56	MG	FA	1627	1/1	0.31	4.71	23,23,23,23	0
56	MG	ED	301	1/1	0.29	4.59	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3062	1/1	0.18	4.58	2,2,2,2	0
56	MG	BA	1638	1/1	0.16	4.54	31,31,31,31	0
56	MG	EA	3088	1/1	0.15	4.46	6,6,6,6	0
56	MG	DA	1612	1/1	0.19	4.43	11,11,11,11	0
56	MG	AA	3107	1/1	0.19	4.41	18,18,18,18	0
56	MG	EA	3132	1/1	0.22	4.38	6,6,6,6	0
56	MG	DA	1621	1/1	0.20	4.36	22,22,22,22	0
56	MG	FA	1605	1/1	0.16	4.33	36,36,36,36	0
56	MG	EA	3061	1/1	0.22	4.29	0,0,0,0	0
56	MG	CA	3010	1/1	0.24	4.28	10,10,10,10	0
56	MG	EA	3050	1/1	0.23	4.27	13,13,13,13	0
56	MG	EA	3027	1/1	0.19	4.17	0,0,0,0	0
56	MG	HA	1632	1/1	0.22	4.16	25,25,25,25	0
56	MG	AA	3115	1/1	0.17	4.09	32,32,32,32	0
56	MG	GA	3005	1/1	0.17	4.07	15,15,15,15	0
56	MG	EA	3078	1/1	0.18	3.94	3,3,3,3	0
56	MG	AA	3091	1/1	0.15	3.89	16,16,16,16	0
56	MG	EA	3108	1/1	0.15	3.88	31,31,31,31	0
56	MG	EA	3009	1/1	0.18	3.84	0,0,0,0	0
56	MG	FA	1611	1/1	0.24	3.84	0,0,0,0	0
56	MG	AA	3041	1/1	0.17	3.81	2,2,2,2	0
56	MG	GA	3033	1/1	0.21	3.78	12,12,12,12	0
56	MG	BA	1625	1/1	0.22	3.77	21,21,21,21	0
56	MG	EA	3025	1/1	0.21	3.75	0,0,0,0	0
56	MG	GA	3120	1/1	0.20	3.74	5,5,5,5	0
56	MG	FA	1608	1/1	0.19	3.72	14,14,14,14	0
56	MG	GA	3030	1/1	0.25	3.70	11,11,11,11	0
56	MG	CA	3119	1/1	0.19	3.60	3,3,3,3	0
56	MG	EA	3126	1/1	0.16	3.57	2,2,2,2	0
56	MG	EA	3031	1/1	0.23	3.57	2,2,2,2	0
56	MG	EA	3052	1/1	0.20	3.47	2,2,2,2	0
56	MG	EA	3064	1/1	0.18	3.44	0,0,0,0	0
56	MG	GA	3091	1/1	0.14	3.43	11,11,11,11	0
56	MG	GA	3009	1/1	0.20	3.39	20,20,20,20	0
56	MG	EA	3122	1/1	0.18	3.39	0,0,0,0	0
56	MG	HA	1602	1/1	0.28	3.35	48,48,48,48	0
56	MG	EA	3114	1/1	0.18	3.33	1,1,1,1	0
56	MG	GA	3029	1/1	0.18	3.27	5,5,5,5	0
56	MG	BA	1615	1/1	0.19	3.20	22,22,22,22	0
56	MG	GA	3083	1/1	0.24	3.16	33,33,33,33	0
56	MG	GA	3020	1/1	0.19	3.10	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3078	1/1	0.24	3.10	29,29,29,29	0
56	MG	GA	3110	1/1	0.19	3.07	12,12,12,12	0
56	MG	GA	3088	1/1	0.17	3.03	8,8,8,8	0
56	MG	EA	3079	1/1	0.21	3.02	0,0,0,0	0
56	MG	EA	3129	1/1	0.22	3.00	0,0,0,0	0
56	MG	CE	301	1/1	0.23	2.95	16,16,16,16	0
56	MG	HA	1603	1/1	0.27	2.94	38,38,38,38	0
56	MG	GA	3072	1/1	0.16	2.94	13,13,13,13	0
56	MG	GA	3051	1/1	0.17	2.88	4,4,4,4	0
56	MG	GA	3106	1/1	0.22	2.85	3,3,3,3	0
56	MG	CA	3028	1/1	0.20	2.84	7,7,7,7	0
56	MG	CA	3123	1/1	0.17	2.81	8,8,8,8	0
56	MG	EA	3118	1/1	0.19	2.80	1,1,1,1	0
56	MG	GA	3042	1/1	0.16	2.79	24,24,24,24	0
56	MG	GA	3047	1/1	0.19	2.73	27,27,27,27	0
56	MG	FA	1640	1/1	0.18	2.69	23,23,23,23	0
56	MG	BA	1619	1/1	0.19	2.69	28,28,28,28	0
56	MG	DA	1631	1/1	0.16	2.68	25,25,25,25	0
56	MG	CA	3030	1/1	0.22	2.67	11,11,11,11	0
56	MG	BA	1622	1/1	0.20	2.63	32,32,32,32	0
56	MG	AA	3042	1/1	0.17	2.62	11,11,11,11	0
56	MG	EA	3085	1/1	0.19	2.62	4,4,4,4	0
56	MG	GA	3108	1/1	0.14	2.61	16,16,16,16	0
56	MG	GA	3048	1/1	0.18	2.59	6,6,6,6	0
56	MG	GA	3004	1/1	0.37	2.59	19,19,19,19	0
56	MG	BA	1618	1/1	0.15	2.57	3,3,3,3	0
56	MG	CA	3107	1/1	0.19	2.52	6,6,6,6	0
56	MG	GA	3010	1/1	0.26	2.50	15,15,15,15	0
56	MG	GA	3129	1/1	0.18	2.49	19,19,19,19	0
56	MG	GA	3061	1/1	0.18	2.47	10,10,10,10	0
56	MG	EA	3034	1/1	0.21	2.47	0,0,0,0	0
56	MG	HA	1639	1/1	0.18	2.39	20,20,20,20	0
56	MG	EA	3131	1/1	0.19	2.38	5,5,5,5	0
56	MG	BV	802	1/1	0.19	2.36	27,27,27,27	0
56	MG	GA	3078	1/1	0.21	2.32	40,40,40,40	0
56	MG	GA	3052	1/1	0.17	2.31	8,8,8,8	0
56	MG	AA	3007	1/1	0.19	2.29	44,44,44,44	0
56	MG	AA	3093	1/1	0.21	2.28	34,34,34,34	0
56	MG	GA	3114	1/1	0.16	2.28	10,10,10,10	0
