



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:05 PM BST

PDB ID : 4V5Y  
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with paromomycin and ribosome recycling factor (RRF).  
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.  
Deposited on : 2007-06-19  
Resolution : 4.45 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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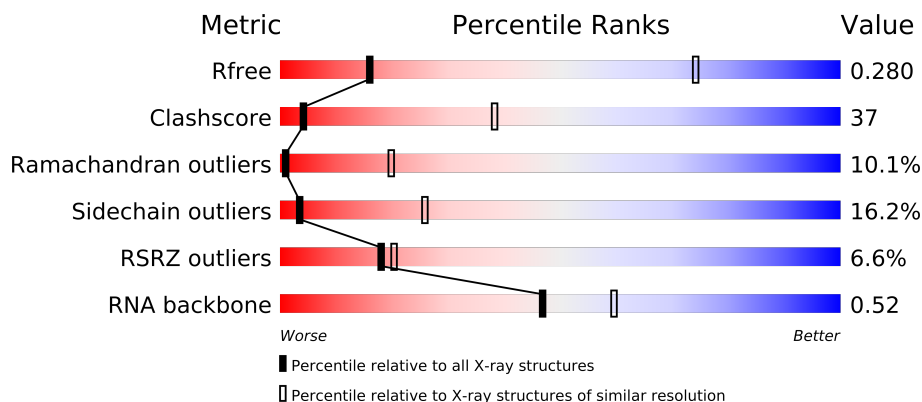
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.45 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	1020 (5.30-3.50)
Clashscore	79885	1285 (5.30-3.50)
Ramachandran outliers	78287	1214 (5.26-3.50)
Sidechain outliers	78261	1195 (5.26-3.50)
RSRZ outliers	66119	1020 (5.30-3.50)
RNA backbone	1838	1030 (6.00-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	1542	
1	CA	1542	
2	AC	232	
2	CC	232	
3	AD	205	
3	CD	205	
4	AE	166	
4	CE	166	
5	AF	135	
5	CF	135	
6	AG	178	
6	CG	178	

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Mol	Chain	Length	Quality of chain
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AN	100	
13	CN	100	
14	AO	89	
14	CO	89	
15	AP	82	
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	70	
21	CU	70	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	
27	DK	123	

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Mol	Chain	Length	Quality of chain
28	BP	114	
28	DP	114	
29	BE	201	
29	DE	201	
30	BY	58	
30	DY	58	
31	B0	56	
31	D0	56	
32	B4	38	
32	D4	38	
33	B1	54	
33	D1	54	
34	B3	64	
34	D3	64	
35	BV	94	
35	DV	94	
36	B2	46	
36	D2	46	
37	BL	144	
37	DL	144	
38	BM	136	
38	DM	136	
39	BX	63	
39	DX	63	
40	BH	149	
40	DH	149	
41	BJ	142	
41	DJ	142	
42	BN	127	
42	DN	127	
43	BO	117	
43	DO	117	
44	BQ	117	
44	DQ	117	
45	BS	110	
45	DS	110	
46	BU	103	
46	DU	103	
47	BF	178	
47	DF	178	
48	BG	176	
48	DG	176	

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Mol	Chain	Length	Quality of chain
49	BR	103	
49	DR	103	
50	BT	100	
50	DT	100	
51	BZ	78	
51	DZ	78	
52	BW	84	
52	DW	84	
53	B6	185	
53	D6	185	

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

Mol	Type	Chain	Res	Geometry	Electron density
54	MG	AA	1608	-	X
54	MG	AA	1614	-	X
54	MG	AA	1617	-	X
54	MG	AA	1619	-	X
54	MG	AA	1621	-	X
54	MG	AA	1622	-	X
54	MG	AA	1623	-	X
54	MG	AA	1624	-	X
54	MG	AA	1625	-	X
54	MG	AA	1626	-	X
54	MG	AA	1627	-	X
54	MG	AA	1632	-	X
54	MG	AA	1633	-	X
54	MG	AA	1637	-	X
54	MG	AA	1639	-	X
54	MG	AA	1647	-	X
54	MG	AA	1651	-	X
54	MG	AA	1652	-	X
54	MG	AA	1656	-	X
54	MG	AA	1657	-	X
54	MG	AA	1658	-	X
54	MG	AA	1659	-	X
54	MG	BB	3017	-	X
54	MG	BB	3018	-	X
54	MG	BB	3020	-	X
54	MG	BB	3028	-	X
54	MG	BB	3033	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
54	MG	BB	3036	-	X
54	MG	BB	3047	-	X
54	MG	BB	3051	-	X
54	MG	BB	3055	-	X
54	MG	BB	3057	-	X
54	MG	BB	3059	-	X
54	MG	BB	3064	-	X
54	MG	BB	3078	-	X
54	MG	BB	3080	-	X
54	MG	BB	3093	-	X
54	MG	BB	3097	-	X
54	MG	BB	3100	-	X
54	MG	BB	3108	-	X
54	MG	CA	1608	-	X
54	MG	CA	1615	-	X
54	MG	CA	1620	-	X
54	MG	CA	1621	-	X
54	MG	CA	1623	-	X
54	MG	CA	1625	-	X
54	MG	CA	1626	-	X
54	MG	CA	1627	-	X
54	MG	CA	1628	-	X
54	MG	CA	1641	-	X
54	MG	CA	1646	-	X
54	MG	CA	1657	-	X
54	MG	CA	1658	-	X
54	MG	CE	201	-	X
54	MG	DB	3028	-	X
54	MG	DB	3030	-	X
54	MG	DB	3036	-	X
54	MG	DB	3052	-	X
54	MG	DB	3058	-	X
54	MG	DB	3065	-	X
54	MG	DB	3068	-	X
54	MG	DB	3083	-	X
54	MG	DB	3086	-	X
54	MG	DB	3101	-	X
54	MG	DB	3108	-	X
54	MG	DB	3111	-	X
55	PAR	BB	3111	-	X
55	PAR	DB	3112	-	X

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 287128 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
1	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
2	CC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
4	CE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	4			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
12	CM	113	Total	C	N	O	S	0	0	0
			876	541	177	155	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
15	CP	80	Total	C	N	O	S	0	0	0
			638	400	126	111	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
16	CQ	81	Total	C	N	O	S	0	0	0
			657	417	122	115	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			
17	CR	55	Total	C	N	O	0	0	0
			455	288	86	81			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
18	CS	80	Total	C	N	O	S	0	0	0
			644	413	121	108	2			

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

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

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
20	CB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

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

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

- Molecule 22 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
22	DA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
23	DB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 24 is a protein called 50S ribosomal protein L11.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			
27	DK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 28 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
30	DY	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L25.

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

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
39	DX	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 40 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
40	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 41 is a protein called 50S ribosomal protein L13.

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

- Molecule 42 is a protein called 50S ribosomal protein L17.

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

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			
47	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 48 is a protein called 50S ribosomal protein L6.

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

- Molecule 49 is a protein called 50S ribosomal protein L21.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
51	DZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 52 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
52	DW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

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

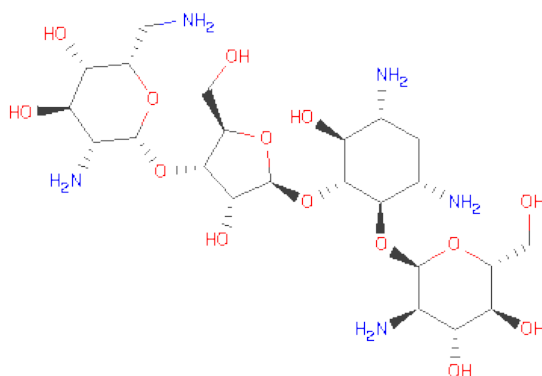


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			
53	D6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	DB	111	Total	Mg	0	0
			111	111		
54	BB	110	Total	Mg	0	0
			110	110		
54	AA	60	Total	Mg	0	0
			60	60		
54	CA	61	Total	Mg	0	0
			61	61		
54	CE	1	Total	Mg	0	0
			1	1		

- Molecule 55 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	AA	1	Total	C	N	O	0	0
			42	23	5	14		
55	BB	1	Total	C	N	O	0	0
			42	23	5	14		
55	CA	1	Total	C	N	O	0	0
			42	23	5	14		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	DB	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	291	Total	O	0	0
			291	291		
57	AL	3	Total	O	0	0
			3	3		
57	AN	4	Total	O	0	0
			4	4		
57	AT	2	Total	O	0	0
			2	2		
57	BB	495	Total	O	0	0
			495	495		
57	BC	6	Total	O	0	0
			6	6		
57	BD	1	Total	O	0	0
			1	1		
57	BE	2	Total	O	0	0
			2	2		
57	BL	1	Total	O	0	0
			1	1		
57	BT	1	Total	O	0	0
			1	1		
57	CA	296	Total	O	0	0
			296	296		
57	CE	3	Total	O	0	0
			3	3		
57	CL	4	Total	O	0	0
			4	4		
57	CN	4	Total	O	0	0
			4	4		