56	MG	HA	1630	1/1	0.16	2.22	40,40,40,40	0
56	MG	AA	3084	1/1	0.20	2.20	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	HA	1607	1/1	0.18	2.20	11,11,11,11	0
56	MG	EA	3107	1/1	0.20	2.18	0,0,0,0	0
56	MG	CA	3037	1/1	0.19	2.18	1,1,1,1	0
56	MG	CA	3039	1/1	0.21	2.17	6,6,6,6	0
56	MG	DA	1616	1/1	0.25	2.14	26,26,26,26	0
56	MG	CA	3077	1/1	0.21	2.13	35,35,35,35	0
56	MG	GA	3111	1/1	0.17	2.12	11,11,11,11	0
56	MG	EA	3102	1/1	0.21	2.12	0,0,0,0	0
56	MG	AA	3033	1/1	0.17	2.12	8,8,8,8	0
56	MG	EA	3053	1/1	0.18	2.08	1,1,1,1	0
56	MG	HA	1615	1/1	0.27	2.08	38,38,38,38	0
56	MG	GA	3045	1/1	0.17	2.06	7,7,7,7	0
56	MG	FA	1615	1/1	0.16	2.05	16,16,16,16	0
56	MG	CA	3016	1/1	0.17	2.03	8,8,8,8	0
56	MG	AA	3035	1/1	0.18	2.01	3,3,3,3	0
56	MG	CA	3066	1/1	0.17	2.00	2,2,2,2	0
56	MG	CA	3024	1/1	0.18	1.98	2,2,2,2	0
56	MG	CB	1201	1/1	0.13	1.87	41,41,41,41	0
56	MG	GA	3095	1/1	0.17	1.86	2,2,2,2	0
56	MG	AA	3036	1/1	0.24	1.85	25,25,25,25	0
56	MG	AA	3037	1/1	0.18	1.84	9,9,9,9	0
56	MG	CA	3086	1/1	0.19	1.83	20,20,20,20	0
56	MG	GA	3066	1/1	0.16	1.83	4,4,4,4	0
56	MG	CA	3049	1/1	0.17	1.82	9,9,9,9	0
56	MG	DA	1615	1/1	0.15	1.81	24,24,24,24	0
56	MG	CA	3111	1/1	0.16	1.76	13,13,13,13	0
56	MG	EA	3039	1/1	0.19	1.75	0,0,0,0	0
56	MG	AB	1202	1/1	0.23	1.74	44,44,44,44	0
56	MG	CA	3092	1/1	0.15	1.72	30,30,30,30	0
56	MG	EA	3002	1/1	0.17	1.72	4,4,4,4	0
56	MG	BA	1609	1/1	0.11	1.61	38,38,38,38	0
56	MG	CA	3003	1/1	0.14	1.59	12,12,12,12	0
56	MG	HA	1614	1/1	0.12	1.54	37,37,37,37	0
56	MG	HA	1633	1/1	0.15	1.54	52,52,52,52	0
56	MG	CA	3060	1/1	0.19	1.53	13,13,13,13	0
56	MG	AA	3019	1/1	0.16	1.52	33,33,33,33	0
56	MG	AA	3017	1/1	0.18	1.50	1,1,1,1	0
56	MG	AC	302	1/1	0.23	1.49	19,19,19,19	0
56	MG	AA	3068	1/1	0.20	1.46	59,59,59,59	0
56	MG	AA	3116	1/1	0.18	1.44	3,3,3,3	0
56	MG	EA	3040	1/1	0.17	1.44	1,1,1,1	0
56	MG	BA	1616	1/1	0.21	1.43	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	EA	3091	1/1	0.13	1.41	11,11,11,11	0
56	MG	AA	3110	1/1	0.21	1.40	4,4,4,4	0
56	MG	AA	3125	1/1	0.16	1.39	23,23,23,23	0
56	MG	GL	201	1/1	0.24	1.39	7,7,7,7	0
56	MG	CA	3100	1/1	0.18	1.35	1,1,1,1	0
56	MG	CA	3103	1/1	0.17	1.35	0,0,0,0	0
56	MG	AA	3066	1/1	0.17	1.34	6,6,6,6	0
56	MG	GA	3104	1/1	0.19	1.31	6,6,6,6	0
56	MG	CA	3046	1/1	0.17	1.31	17,17,17,17	0
56	MG	FA	1620	1/1	0.16	1.30	6,6,6,6	0
56	MG	EA	3014	1/1	0.18	1.29	0,0,0,0	0
56	MG	EA	3103	1/1	0.20	1.28	10,10,10,10	0
56	MG	CA	3017	1/1	0.17	1.28	2,2,2,2	0
56	MG	EA	3130	1/1	0.23	1.24	29,29,29,29	0
56	MG	CA	3098	1/1	0.19	1.23	10,10,10,10	0
56	MG	GA	3082	1/1	0.14	1.22	35,35,35,35	0
56	MG	GB	1203	1/1	0.13	1.19	16,16,16,16	0
56	MG	GA	3098	1/1	0.14	1.19	25,25,25,25	0
56	MG	GA	3023	1/1	0.17	1.15	7,7,7,7	0
56	MG	AA	3124	1/1	0.16	1.15	9,9,9,9	0
56	MG	AA	3120	1/1	0.19	1.14	6,6,6,6	0
56	MG	CA	3106	1/1	0.17	1.13	13,13,13,13	0
56	MG	GA	3013	1/1	0.20	1.12	1,1,1,1	0
56	MG	AA	3106	1/1	0.18	1.12	9,9,9,9	0
56	MG	CA	3038	1/1	0.19	1.12	7,7,7,7	0
56	MG	CA	3034	1/1	0.19	1.11	18,18,18,18	0
56	MG	CA	3075	1/1	0.20	1.11	20,20,20,20	0
56	MG	EA	3003	1/1	0.13	1.10	6,6,6,6	0
56	MG	CA	3023	1/1	0.18	1.09	5,5,5,5	0
56	MG	GA	3105	1/1	0.16	1.08	3,3,3,3	0
56	MG	HA	1606	1/1	0.15	1.06	17,17,17,17	0
56	MG	EA	3024	1/1	0.18	1.03	0,0,0,0	0
56	MG	GA	3024	1/1	0.17	1.02	8,8,8,8	0
56	MG	DA	1637	1/1	0.13	1.01	23,23,23,23	0
56	MG	CA	3084	1/1	0.20	1.01	4,4,4,4	0
56	MG	GA	3001	1/1	0.16	1.00	32,32,32,32	0
56	MG	AA	3105	1/1	0.18	0.99	12,12,12,12	0
56	MG	CA	3090	1/1	0.14	0.99	20,20,20,20	0
56	MG	CA	3072	1/1	0.15	0.98	11,11,11,11	0
56	MG	EA	3074	1/1	0.17	0.95	4,4,4,4	0
56	MG	AA	3046	1/1	0.16	0.94	7,7,7,7	0
56	MG	CA	3033	1/1	0.17	0.94	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	GA	3027	1/1	0.16	0.93	6,6,6,6	0
56	MG	EA	3113	1/1	0.17	0.90	0,0,0,0	0
56	MG	AA	3108	1/1	0.15	0.90	21,21,21,21	0
56	MG	GA	3122	1/1	0.18	0.89	14,14,14,14	0
56	MG	EA	3111	1/1	0.20	0.89	2,2,2,2	0
56	MG	CA	3020	1/1	0.16	0.89	19,19,19,19	0
56	MG	GA	3002	1/1	0.15	0.86	14,14,14,14	0
56	MG	AA	3023	1/1	0.17	0.83	3,3,3,3	0
56	MG	CA	3105	1/1	0.17	0.81	6,6,6,6	0
56	MG	EA	3017	1/1	0.16	0.78	3,3,3,3	0
56	MG	ED	302	1/1	0.17	0.78	2,2,2,2	0
56	MG	EA	3109	1/1	0.16	0.78	8,8,8,8	0
56	MG	AA	3056	1/1	0.17	0.74	24,24,24,24	0
56	MG	AA	3025	1/1	0.17	0.73	8,8,8,8	0
56	MG	EA	3119	1/1	0.21	0.70	0,0,0,0	0
56	MG	EA	3008	1/1	0.18	0.69	1,1,1,1	0
56	MG	EA	3104	1/1	0.17	0.67	1,1,1,1	0
56	MG	AA	3073	1/1	0.16	0.67	8,8,8,8	0
56	MG	GA	3085	1/1	0.15	0.66	16,16,16,16	0
56	MG	AA	3103	1/1	0.16	0.65	10,10,10,10	0
56	MG	GA	3008	1/1	0.20	0.62	12,12,12,12	0
56	MG	BA	1626	1/1	0.15	0.58	36,36,36,36	0
56	MG	AT	201	1/1	0.19	0.57	36,36,36,36	0
56	MG	EA	3046	1/1	0.16	0.57	9,9,9,9	0
56	MG	AA	3049	1/1	0.16	0.55	3,3,3,3	0
56	MG	EA	3057	1/1	0.14	0.54	15,15,15,15	0
56	MG	CA	3115	1/1	0.14	0.50	12,12,12,12	0
56	MG	CA	3008	1/1	0.17	0.50	15,15,15,15	0
56	MG	GA	3018	1/1	0.28	0.50	36,36,36,36	0
56	MG	EA	3128	1/1	0.16	0.49	4,4,4,4	0
56	MG	GA	3050	1/1	0.14	0.48	9,9,9,9	0
56	MG	EA	3080	1/1	0.18	0.48	3,3,3,3	0
56	MG	EB	1203	1/1	0.13	0.47	3,3,3,3	0
56	MG	CA	3122	1/1	0.17	0.46	7,7,7,7	0
56	MG	HA	1609	1/1	0.11	0.46	29,29,29,29	0
56	MG	EA	3018	1/1	0.15	0.45	8,8,8,8	0
56	MG	AA	3044	1/1	0.14	0.43	17,17,17,17	0
56	MG	AA	3024	1/1	0.17	0.43	20,20,20,20	0
56	MG	FA	1632	1/1	0.13	0.43	28,28,28,28	0
56	MG	EA	3092	1/1	0.14	0.43	7,7,7,7	0
56	MG	HA	1627	1/1	0.13	0.42	24,24,24,24	0
56	MG	CA	3068	1/1	0.14	0.42	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	EA	3028	1/1	0.17	0.42	1,1,1,1	0
56	MG	GA	3065	1/1	0.14	0.42	3,3,3,3	0
56	MG	HA	1608	1/1	0.16	0.41	14,14,14,14	0
56	MG	CA	3089	1/1	0.14	0.41	2,2,2,2	0
56	MG	GA	3049	1/1	0.16	0.41	8,8,8,8	0
56	MG	CA	3009	1/1	0.14	0.39	18,18,18,18	0
56	MG	CA	3054	1/1	0.16	0.38	6,6,6,6	0
56	MG	EA	3051	1/1	0.15	0.37	0,0,0,0	0
56	MG	EA	3081	1/1	0.15	0.37	3,3,3,3	0
56	MG	DA	1609	1/1	0.16	0.37	16,16,16,16	0
56	MG	EA	3068	1/1	0.15	0.35	35,35,35,35	0
56	MG	CD	301	1/1	0.18	0.34	3,3,3,3	0
56	MG	FA	1626	1/1	0.15	0.33	15,15,15,15	0
56	MG	DA	1632	1/1	0.16	0.32	28,28,28,28	0
56	MG	CA	3093	1/1	0.13	0.31	25,25,25,25	0
56	MG	DA	1605	1/1	0.14	0.28	28,28,28,28	0
56	MG	CA	3002	1/1	0.13	0.23	17,17,17,17	0
56	MG	GA	3025	1/1	0.14	0.21	18,18,18,18	0
56	MG	CA	3044	1/1	0.15	0.21	22,22,22,22	0
56	MG	GA	3022	1/1	0.17	0.19	16,16,16,16	0
56	MG	AA	3130	1/1	0.16	0.15	27,27,27,27	0
56	MG	EA	3012	1/1	0.17	0.15	1,1,1,1	0
56	MG	EA	3112	1/1	0.14	0.13	5,5,5,5	0
56	MG	FA	1641	1/1	0.15	0.12	18,18,18,18	0
56	MG	AA	3081	1/1	0.13	0.10	16,16,16,16	0
56	MG	GA	3076	1/1	0.15	0.09	23,23,23,23	0
56	MG	EA	3077	1/1	0.12	0.08	14,14,14,14	0
56	MG	DA	1601	1/1	0.13	0.06	37,37,37,37	0
56	MG	AA	3012	1/1	0.19	0.06	7,7,7,7	0
56	MG	EA	3106	1/1	0.16	0.05	0,0,0,0	0
56	MG	HA	1635	1/1	0.14	0.03	17,17,17,17	0
56	MG	AA	3011	1/1	0.18	0.03	18,18,18,18	0
56	MG	EA	3066	1/1	0.17	0.02	0,0,0,0	0
56	MG	BA	1601	1/1	0.13	0.02	33,33,33,33	0
56	MG	BA	1636	1/1	0.14	0.02	40,40,40,40	0
56	MG	AA	3065	1/1	0.15	0.01	2,2,2,2	0
56	MG	CA	3125	1/1	0.14	0.01	9,9,9,9	0