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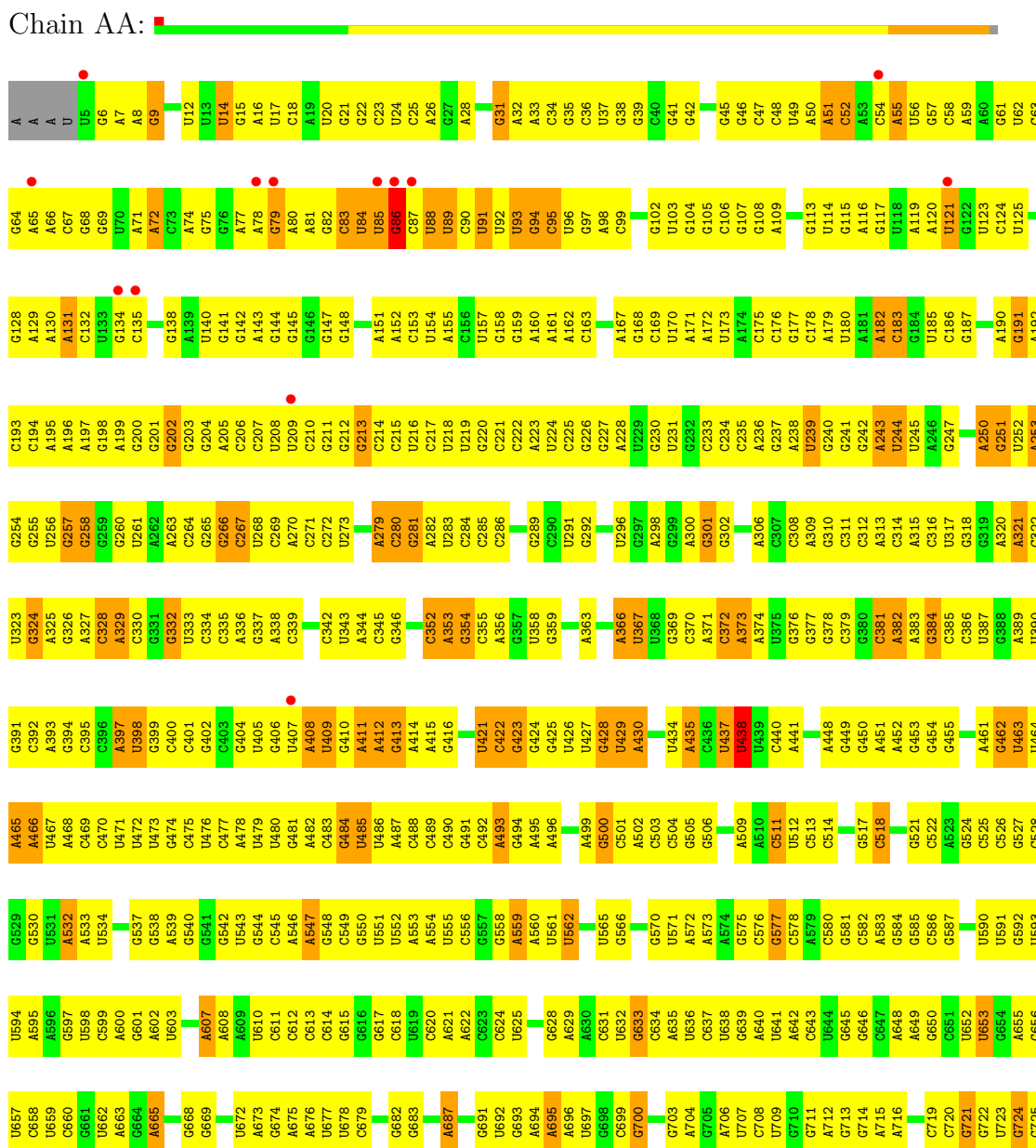
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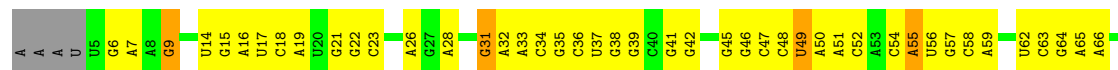
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CP	1	Total 1	O 1	0	0
57	CT	1	Total 1	O 1	0	0
57	DB	502	Total 502	O 502	0	0
57	DC	4	Total 4	O 4	0	0
57	DD	1	Total 1	O 1	0	0
57	DE	1	Total 1	O 1	0	0
57	DL	2	Total 2	O 2	0	0
57	DQ	1	Total 1	O 1	0	0
57	DR	1	Total 1	O 1	0	0

### 3 Residue-property plots

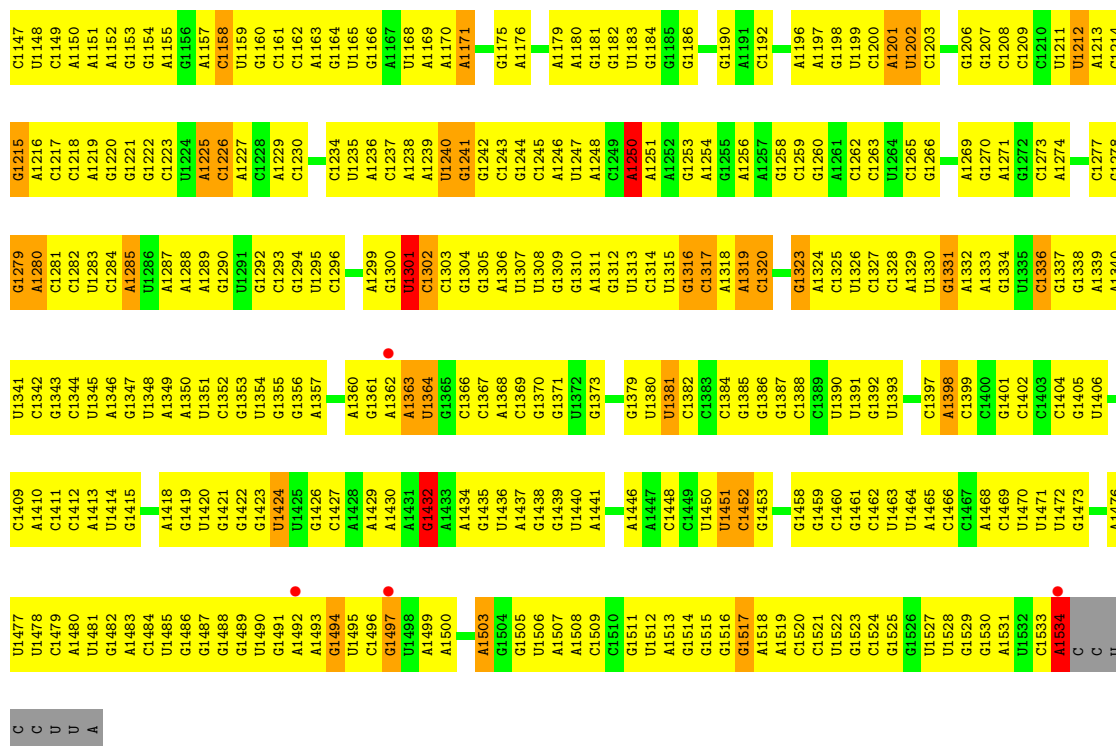
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: 16S rRNA