56	MG	AA	3072	1/1	0.16	0.01	7,7,7,7	0
56	MG	AA	3043	1/1	0.14	0.00	21,21,21,21	0
56	MG	CA	3041	1/1	0.13	-0.01	13,13,13,13	0
56	MG	DA	1634	1/1	0.13	-0.04	33,33,33,33	0
56	MG	AA	3058	1/1	0.18	-0.04	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3119	1/1	0.15	-0.04	13,13,13,13	0
56	MG	GA	3124	1/1	0.12	-0.06	16,16,16,16	0
56	MG	AA	3039	1/1	0.17	-0.06	5,5,5,5	0
56	MG	EA	3023	1/1	0.16	-0.07	2,2,2,2	0
56	MG	AA	3101	1/1	0.16	-0.07	7,7,7,7	0
56	MG	AD	301	1/1	0.15	-0.08	6,6,6,6	0
56	MG	EA	3062	1/1	0.17	-0.08	0,0,0,0	0
56	MG	CA	3112	1/1	0.14	-0.09	4,4,4,4	0
56	MG	AA	3045	1/1	0.14	-0.09	18,18,18,18	0
56	MG	DU	101	1/1	0.39	-0.10	36,36,36,36	0
56	MG	HA	1628	1/1	0.14	-0.11	30,30,30,30	0
56	MG	AA	3069	1/1	0.14	-0.11	6,6,6,6	0
58	GCP	DV	801	32/32	0.14	-0.12	20,38,49,52	0
56	MG	GA	3026	1/1	0.14	-0.13	6,6,6,6	0
56	MG	CA	3032	1/1	0.16	-0.16	3,3,3,3	0
56	MG	DA	1608	1/1	0.14	-0.18	14,14,14,14	0
56	MG	BA	1617	1/1	0.14	-0.18	25,25,25,25	0
56	MG	EA	3096	1/1	0.15	-0.18	15,15,15,15	0
56	MG	CA	3129	1/1	0.15	-0.20	9,9,9,9	0
56	MG	CA	3109	1/1	0.12	-0.21	26,26,26,26	0
56	MG	HA	1623	1/1	0.12	-0.21	18,18,18,18	0
56	MG	AA	3074	1/1	0.17	-0.24	9,9,9,9	0
56	MG	CA	3063	1/1	0.15	-0.25	2,2,2,2	0
56	MG	GA	3071	1/1	0.15	-0.26	20,20,20,20	0
56	MG	EA	3098	1/1	0.15	-0.28	6,6,6,6	0
56	MG	GA	3003	1/1	0.12	-0.28	15,15,15,15	0
58	GCP	BV	801	32/32	0.13	-0.29	17,36,43,49	0
56	MG	EA	3095	1/1	0.16	-0.30	5,5,5,5	0
56	MG	EA	3029	1/1	0.17	-0.30	0,0,0,0	0
56	MG	EA	3072	1/1	0.14	-0.31	8,8,8,8	0
56	MG	HA	1619	1/1	0.15	-0.33	34,34,34,34	0
56	MG	CA	3134	1/1	0.16	-0.33	23,23,23,23	0
56	MG	BA	1621	1/1	0.25	-0.33	52,52,52,52	0
56	MG	HA	1605	1/1	0.12	-0.34	39,39,39,39	0
56	MG	AA	3032	1/1	0.15	-0.34	14,14,14,14	0
56	MG	EB	1201	1/1	0.12	-0.35	26,26,26,26	0
56	MG	GC	301	1/1	0.15	-0.35	4,4,4,4	0
56	MG	DA	1624	1/1	0.16	-0.36	48,48,48,48	0
56	MG	AA	3013	1/1	0.15	-0.38	5,5,5,5	0
56	MG	DV	802	1/1	0.12	-0.38	34,34,34,34	0
56	MG	GA	3012	1/1	0.17	-0.39	2,2,2,2	0
58	GCP	FV	801	32/32	0.19	-0.40	43,58,69,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3078	1/1	0.11	-0.41	25,25,25,25	0
56	MG	AA	3030	1/1	0.16	-0.43	13,13,13,13	0
56	MG	AA	3031	1/1	0.15	-0.44	8,8,8,8	0
56	MG	EA	3036	1/1	0.14	-0.45	1,1,1,1	0
56	MG	DA	1639	1/1	0.11	-0.46	40,40,40,40	0
56	MG	AA	3080	1/1	0.17	-0.47	7,7,7,7	0
56	MG	AA	3014	1/1	0.16	-0.48	4,4,4,4	0
56	MG	AA	3047	1/1	0.12	-0.48	30,30,30,30	0
56	MG	GA	3096	1/1	0.15	-0.48	4,4,4,4	0
56	MG	CA	3130	1/1	0.15	-0.51	1,1,1,1	0
56	MG	HV	802	1/1	0.15	-0.53	38,38,38,38	0
56	MG	AB	1203	1/1	0.11	-0.53	14,14,14,14	0
56	MG	DA	1619	1/1	0.12	-0.53	33,33,33,33	0
56	MG	CA	3124	1/1	0.15	-0.54	0,0,0,0	0
56	MG	BU	101	1/1	0.27	-0.55	39,39,39,39	0
56	MG	GA	3016	1/1	0.14	-0.55	9,9,9,9	0
56	MG	BA	1629	1/1	0.15	-0.55	41,41,41,41	0
56	MG	AA	3015	1/1	0.16	-0.56	22,22,22,22	0
56	MG	FA	1601	1/1	0.13	-0.57	28,28,28,28	0
56	MG	CA	3132	1/1	0.15	-0.57	2,2,2,2	0
56	MG	EA	3022	1/1	0.14	-0.62	0,0,0,0	0
56	MG	DA	1642	1/1	0.17	-0.62	29,29,29,29	0
56	MG	BA	1630	1/1	0.11	-0.67	25,25,25,25	0
56	MG	HE	201	1/1	0.24	-0.67	39,39,39,39	0
56	MG	GA	3038	1/1	0.14	-0.70	11,11,11,11	0
56	MG	HA	1638	1/1	0.12	-0.72	26,26,26,26	0
56	MG	GA	3121	1/1	0.15	-0.72	4,4,4,4	0
56	MG	CA	3050	1/1	0.12	-0.73	12,12,12,12	0
56	MG	AA	3096	1/1	0.15	-0.73	33,33,33,33	0
56	MG	HA	1617	1/1	0.18	-0.75	62,62,62,62	0
56	MG	CA	3047	1/1	0.12	-0.75	31,31,31,31	0
56	MG	CA	3070	1/1	0.12	-0.75	4,4,4,4	0
56	MG	AB	1201	1/1	0.10	-0.76	38,38,38,38	0
56	MG	GA	3006	1/1	0.12	-0.77	25,25,25,25	0
56	MG	EB	1202	1/1	0.11	-0.77	19,19,19,19	0
56	MG	CA	3018	1/1	0.10	-0.78	26,26,26,26	0
56	MG	AA	3070	1/1	0.15	-0.78	11,11,11,11	0
56	MG	EC	301	1/1	0.14	-0.78	1,1,1,1	0
56	MG	BA	1640	1/1	0.13	-0.79	33,33,33,33	0
56	MG	CB	1203	1/1	0.11	-0.79	6,6,6,6	0
56	MG	CA	3128	1/1	0.15	-0.80	6,6,6,6	0
56	MG	EA	3006	1/1	0.12	-0.87	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3069	1/1	0.09	-0.87	45,45,45,45	0
56	MG	GA	3054	1/1	0.13	-0.88	1,1,1,1	0
56	MG	GA	3119	1/1	0.14	-0.90	5,5,5,5	0
56	MG	EA	3105	1/1	0.14	-0.91	4,4,4,4	0
56	MG	FA	1629	1/1	0.13	-0.94	16,16,16,16	0
56	MG	AA	3067	1/1	0.08	-0.96	29,29,29,29	0
56	MG	CA	3059	1/1	0.16	-0.96	3,3,3,3	0
57	ZN	C4	102	1/1	0.08	-0.96	76,76,76,76	0
56	MG	EA	3097	1/1	0.16	-0.97	2,2,2,2	0
56	MG	FV	802	1/1	0.13	-1.00	48,48,48,48	0
56	MG	HA	1629	1/1	0.12	-1.01	17,17,17,17	0
56	MG	CA	3035	1/1	0.14	-1.04	3,3,3,3	0
56	MG	EA	3047	1/1	0.10	-1.04	6,6,6,6	0
56	MG	GA	3036	1/1	0.12	-1.04	35,35,35,35	0
56	MG	HA	1637	1/1	0.10	-1.04	47,47,47,47	0
57	ZN	A4	101	1/1	0.08	-1.04	63,63,63,63	0
56	MG	AA	3127	1/1	0.12	-1.05	16,16,16,16	0
56	MG	BA	1604	1/1	0.12	-1.05	20,20,20,20	0
56	MG	EA	3100	1/1	0.14	-1.05	0,0,0,0	0
56	MG	AA	3008	1/1	0.12	-1.07	15,15,15,15	0
56	MG	FA	1631	1/1	0.07	-1.07	21,21,21,21	0
56	MG	DA	1622	1/1	0.08	-1.08	37,37,37,37	0
56	MG	FA	1635	1/1	0.12	-1.09	8,8,8,8	0
56	MG	GA	3074	1/1	0.14	-1.09	2,2,2,2	0
56	MG	CA	3099	1/1	0.12	-1.11	17,17,17,17	0
56	MG	CB	1202	1/1	0.10	-1.14	55,55,55,55	0
56	MG	BA	1634	1/1	0.12	-1.14	14,14,14,14	0
58	GCP	HV	801	32/32	0.12	-1.14	24,48,54,56	0
56	MG	EA	3048	1/1	0.12	-1.15	11,11,11,11	0
56	MG	DA	1617	1/1	0.14	-1.16	45,45,45,45	0
56	MG	FU	101	1/1	0.14	-1.16	24,24,24,24	0
56	MG	GA	3077	1/1	0.12	-1.17	33,33,33,33	0
56	MG	AA	3071	1/1	0.12	-1.17	3,3,3,3	0
56	MG	EA	3033	1/1	0.16	-1.17	1,1,1,1	0
56	MG	AA	3097	1/1	0.16	-1.20	8,8,8,8	0
56	MG	CA	3113	1/1	0.11	-1.20	14,14,14,14	0
56	MG	CA	3045	1/1	0.13	-1.21	21,21,21,21	0
56	MG	EA	3070	1/1	0.14	-1.21	3,3,3,3	0
56	MG	EA	3035	1/1	0.14	-1.22	0,0,0,0	0
56	MG	CA	3083	1/1	0.11	-1.22	22,22,22,22	0
56	MG	EA	3044	1/1	0.13	-1.23	11,11,11,11	0
56	MG	FA	1633	1/1	0.11	-1.23	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	GA	3099	1/1	0.14	-1.25	12,12,12,12	0
56	MG	CA	3120	1/1	0.14	-1.30	3,3,3,3	0
56	MG	GA	3089	1/1	0.10	-1.31	14,14,14,14	0
56	MG	BA	1623	1/1	0.10	-1.31	24,24,24,24	0
56	MG	HA	1616	1/1	0.14	-1.34	33,33,33,33	0
56	MG	AE	301	1/1	0.12	-1.36	11,11,11,11	0
56	MG	GA	3107	1/1	0.13	-1.39	27,27,27,27	0
56	MG	GA	3053	1/1	0.13	-1.40	4,4,4,4	0
56	MG	GA	3116	1/1	0.13	-1.40	3,3,3,3	0
56	MG	AA	3087	1/1	0.13	-1.41	31,31,31,31	0
57	ZN	G4	101	1/1	0.09	-1.43	69,69,69,69	0
56	MG	GA	3069	1/1	0.12	-1.43	63,63,63,63	0
56	MG	BA	1602	1/1	0.12	-1.44	15,15,15,15	0
56	MG	BA	1603	1/1	0.08	-1.45	21,21,21,21	0
56	MG	CA	3027	1/1	0.09	-1.46	2,2,2,2	0
56	MG	AA	3111	1/1	0.15	-1.46	21,21,21,21	0
56	MG	CA	3042	1/1	0.11	-1.46	8,8,8,8	0
56	MG	CA	3116	1/1	0.12	-1.48	13,13,13,13	0
56	MG	AA	3079	1/1	0.15	-1.49	11,11,11,11	0
56	MG	CA	3056	1/1	0.11	-1.49	7,7,7,7	0
56	MG	EA	3115	1/1	0.12	-1.50	2,2,2,2	0
56	MG	EA	3124	1/1	0.11	-1.51	5,5,5,5	0
56	MG	AA	3128	1/1	0.13	-1.52	2,2,2,2	0
56	MG	EA	3071	1/1	0.12	-1.54	2,2,2,2	0
56	MG	FA	1617	1/1	0.13	-1.57	9,9,9,9	0
56	MG	FA	1606	1/1	0.10	-1.58	13,13,13,13	0
56	MG	AA	3061	1/1	0.14	-1.58	6,6,6,6	0
56	MG	AA	3100	1/1	0.10	-1.60	6,6,6,6	0
56	MG	BA	1613	1/1	0.13	-1.63	38,38,38,38	0
56	MG	CA	3021	1/1	0.13	-1.64	10,10,10,10	0
56	MG	AA	3076	1/1	0.10	-1.65	21,21,21,21	0
56	MG	EA	3101	1/1	0.10	-1.66	26,26,26,26	0
56	MG	AA	3051	1/1	0.08	-1.68	4,4,4,4	0
56	MG	EA	3045	1/1	0.14	-1.68	1,1,1,1	0
56	MG	AA	3090	1/1	0.10	-1.68	23,23,23,23	0
56	MG	DA	1606	1/1	0.10	-1.71	26,26,26,26	0
56	MG	EA	3005	1/1	0.11	-1.71	27,27,27,27	0
56	MG	AA	3113	1/1	0.11	-1.71	8,8,8,8	0
56	MG	CA	3001	1/1	0.12	-1.72	10,10,10,10	0
56	MG	EA	3084	1/1	0.16	-1.72	2,2,2,2	0
56	MG	CA	3064	1/1	0.09	-1.73	1,1,1,1	0
56	MG	AA	3088	1/1	0.12	-1.75	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3015	1/1	0.14	-1.76	14,14,14,14	0
56	MG	DA	1641	1/1	0.12	-1.78	30,30,30,30	0
56	MG	BE	201	1/1	0.10	-1.79	43,43,43,43	0
56	MG	CA	3006	1/1	0.08	-1.80	15,15,15,15	0
56	MG	FA	1638	1/1	0.10	-1.82	33,33,33,33	0
56	MG	A3	101	1/1	0.09	-1.82	13,13,13,13	0
56	MG	CA	3108	1/1	0.13	-1.82	3,3,3,3	0
56	MG	FA	1637	1/1	0.11	-1.83	34,34,34,34	0
56	MG	AA	3112	1/1	0.09	-1.83	7,7,7,7	0
56	MG	EA	3116	1/1	0.14	-1.88	0,0,0,0	0
57	ZN	E4	101	1/1	0.09	-1.90	54,54,54,54	0
56	MG	CA	3133	1/1	0.11	-1.91	13,13,13,13	0
56	MG	AA	3001	1/1	0.10	-1.92	11,11,11,11	0
56	MG	AA	3064	1/1	0.13	-1.92	20,20,20,20	0
56	MG	FA	1613	1/1	0.11	-1.98	9,9,9,9	0
56	MG	GA	3132	1/1	0.12	-1.98	7,7,7,7	0
56	MG	AA	3004	1/1	0.10	-1.98	34,34,34,34	0
56	MG	EA	3058	1/1	0.12	-1.98	6,6,6,6	0
56	MG	AA	3126	1/1	0.09	-1.99	3,3,3,3	0
56	MG	BA	1627	1/1	0.07	-2.02	25,25,25,25	0
56	MG	GA	3056	1/1	0.11	-2.04	4,4,4,4	0
56	MG	CA	3080	1/1	0.13	-2.06	8,8,8,8	0
56	MG	CA	3019	1/1	0.08	-2.06	22,22,22,22	0
56	MG	GA	3097	1/1	0.16	-2.07	26,26,26,26	0
56	MG	GA	3075	1/1	0.13	-2.08	7,7,7,7	0
56	MG	CA	3062	1/1	0.13	-2.10	5,5,5,5	0
56	MG	BA	1605	1/1	0.11	-2.11	21,21,21,21	0
56	MG	AA	3027	1/1	0.13	-2.13	8,8,8,8	0
56	MG	AA	3016	1/1	0.11	-2.14	10,10,10,10	0
56	MG	EA	3076	1/1	0.09	-2.15	18,18,18,18	0
56	MG	CA	3131	1/1	0.10	-2.16	0,0,0,0	0
56	MG	AA	3021	1/1	0.09	-2.16	11,11,11,11	0
56	MG	AA	3006	1/1	0.08	-2.17	38,38,38,38	0
56	MG	GA	3130	1/1	0.09	-2.19	9,9,9,9	0
56	MG	GA	3064	1/1	0.11	-2.21	9,9,9,9	0
56	MG	FA	1618	1/1	0.10	-2.21	28,28,28,28	0
56	MG	DA	1604	1/1	0.09	-2.23	23,23,23,23	0
56	MG	EA	3001	1/1	0.11	-2.28	9,9,9,9	0
56	MG	BA	1632	1/1	0.10	-2.29	40,40,40,40	0
56	MG	EA	3059	1/1	0.12	-2.29	1,1,1,1	0
56	MG	FA	1616	1/1	0.15	-2.33	16,16,16,16	0
56	MG	GA	3112	1/1	0.10	-2.34	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3048	1/1	0.13	-2.37	2,2,2,2	0
56	MG	AA	3085	1/1	0.08	-2.39	30,30,30,30	0
56	MG	EA	3037	1/1	0.12	-2.41	2,2,2,2	0
56	MG	CA	3031	1/1	0.13	-2.41	11,11,11,11	0
56	MG	GA	3057	1/1	0.09	-2.42	22,22,22,22	0
56	MG	EA	3010	1/1	0.15	-2.43	11,11,11,11	0
56	MG	GA	3055	1/1	0.11	-2.43	12,12,12,12	0
56	MG	AA	3121	1/1	0.08	-2.44	20,20,20,20	0
56	MG	EA	3016	1/1	0.10	-2.45	6,6,6,6	0
56	MG	BA	1611	1/1	0.12	-2.45	15,15,15,15	0
56	MG	CA	3071	1/1	0.14	-2.46	2,2,2,2	0
56	MG	FA	1602	1/1	0.10	-2.46	23,23,23,23	0
56	MG	BA	1628	1/1	0.13	-2.47	26,26,26,26	0
56	MG	CA	3067	1/1	0.11	-2.49	4,4,4,4	0
56	MG	CA	3004	1/1	0.09	-2.53	6,6,6,6	0
56	MG	GA	3035	1/1	0.11	-2.58	15,15,15,15	0
56	MG	CB	1204	1/1	0.06	-2.60	16,16,16,16	0
56	MG	GA	3062	1/1	0.12	-2.62	18,18,18,18	0
56	MG	HA	1640	1/1	0.10	-2.62	15,15,15,15	0
56	MG	CA	3043	1/1	0.11	-2.62	5,5,5,5	0
56	MG	CA	3058	1/1	0.11	-2.69	5,5,5,5	0
56	MG	AB	1204	1/1	0.07	-2.70	8,8,8,8	0
56	MG	EA	3054	1/1	0.12	-2.72	5,5,5,5	0
56	MG	AA	3020	1/1	0.13	-2.73	24,24,24,24	0
56	MG	CA	3104	1/1	0.14	-2.73	4,4,4,4	0
56	MG	DA	1607	1/1	0.14	-2.75	16,16,16,16	0
56	MG	AA	3022	1/1	0.10	-2.81	8,8,8,8	0
56	MG	DA	1635	1/1	0.07	-2.86	38,38,38,38	0
56	MG	AA	3129	1/1	0.10	-2.91	20,20,20,20	0
56	MG	AA	3104	1/1	0.12	-2.94	12,12,12,12	0
56	MG	FA	1630	1/1	0.09	-2.94	16,16,16,16	0
56	MG	CA	3101	1/1	0.14	-2.96	10,10,10,10	0
56	MG	EA	3021	1/1	0.10	-2.96	5,5,5,5	0
56	MG	CA	3110	1/1	0.10	-2.96	20,20,20,20	0
56	MG	FA	1604	1/1	0.06	-2.97	33,33,33,33	0
56	MG	GA	3079	1/1	0.10	-2.97	18,18,18,18	0
56	MG	AA	3122	1/1	0.12	-3.00	2,2,2,2	0
56	MG	GA	3028	1/1	0.11	-3.07	10,10,10,10	0
56	MG	CA	3014	1/1	0.11	-3.08	9,9,9,9	0
56	MG	GA	3043	1/1	0.10	-3.08	8,8,8,8	0
56	MG	EA	3056	1/1	0.08	-3.09	2,2,2,2	0
56	MG	CA	3102	1/1	0.07	-3.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	EA	3090	1/1	0.07	-3.12	29,29,29,29	0
56	MG	FA	1607	1/1	0.10	-3.15	18,18,18,18	0
56	MG	CA	3082	1/1	0.12	-3.16	15,15,15,15	0
56	MG	C4	101	1/1	0.06	-3.19	22,22,22,22	0
56	MG	BA	1620	1/1	0.05	-3.19	20,20,20,20	0
56	MG	AA	3038	1/1	0.12	-3.19	6,6,6,6	0
56	MG	GA	3021	1/1	0.13	-3.19	9,9,9,9	0
56	MG	GA	3117	1/1	0.07	-3.21	22,22,22,22	0
56	MG	CA	3022	1/1	0.13	-3.27	0,0,0,0	0
56	MG	AA	3034	1/1	0.11	-3.28	14,14,14,14	0
56	MG	GA	3046	1/1	0.08	-3.29	35,35,35,35	0
56	MG	BA	1639	1/1	0.11	-3.32	19,19,19,19	0
56	MG	EA	3065	1/1	0.10	-3.32	0,0,0,0	0
56	MG	EA	3063	1/1	0.13	-3.34	1,1,1,1	0
56	MG	CA	3088	1/1	0.10	-3.41	28,28,28,28	0
56	MG	AA	3086	1/1	0.07	-3.42	35,35,35,35	0
56	MG	EA	3094	1/1	0.10	-3.44	15,15,15,15	0
56	MG	CA	3061	1/1	0.11	-3.45	3,3,3,3	0
56	MG	DA	1603	1/1	0.12	-3.48	22,22,22,22	0
56	MG	EA	3082	1/1	0.07	-3.48	13,13,13,13	0
56	MG	AA	3040	1/1	0.11	-3.49	24,24,24,24	0
56	MG	HA	1631	1/1	0.10	-3.52	28,28,28,28	0
56	MG	DA	1611	1/1	0.10	-3.52	15,15,15,15	0
56	MG	GA	3090	1/1	0.05	-3.54	26,26,26,26	0
56	MG	AA	3099	1/1	0.12	-3.58	15,15,15,15	0
56	MG	DA	1630	1/1	0.11	-3.61	34,34,34,34	0
56	MG	GA	3101	1/1	0.07	-3.63	15,15,15,15	0
56	MG	HA	1622	1/1	0.09	-3.64	36,36,36,36	0
56	MG	EA	3089	1/1	0.09	-3.66	5,5,5,5	0
56	MG	EA	3013	1/1	0.13	-3.69	0,0,0,0	0
56	MG	GA	3032	1/1	0.12	-3.69	8,8,8,8	0
56	MG	AA	3095	1/1	0.09	-3.71	9,9,9,9	0
56	MG	DA	1614	1/1	0.11	-3.74	44,44,44,44	0
56	MG	HA	1634	1/1	0.11	-3.74	24,24,24,24	0
56	MG	CA	3095	1/1	0.10	-3.79	21,21,21,21	0
56	MG	EA	3117	1/1	0.10	-3.83	11,11,11,11	0
56	MG	AA	3003	1/1	0.10	-3.83	26,26,26,26	0
56	MG	AA	3118	1/1	0.10	-3.83	11,11,11,11	0
56	MG	CA	3036	1/1	0.08	-3.90	19,19,19,19	0
56	MG	AA	3063	1/1	0.07	-3.92	9,9,9,9	0
56	MG	DA	1613	1/1	0.09	-3.93	12,12,12,12	0
56	MG	CA	3012	1/1	0.11	-4.04	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3094	1/1	0.07	-4.05	34,34,34,34	0
56	MG	CA	3126	1/1	0.11	-4.08	7,7,7,7	0
56	MG	GA	3128	1/1	0.09	-4.09	20,20,20,20	0
56	MG	EA	3038	1/1	0.10	-4.12	2,2,2,2	0
56	MG	BA	1633	1/1	0.09	-4.13	35,35,35,35	0
56	MG	EA	3086	1/1	0.07	-4.14	34,34,34,34	0
56	MG	AA	3053	1/1	0.10	-4.18	6,6,6,6	0
56	MG	EA	3133	1/1	0.11	-4.24	32,32,32,32	0
56	MG	EA	3004	1/1	0.09	-4.26	13,13,13,13	0
56	MG	EA	3019	1/1	0.07	-4.26	13,13,13,13	0
56	MG	DA	1610	1/1	0.04	-4.26	48,48,48,48	0
56	MG	FA	1614	1/1	0.11	-4.32	5,5,5,5	0
56	MG	HA	1624	1/1	0.09	-4.33	14,14,14,14	0
56	MG	AA	3002	1/1	0.09	-4.37	20,20,20,20	0
56	MG	GB	1201	1/1	0.07	-4.41	38,38,38,38	0
56	MG	EA	3083	1/1	0.12	-4.42	1,1,1,1	0
56	MG	EA	3093	1/1	0.07	-4.46	21,21,21,21	0
56	MG	AA	3092	1/1	0.05	-4.56	31,31,31,31	0
56	MG	GA	3113	1/1	0.09	-4.58	26,26,26,26	0
56	MG	DA	1633	1/1	0.04	-4.60	45,45,45,45	0
56	MG	CA	3055	1/1	0.11	-4.75	20,20,20,20	0
56	MG	DA	1626	1/1	0.06	-4.77	24,24,24,24	0
56	MG	CA	3057	1/1	0.09	-4.84	1,1,1,1	0
56	MG	GA	3109	1/1	0.06	-4.92	9,9,9,9	0
56	MG	AA	3077	1/1	0.07	-4.94	36,36,36,36	0
56	MG	AA	3057	1/1	0.07	-4.97	18,18,18,18	0
56	MG	GA	3031	1/1	0.12	-4.99	4,4,4,4	0
56	MG	AA	3089	1/1	0.08	-5.00	26,26,26,26	0
56	MG	EA	3032	1/1	0.13	-5.08	0,0,0,0	0
56	MG	CA	3081	1/1	0.12	-5.08	10,10,10,10	0
56	MG	GA	3041	1/1	0.08	-5.14	10,10,10,10	0
56	MG	DA	1627	1/1	0.10	-5.17	21,21,21,21	0
56	MG	CA	3065	1/1	0.09	-5.17	1,1,1,1	0
56	MG	GB	1204	1/1	0.08	-5.17	21,21,21,21	0
56	MG	BA	1608	1/1	0.10	-5.20	22,22,22,22	0
56	MG	BA	1610	1/1	0.07	-5.25	19,19,19,19	0
56	MG	FA	1603	1/1	0.12	-5.33	30,30,30,30	0
56	MG	AA	3082	1/1	0.03	-5.36	29,29,29,29	0
56	MG	EA	3026	1/1	0.09	-5.45	28,28,28,28	0
56	MG	CA	3048	1/1	0.09	-5.55	13,13,13,13	0
56	MG	GA	3127	1/1	0.11	-5.58	1,1,1,1	0
56	MG	DA	1638	1/1	0.05	-5.61	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	FA	1619	1/1	0.09	-5.68	25,25,25,25	0
56	MG	DA	1625	1/1	0.09	-5.70	23,23,23,23	0
56	MG	FA	1625	1/1	0.06	-5.72	18,18,18,18	0
56	MG	GA	3007	1/1	0.06	-5.78	28,28,28,28	0
56	MG	GA	3015	1/1	0.07	-5.80	18,18,18,18	0
56	MG	CA	3087	1/1	0.04	-5.87	29,29,29,29	0
56	MG	GA	3134	1/1	0.05	-6.00	16,16,16,16	0
56	MG	GA	3126	1/1	0.09	-6.14	18,18,18,18	0
56	MG	GA	3125	1/1	0.09	-6.28	5,5,5,5	0
56	MG	EB	1204	1/1	0.05	-6.31	12,12,12,12	0
56	MG	BA	1631	1/1	0.06	-6.35	28,28,28,28	0
56	MG	CA	3029	1/1	0.07	-6.36	8,8,8,8	0
56	MG	CA	3127	1/1	0.07	-6.55	11,11,11,11	0
56	MG	AA	3052	1/1	0.11	-6.76	2,2,2,2	0
56	MG	EA	3075	1/1	0.11	-6.88	10,10,10,10	0
56	MG	CA	3025	1/1	0.10	-7.26	7,7,7,7	0
56	MG	AA	3050	1/1	0.07	-7.31	7,7,7,7	0
56	MG	GA	3092	1/1	0.06	-7.32	17,17,17,17	0
56	MG	CA	3026	1/1	0.10	-7.43	5,5,5,5	0
56	MG	GA	3058	1/1	0.11	-7.48	17,17,17,17	0
56	MG	FA	1622	1/1	0.07	-7.51	15,15,15,15	0
56	MG	EA	3041	1/1	0.09	-7.54	2,2,2,2	0
56	MG	DA	1623	1/1	0.05	-7.60	12,12,12,12	0
56	MG	HA	1636	1/1	0.04	-7.80	21,21,21,21	0
56	MG	EA	3007	1/1	0.06	-7.83	15,15,15,15	0
56	MG	FA	1634	1/1	0.06	-8.06	19,19,19,19	0
56	MG	GA	3011	1/1	0.09	-8.19	46,46,46,46	0
56	MG	DA	1620	1/1	0.06	-8.41	22,22,22,22	0
56	MG	CA	3076	1/1	0.08	-8.70	25,25,25,25	0
56	MG	EA	3125	1/1	0.09	-8.75	3,3,3,3	0
56	MG	AA	3114	1/1	0.07	-8.82	1,1,1,1	0
56	MG	AA	3054	1/1	0.12	-9.15	11,11,11,11	0
56	MG	CA	3117	1/1	0.06	-9.17	7,7,7,7	0
56	MG	AA	3026	1/1	0.07	-9.30	10,10,10,10	0
56	MG	EA	3110	1/1	0.10	-10.11	24,24,24,24	0
56	MG	EA	3127	1/1	0.14	-10.25	0,0,0,0	0
56	MG	CA	3053	1/1	0.11	-10.92	5,5,5,5	0
56	MG	GA	3017	1/1	0.09	-10.96	24,24,24,24	0
56	MG	GA	3086	1/1	0.03	-11.00	26,26,26,26	0
56	MG	EA	3043	1/1	0.10	-11.40	4,4,4,4	0
56	MG	DA	1618	1/1	0.08	-11.72	33,33,33,33	0
56	MG	AA	3075	1/1	0.08	-12.38	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	GA	3019	1/1	0.10	-14.50	5,5,5,5	0
56	MG	CA	3013	1/1	0.08	-15.53	7,7,7,7	0
56	MG	AA	3029	1/1	0.09	-16.00	21,21,21,21	0
56	MG	CA	3052	1/1	0.08	-19.11	10,10,10,10	0
56	MG	CA	3074	1/1	0.05	-20.41	19,19,19,19	0
56	MG	AA	3094	1/1	0.06	-22.94	20,20,20,20	0
56	MG	HA	1618	1/1	0.07	-39.55	19,19,19,19	0
56	MG	BA	1624	1/1	0.10	-45.00	28,28,28,28	0
56	MG	CA	3007	1/1	0.08	-51.44	15,15,15,15	0
56	MG	EA	3030	1/1	0.15	-	0,0,0,0	0
56	MG	HC	401	1/1	0.45	-	49,49,49,49	0
56	MG	GA	3093	1/1	0.46	-	28,28,28,28	0
56	MG	BL	201	1/1	0.27	-	51,51,51,51	0
56	MG	HA	1620	1/1	0.08	-	14,14,14,14	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.