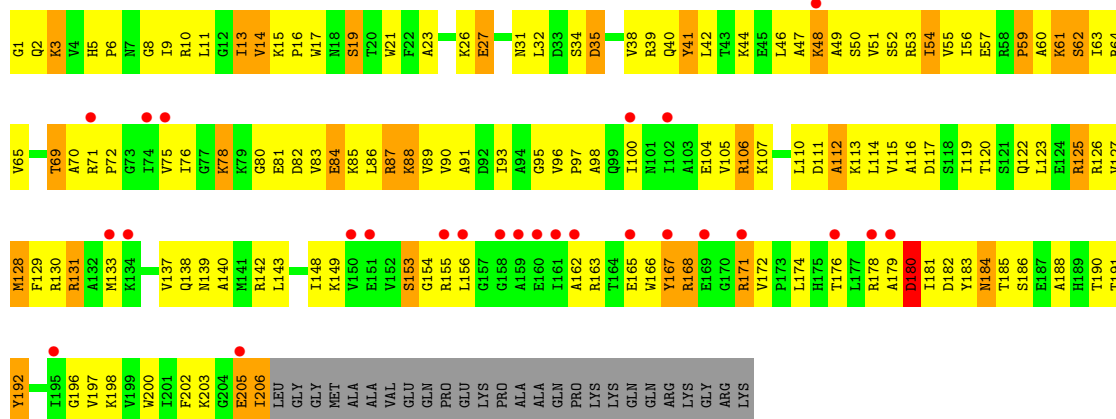


A1080	A1081	A1019	U952	G877	A807	G741	A663	A800	U534	U471	A397	G331	G265	A205	A139	G69
U1082	G1020	G1020	G953	A878	C808	G742	G664	G601	A535	U472	U398	G332	G266	C206	U140	U70
U1083	A1021	C880	U954	C879	G809	A743	A665	U603	C536	U473	G399	U333	G267	C207	G141	A71
G1084	A1022	G881	U956	G881	C811	A746	U672	A607	G538	C475	C400	C334	U268	U208	G142	A72
U1085	U1023	G882	U957	C882	G812	A747	A673	A608	A539	C476	C401	C335	C269	C209	G143	C73
U1086	G1024	C883	A958	C883	G813	G748	A674	A609	G540	C477	C402	C336	A270	C210	G144	A74
G1087	U1025	U884	A959	U884	G814	G748	A675	A610	G541	A478	G404	A338	C271	G211	G145	
	G1026	G886	U960	G886	A815	G749	A676	C611	G542	U479	U405	C339	C272	G212	G146	A80
	C1027	A816	U961	G887	A817	C750	A677	C612	G544	U480	G406		U273	G213	G147	A81
	C1028	C817			C818	A753	C679	C613	C545	A482	U407			G214	G148	
	G966	G818	G966	G838	A819	C754	A687	G614	A546	A483	U409			C215	A151	U84
	C967	U820	A968	C899	U821	G755		G615	A547	G484	G410			C216	A152	U85
	A969	A900	A969	A900	G821	C756		G616	G548	U485	A411			C217	A153	G86
	C1096	G1032	C970	A901	U822	G761	G691	G617	C549	U486	A412			U218	C153	G87
	C1097	G1033	G971	G902	U823	U762	U692	C618	G550	A487	A413			U219	U154	U88
	C1098	G1034	G972	G903	A825	G763	G693	U619	G551	C488	A414			C221	C156	U89
	G1099	A1035	G973	U904	C826	G764	A694	C620	U552	A489	A415			C222	G157	U91
	C1100	A1036	U974	U905	U827	C765	A695	A821	A553	C490	G416			A223	G158	U92
	A1101	C1037	A975	A906	U828	A766	A696	A822	A554	G491				U224	G159	U93
	A1102	C1038	A976	A907	G829	A767	U697	C623	U555	C492	C422			U225	A160	U94
	C1103	G1039	A977	A908		A768	U698	C624	U556	A493	C423			G226	A161	C95
	G1104	U1040	A978	A909	G832	G769	C699	U625	G557	G494	G424			U227	A162	C96
	A1105	A1041	C979	C910	G833	A770	G700		G558	A495	G425			A228	U96	U97
	G1106	G1043	C980	U911	U834	C770			A559	A496				U229	G97	
			U981	C912	U835	G771	G703	G828	A560		U426			G230	A167	A98
			U982	A913	A704	U772	A704	A829	U561	A499	U427			U231	G168	C99
			A983	A914	G705	U773	G706	G830	U562	G500	G428			G232	C169	
			G984	A915	A706	G775	G707	U632		C501	U429			C233	U170	G102
			U985	U916	U707	A776	G708	G833	G566	A502	A430			C234	A171	U103
			U986	G917	C708	A777		C834		C503				C235	A172	G104
			G987	A918	U709	G778	U709	A635	G570	C504	U434			A236	U173	G105
				U919	G844	G779	G710	U636	U571	G505	C436			G237	C106	C106
				U920	A845	A780	G711	U637	A572	G506	U437			U238	G107	G108
				U921	G847	A781	G712	U638	A573		U438			G240	G177	A109
				G922	C848	A782	G713	G639	A574	A509	U439			G241	C178	
				A923	G849	C783	G714	A640	G575	A510	U440			G242	A179	G113
				C924		A784	A715	U641	C576	C511	A441			A243	U180	U114
				G925		G785	A716	A642	G577	U512				U244	G181	G115
				G926		G786		C643	C578	C513				U245	A182	A116
				G927		G787		U644	C579	C514				A246	C183	G117
						U788		G645	C580	G515	A448			G247	U118	
						U789		G646	G581	G516	G449			C248	A119	
						A789		C647	G581	G517	A451			U249	A120	
						G791		A648	G584	C518	A452			A250	A190	U121
						A792		A649	G585		G453			G251	G191	G122
						U793		G650	C586	G521	C454			U252	A192	U123
						A794		C651	G587	G522	G455			A253	C193	G124
						C795		U652		A523				G254	C194	U125
						C796		U653	U590	G524	A461			G255	A195	
						C797		U654	U591	C525	G462			U256	A196	G128
						U798		A655	U592	C526	U463			G257	A197	A129
								G656	U593	G527	U464			G258	G198	A130
								U657	U594	G528	A465			G259	A199	A131
						U801		G658	A595	G529	A466			G260	G200	C132
						A802		U659	A596	G530	U467			U261	G201	
						G803		C660	A597	U531	A468			A262	G202	C135
						U804		G661	U598	A532	A469			G263	A329	
						C805		U662	C599	A533	C470			C264	G204	G138
						C906										



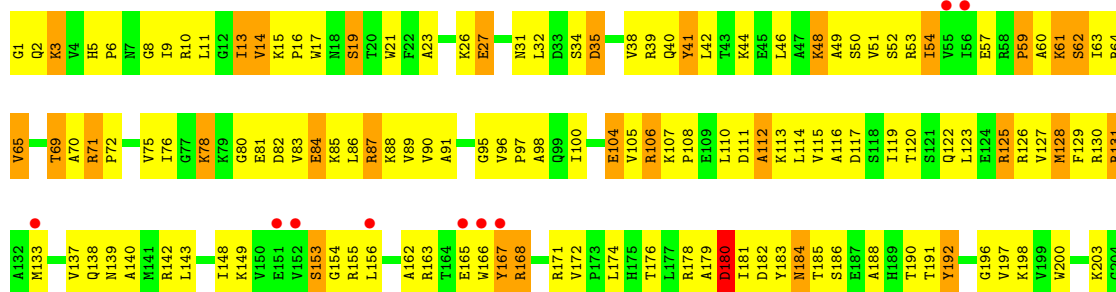
### • Molecule 2: 30S ribosomal protein S3

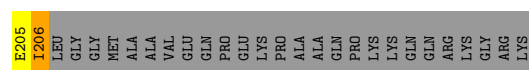
Chain AC:



### • Molecule 2: 30S ribosomal protein S3

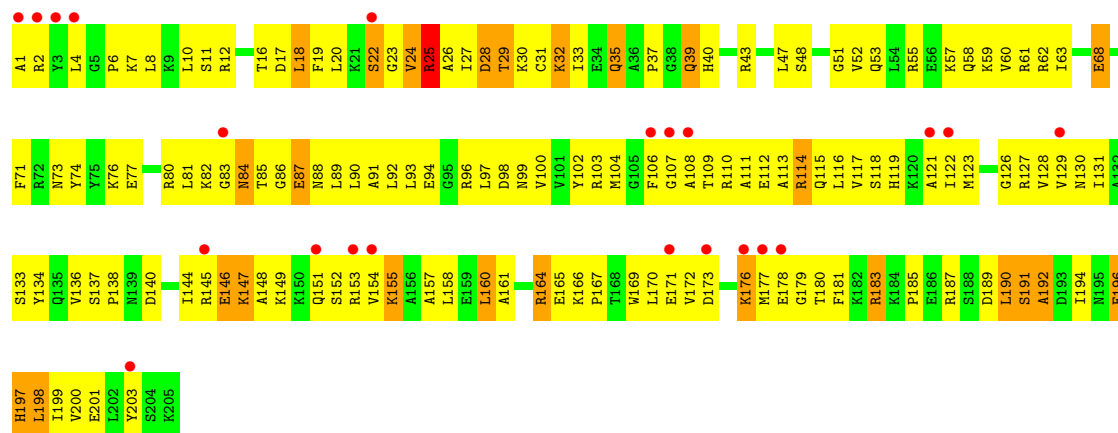
Chain CC:





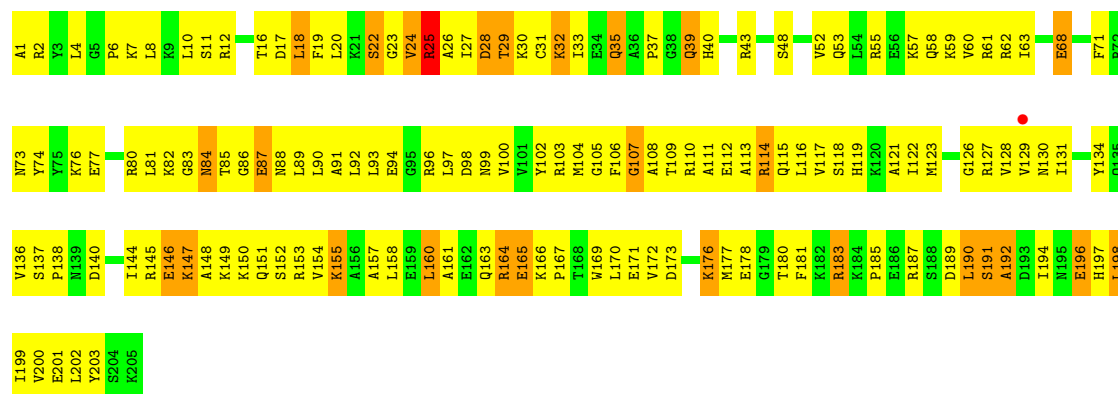
• Molecule 3: 30S ribosomal protein S4

Chain AD:



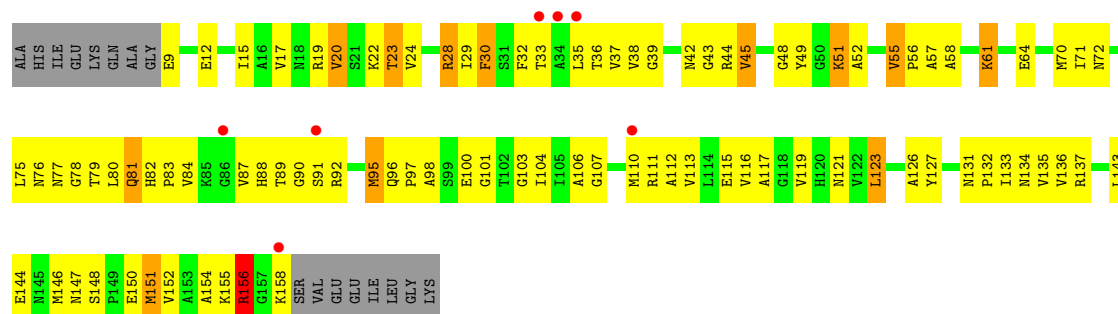
• Molecule 3: 30S ribosomal protein S4

Chain CD:



• Molecule 4: 30S ribosomal protein S5

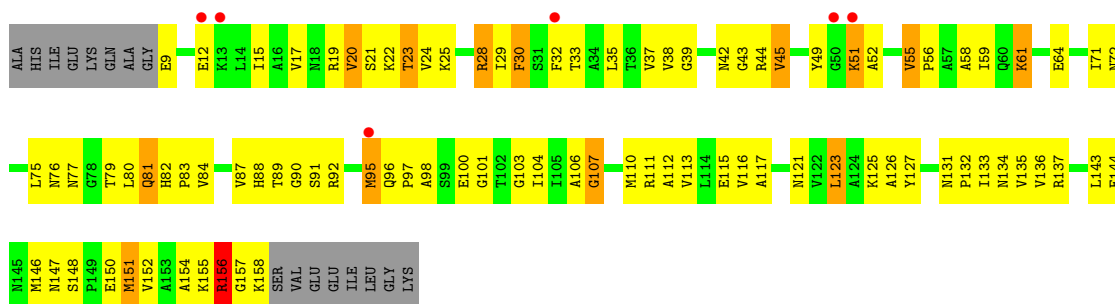
Chain AE:



• Molecule 4: 30S ribosomal protein S5

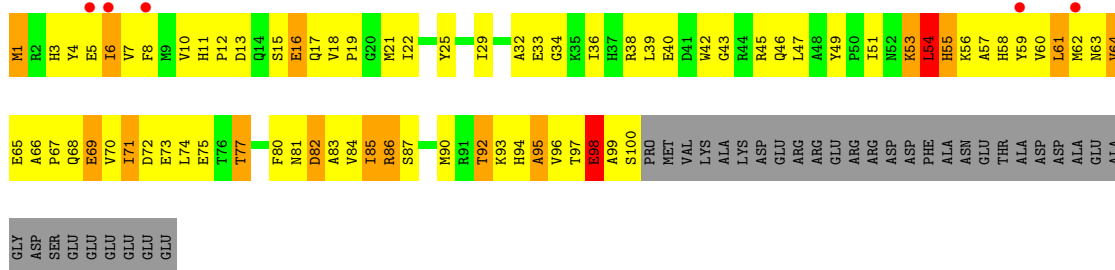
Chain CE:





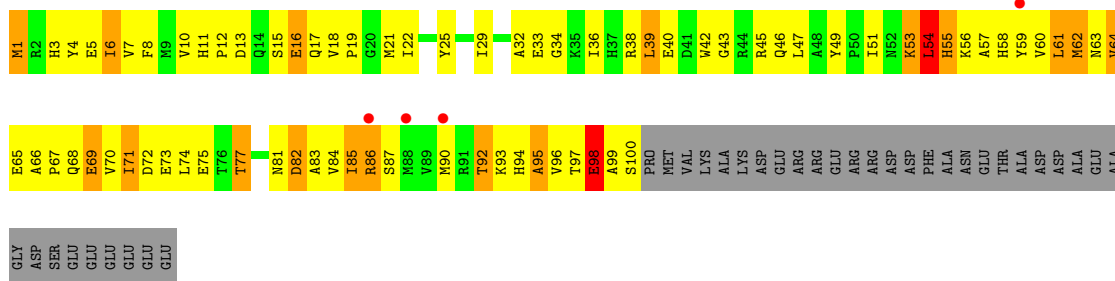
• Molecule 5: 30S ribosomal protein S6

Chain AF:



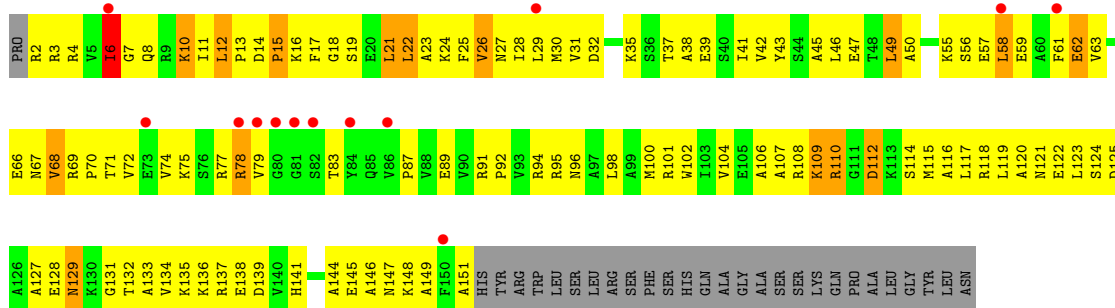
• Molecule 5: 30S ribosomal protein S6

Chain CF:



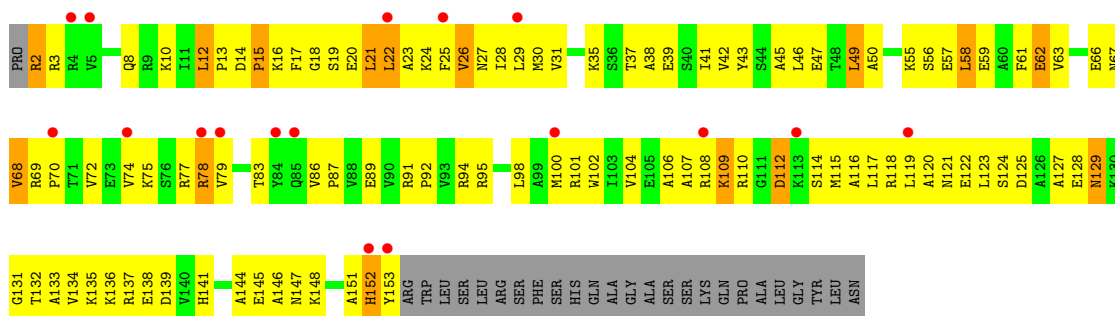
• Molecule 6: 30S ribosomal protein S7

Chain AG:



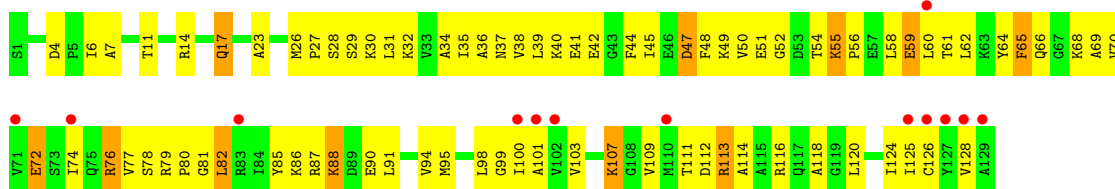
• Molecule 6: 30S ribosomal protein S7

Chain CG:



• Molecule 7: 30S ribosomal protein S8

Chain AH:



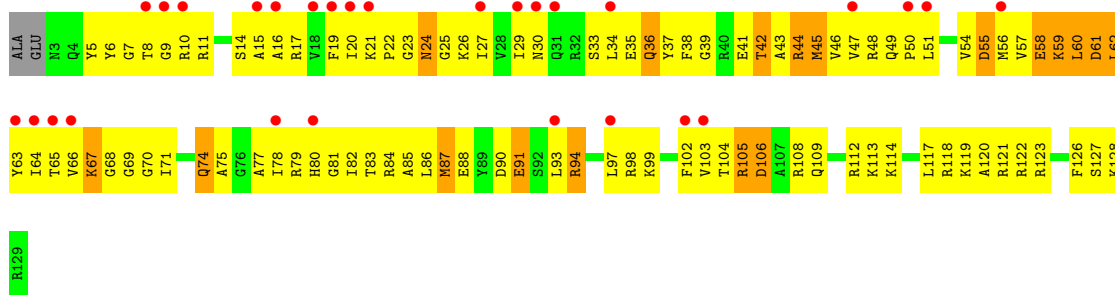
• Molecule 7: 30S ribosomal protein S8

Chain CH:



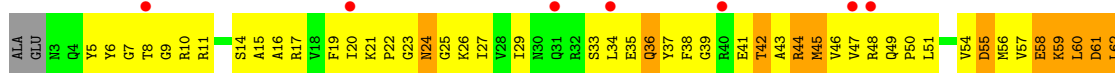
• Molecule 8: 30S ribosomal protein S9

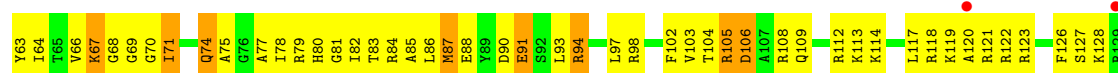
Chain AI:



• Molecule 8: 30S ribosomal protein S9

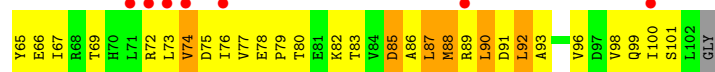
Chain CI:





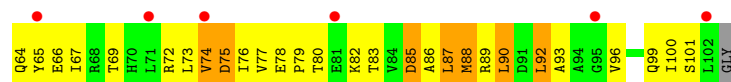
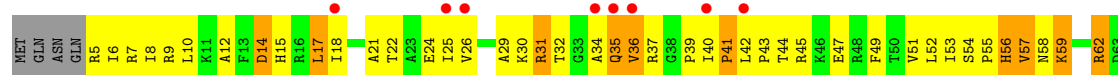
• Molecule 9: 30S ribosomal protein S10

Chain AJ:



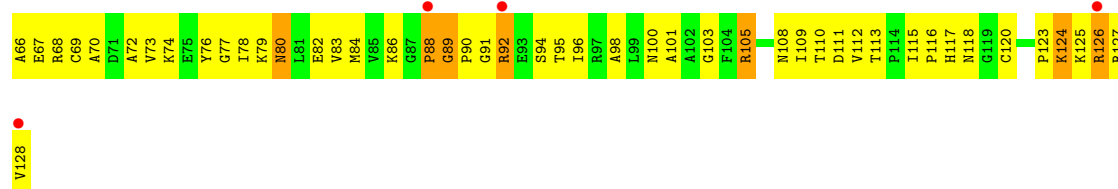
• Molecule 9: 30S ribosomal protein S10

Chain CJ:



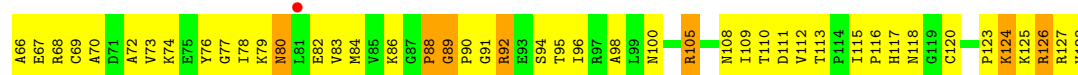
• Molecule 10: 30S ribosomal protein S11

Chain AK:



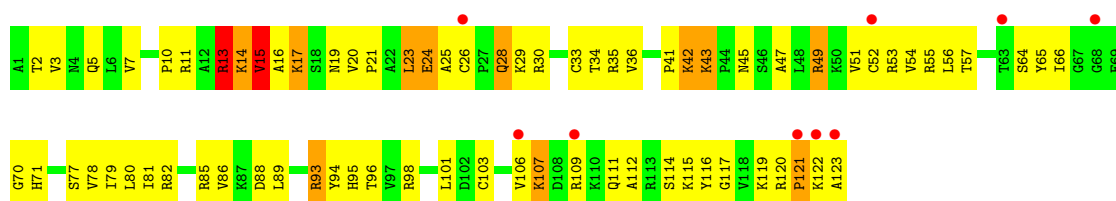
• Molecule 10: 30S ribosomal protein S11

Chain CK:



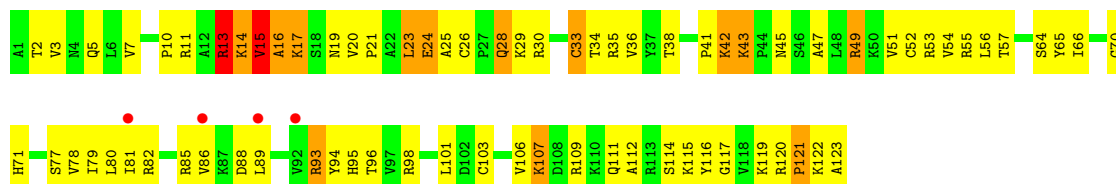
• Molecule 11: 30S ribosomal protein S12

Chain AL:



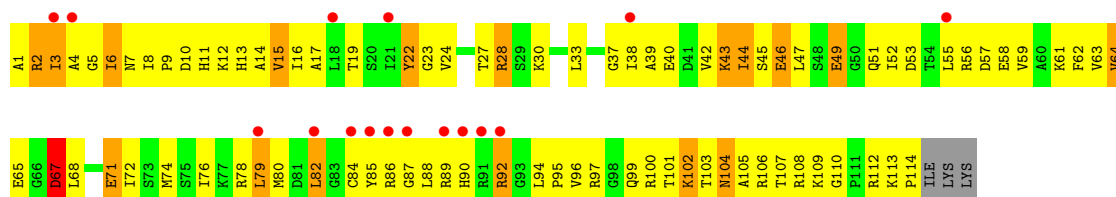
• Molecule 11: 30S ribosomal protein S12

Chain CL:



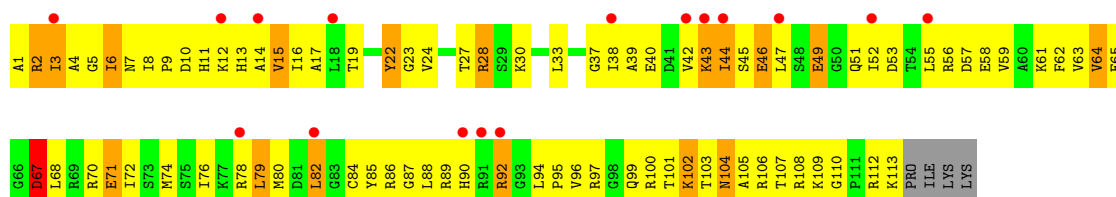
• Molecule 12: 30S ribosomal protein S13

Chain AM:



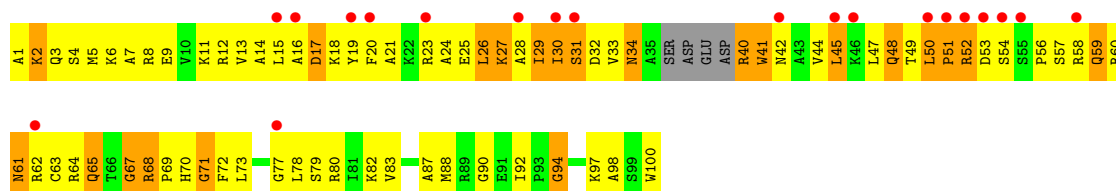
• Molecule 12: 30S ribosomal protein S13

Chain CM:



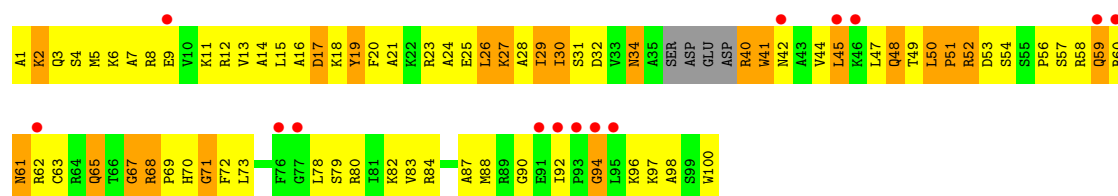
• Molecule 13: 30S ribosomal protein S14

Chain AN:



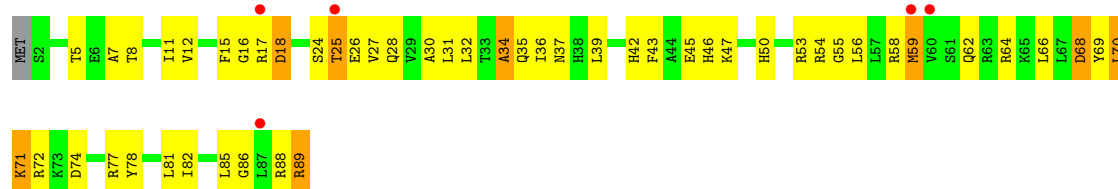
• Molecule 13: 30S ribosomal protein S14

Chain CN:



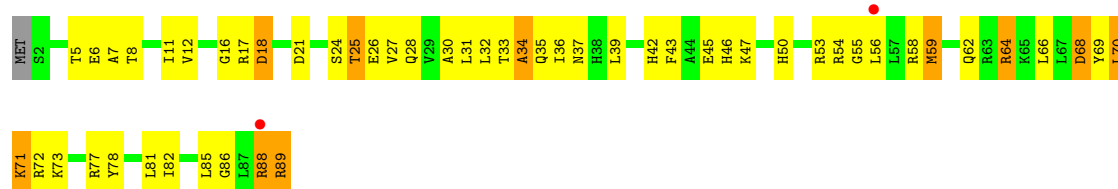
• Molecule 14: 30S ribosomal protein S15

Chain AO:



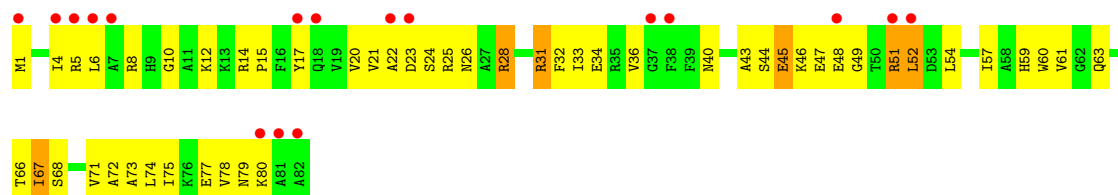
• Molecule 14: 30S ribosomal protein S15

Chain CO:



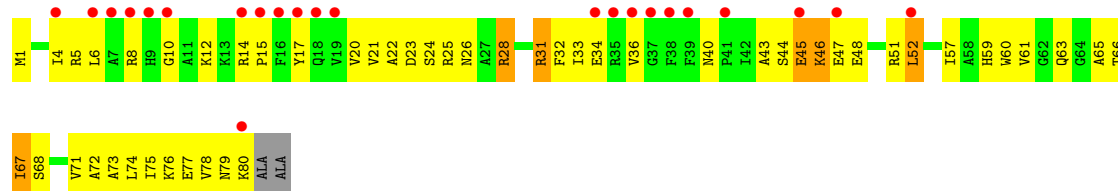
• Molecule 15: 30S ribosomal protein S16

Chain AP:



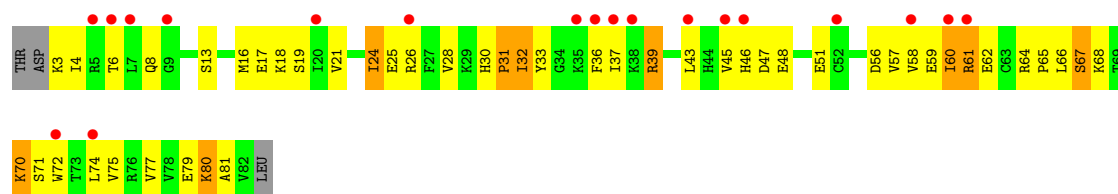
• Molecule 15: 30S ribosomal protein S16

Chain CP:



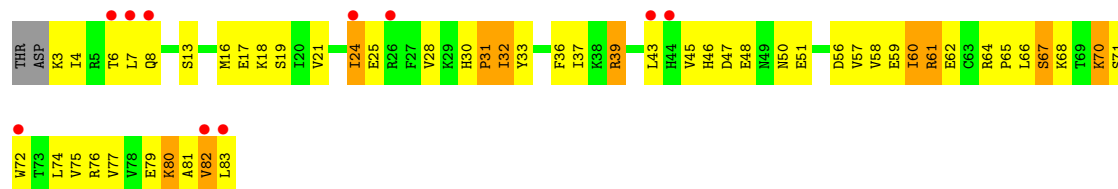
• Molecule 16: 30S ribosomal protein S17

Chain AQ:



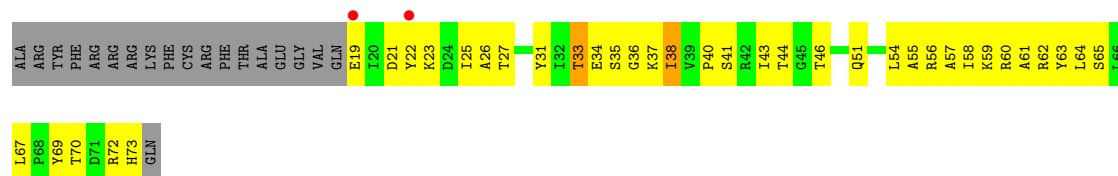
- Molecule 16: 30S ribosomal protein S17

Chain CQ:



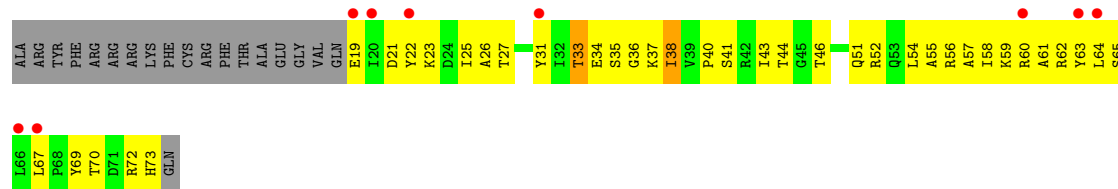
- Molecule 17: 30S ribosomal protein S18

Chain AR:



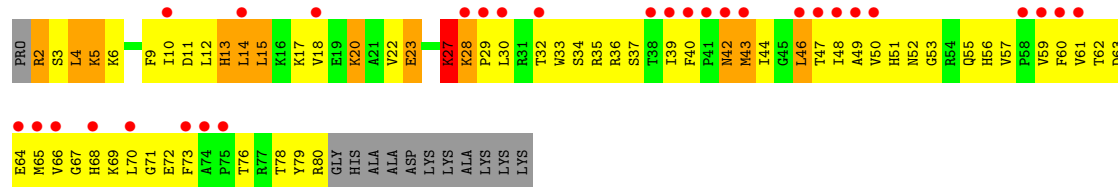
- Molecule 17: 30S ribosomal protein S18

Chain CR:



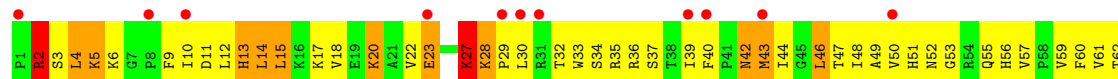
- Molecule 18: 30S ribosomal protein S19

Chain AS:



- Molecule 18: 30S ribosomal protein S19

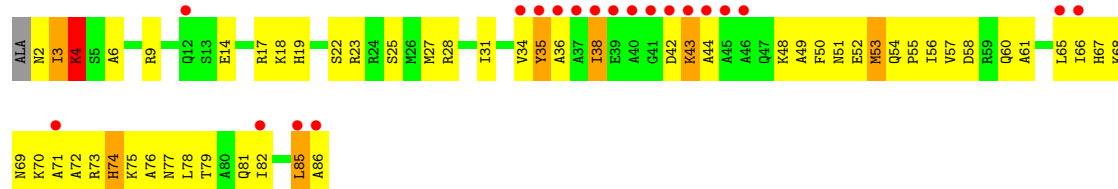
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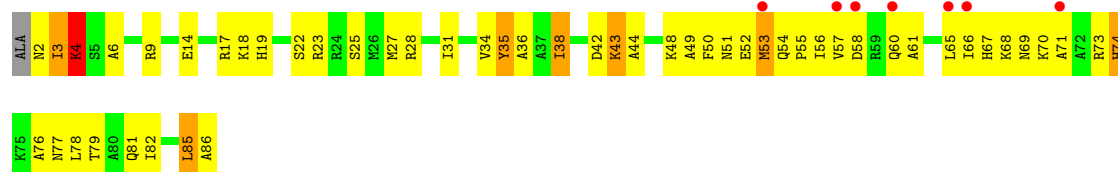
• Molecule 19: 30S ribosomal protein S20

Chain AT:



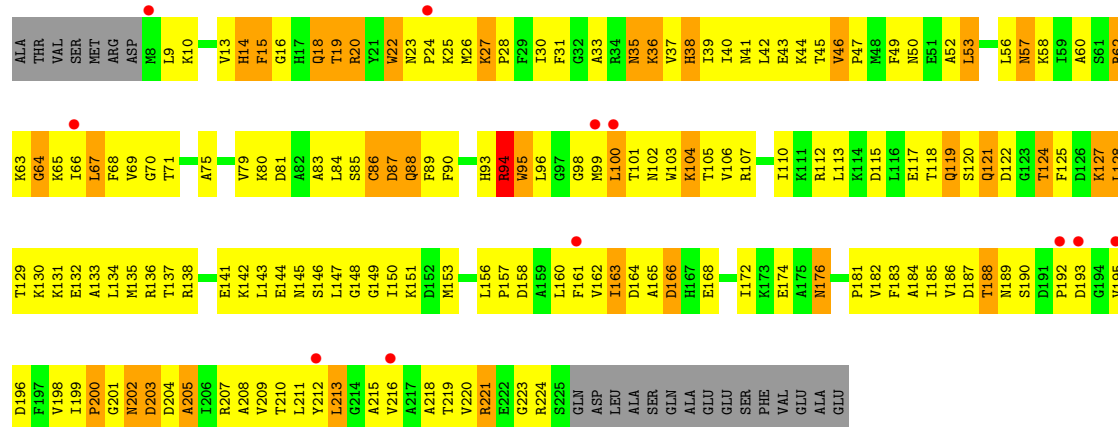
• Molecule 19: 30S ribosomal protein S20

Chain CT:



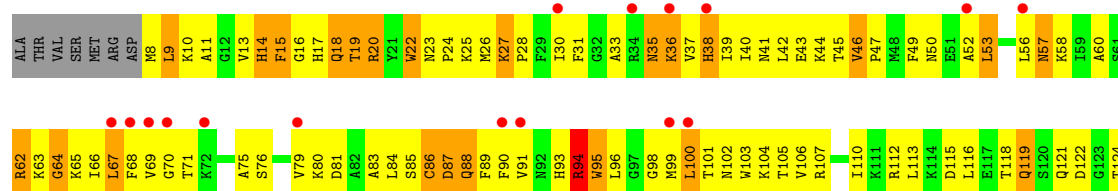
• Molecule 20: 30S ribosomal protein S2

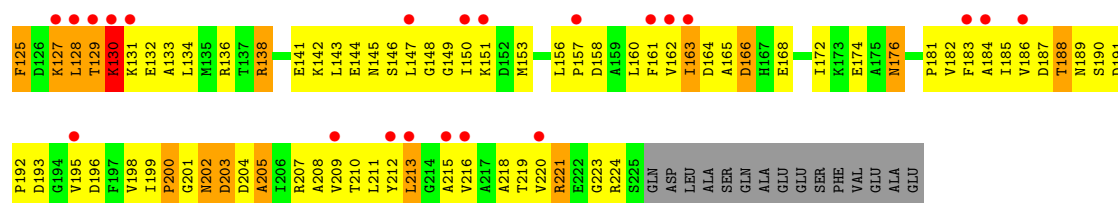
Chain AB:



• Molecule 20: 30S ribosomal protein S2

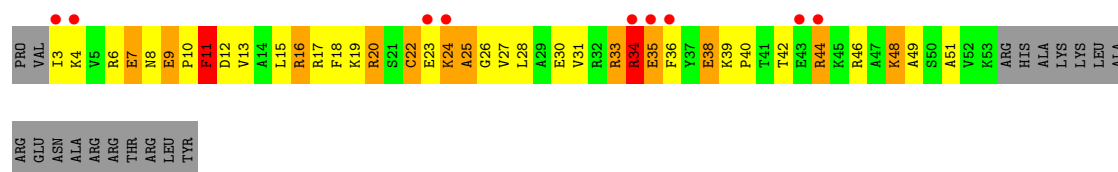
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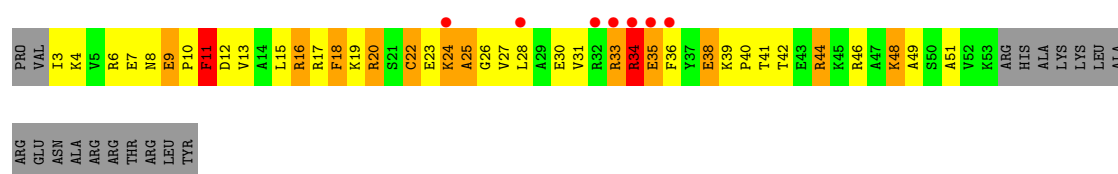
• Molecule 21: 30S ribosomal protein S21

Chain AU:



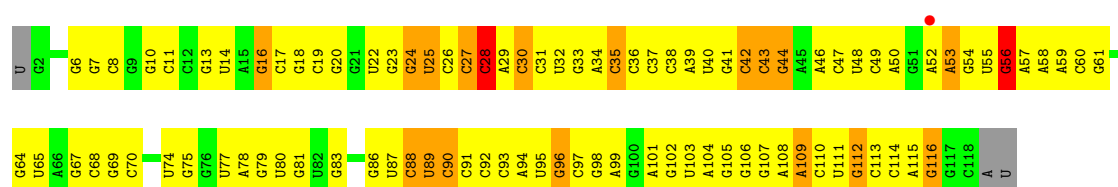
• Molecule 21: 30S ribosomal protein S21

Chain CU:



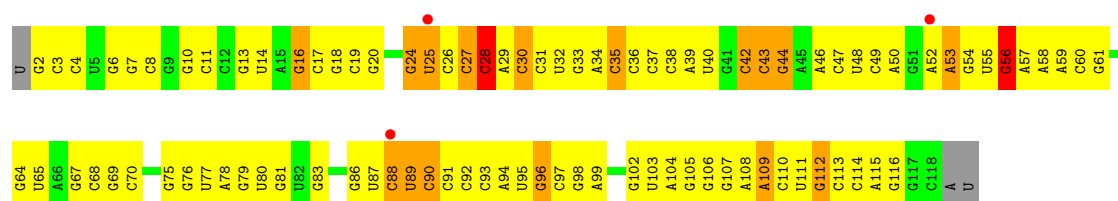
• Molecule 22: 5S rRNA

Chain BA:



• Molecule 22: 5S rRNA

Chain DA:



• Molecule 23: 23S rRNA

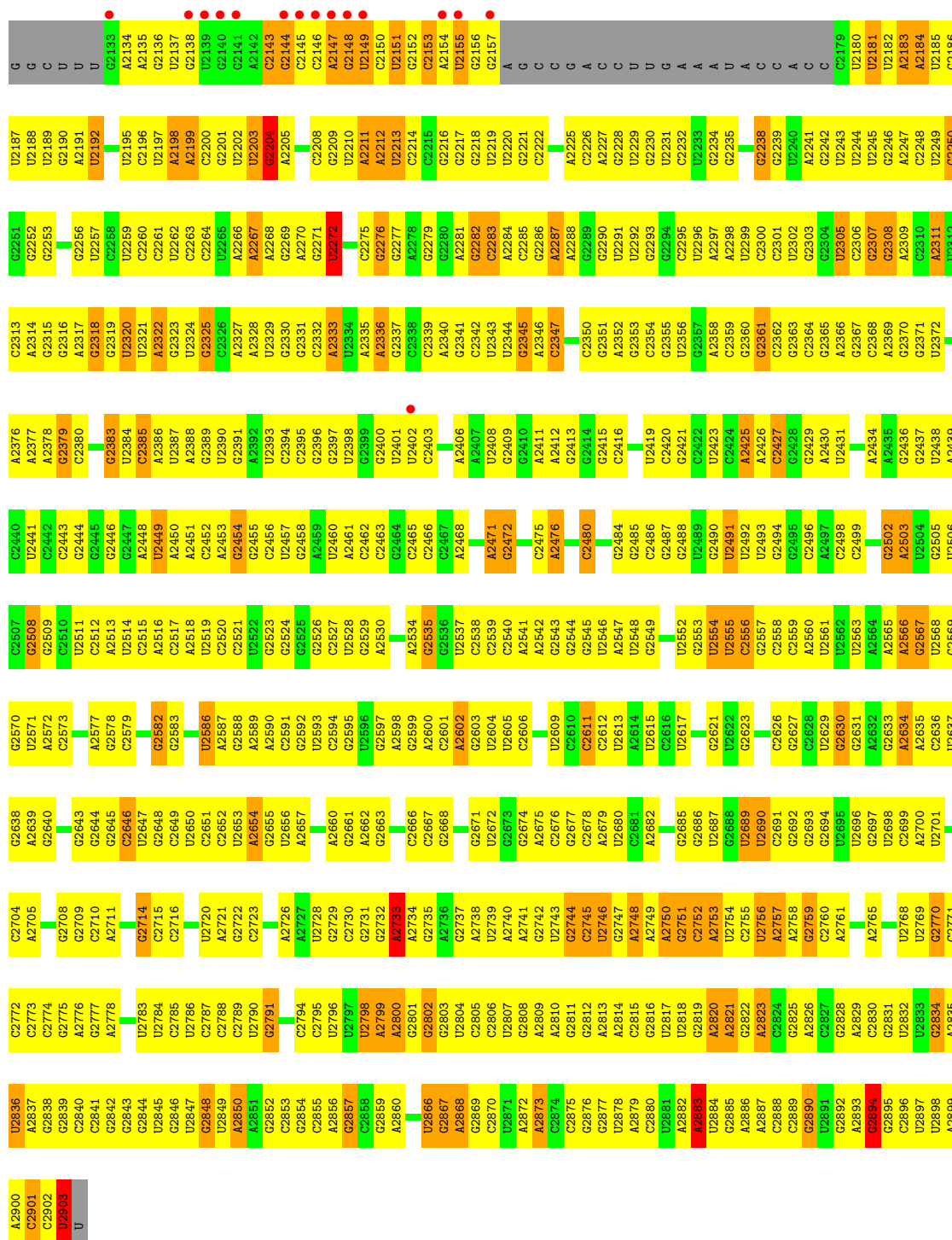
Chain BB:





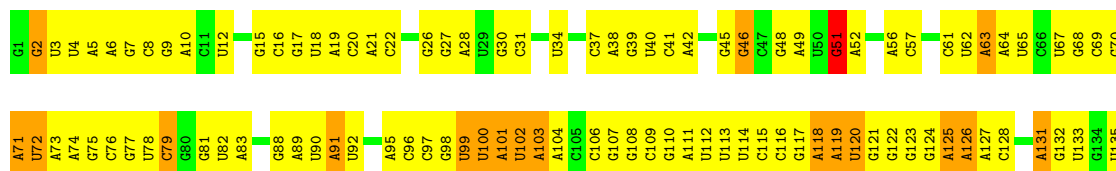
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A1069	A1008	G938	C876	C814	U742	G681	G617	G551	A483	G411	A340	G272	A204	A142	G77
A1070	A1009	A941	A877	C815	A743	G682	G618	U552	C485	C413	C341	G273	G205	C143	U78
G1071	A1010	G942	A878	C816	U744	U683	G619	G553	C486	C414	A345	C274	C208	A144	C79
C1072	G1011	G943	G	C817	G745	G684	G620	U554		C415	A346	C275	C209	C145	G80
	U1012	C944	G	G818	U746	A685	A621		C490	A415		U276	C210	A146	G81
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A1076	A1014	C946	G	A820	A753	C687	C623		A492	C417	G359	A278	U148	U149	A83
	U1015	A947	U	C822	U754	U688	G624		A493	C418	G359	A279	A149	A150	G88
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C1092	A1028	U962	C	C835	G772	U702	G638		A507		U366	U297	A227	C163	A101
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	U1033	C968		C840	U779	G707	A643		A512	U440	G372		G232	G168	G106
	G1034	G969		G841	U780	G708	A644		A513	U441	U373		A233	G169	G107
	U1035	U970		U842	G781	U709	C645		A514	U442			U234	U170	G108
	G1036	G971		G843	A782	U710	U646		A515	G443			U235	U171	
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	A1039	G974		U846	G785	U714	G649		C518	G446	G379		C238	U174	
	U1040			U847	G786	A715	C650		U519		G380			G175	
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	G1055	G992		G862	G801	A730			A538	G466	C398		C257	A190	
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	G1063	A1000		U872		G738	A677		A547	C336				C198	
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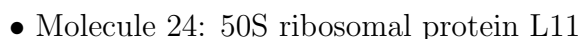
• Molecule 23: 23S rRNA

Chain DB:

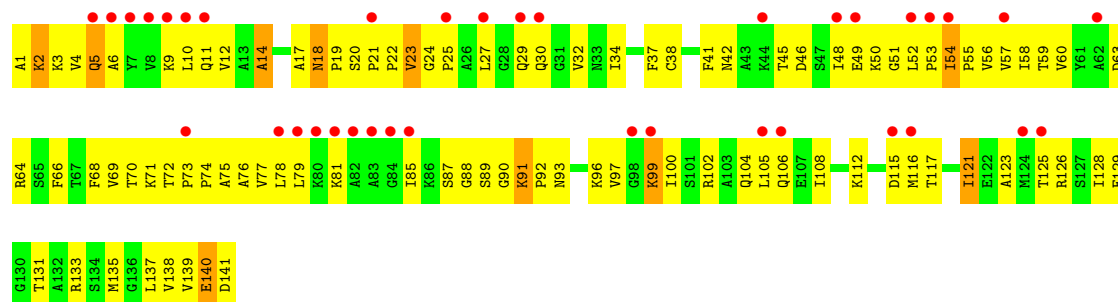




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U	A	G	C1986	C1986	U	A1786	A1722	C1656	A1579	G1517	G1452	U1390	C1257	U1188
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C	C	A	A2058	U1993	U1858	G1792	C1728	G1663	C1585	U1523	U1397	G1331	G1266	A1194
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G	A	A	A2060	U1995	G1860	A1794	G1730	A1665	G1587	A1525	U1400	A1336	A1268	C1196
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G	A	G	C2063	A1998	G1863	G1797	G1733	A1668	A1590	A1528	U1403	G1339	G1271	U1199
G	G	G	C2064	C1999	U1864	G1798	G1734	A1669	A1591	A1529	A1404	U1272	A1277	C1200
A	A	A	C2065	C2000	U1865	G1799	A1735	A1670	C1592	U1593	U1405	U1340	U1273	U1201
G	A	G	C2066	C2001	A1866	C1800	U1736	G1671	A1593	A1532	U1406	G1341	A1274	G1202
G	G	G	G2067	G2002	G1867	U	G1737	A1672	U1594	U1533	G1407	U1342	A1275	U1203
U	U	U	U2068	U1930	C1868	C1804	G1738	G1673	C1595	U1534	U1408	U1344	A1276	A1204
C	C	C	G2069	U1931	G1869	A1805	A1739	A1674	A1596	U1535	U1409	U1345	G1277	A1205
U	U	U	A2070	A1932	C1870	U	G1740	C1675	A1597	A1536	G1410	G1346	G1278	G1206
U	U	U	A2071	G1933	A1871	A1809	C1741	A1676	A1598	G1537	U1411	A1347	U	G1210
C	C	U	C2072	G2010	A1872	A1810	U1742	G1682	U1599	G1538	U1412	C1348	A1283	G1211
G	A	U	C2073	U2011	G1873	G1811	G1743	A1677	U1599	U1539	U1413	C1349	A1285	G1212
G	A	U	U2074	G2012	C1874	U1812	A1744	A1678	C1600	G1540	C1414	C1350	A1286	A1213
A	A	U	U2075	A2013	U1875	G1813	A1745	A1680	U1603	C1541	U1415	U1351	A1287	G1215
A	A	U	U2076	A2014	G1814	A1814	A1746	G1681	U	U1542	G1416	U1352	A1288	U1219
G	G	U	A2077	A2015	U1885	A1815	U1747	G1682	C1607	G1543	G1417	A1353	A1291	G1220
G	G	U	C2078	A2016	A1886	A1816	C1748	U1688	A1608	G1544	G1418	A1354	G1292	G1221
U	U	U	U2079	U2017	C1887	G1817	A1749	G1686	A1609	A1545	A1419	G1355	G1297	G1228
A	A	U	A2080	G2018	C1888	U1818	G1750	C1685	A1610	G1546	A1420	G1356	C1298	A1230
U	U	U	U2081	A2019	U1889	A1819	U1751	G1686	G1611	G1547	G1421	G1357	U	U1231
A	A	U	A2082	A2020	A1890	U1820	C1752	G1687	C1612	U1548	G1422	G1358	G1299	U1234
C	C	U	G2083	C2021	G1884	A1821	G1753	U1688	G1613	A1549	G1423	A1359	A1301	G1235
C	C	U	C2084	U2022	A1885	C1822	A1754	A1689	A1614	C1550	G1424	G1360	A1302	G1236
U	U	U	U2085	C2023	C1886	G1823	A1755	A1690	G1615	A1551	U1487	G1361	G1303	G1237
U	U	U	U2086	G2024	C1887	G1824	G1756	C1691	A1616	A1552	G1426	U	A1304	G1238
A	A	U	G2087	G2025	G1888	U1825	A1757	U1692	C1617	U1553	A1427	A1365	A1305	G1239
A	A	U	A2088	U2026	A1889	U1826	U1758	U1693	U	U1554	C1428	A1366	G1306	U1240
C	C	U	C2089	G2027	A1890	U1827	G1759	C1694	G1622	G1555	G1429	A1367	A1307	U1241
C	C	U	A2090	U2028	G1891	G1828	C1760	G1765	G1623	U	A1431	G1368	A1308	A1241
C	C	U	C2091	G2029	C1892	A1829	C1761	G1766	A1624	U1559	G1432	C1370	G1309	U1242
C	C	U	U2092	A2030	C1893	C1830	A1762	C1768	U	U1560	U1433	A1371	G1310	C1243
C	C	U	G2093	A2031	C1894	G1831	G1763	U	G1628	C1561	A1434	A1433	A1304	A1244
C	C	U	C2094	G2032	G1895	C1832	C1764	U	U1562	U1561	U1440	A1378	U1313	G1245
C	C	U	A2095	A2033	G1896	C1833	U1765	A1705	G1633	C1562	G1435	U1372	C1314	A1246
C	C	U	C2096	U2034	G1897	U1834	G1766	C1706	A1634	U1563	G1436	A1373	G1315	A1247
C	C	U	A2097	G2035	U1898	G1835	G1767	U1712	A1635	C1564	G1500	G1374	C1316	U1248
C	C	U	U2098	C2036	A1900	C1836	C1768	U1708	U1636	A1565	G1501	C1375	G1317	U1249
C	C	U	G2099	A2037	A1901	C1837	U1709	U1714	A1637	A1566	U1438	C1376	U1318	G1250
C	C	U	U2100	G2038	C1901	U1838	A1773	G1715	G1638	G1567	A1504	A1379	U1319	C1251
C	C	U	A2101	U2039	C1902	G1839	C1774	U1716	C1639	U1568	U1441	U1379	C1320	A1252
C	C	U	G2102	G2040	G1903	U1842	U1775	U1717	A1640	A1569	G1442	G1380	G1321	A1321
A	A	U	C2103	U2041	G1904	G1843	G1776	A1713	A1641	A1570	U1443	G1381	U1247	U1253
C	C	U	A2042	C1905	C1843	C1844	U1777	U1714	U1647	A1571	G1444	G1382	U1248	U1254
C	C	U	U2105	G1906	G1907	C1845	U1778	G1715	U1648	A1572	G1445	A1383	U1318	G1255
U	U	U	G2106	C1907	G1908	G1846	U1779	U1716	U1649	G1573	G1446	A1384	C1319	C1256
U	U	U	A2107	C1974	U1908	G1847	U1782	U1717	U1650	A1574	C1447	A1385	G1320	A1257
G	G	G	A2108	U	C1909	A1847	U1782	G1718	A1652	C1575	G1448	G1448	G1386	A1258

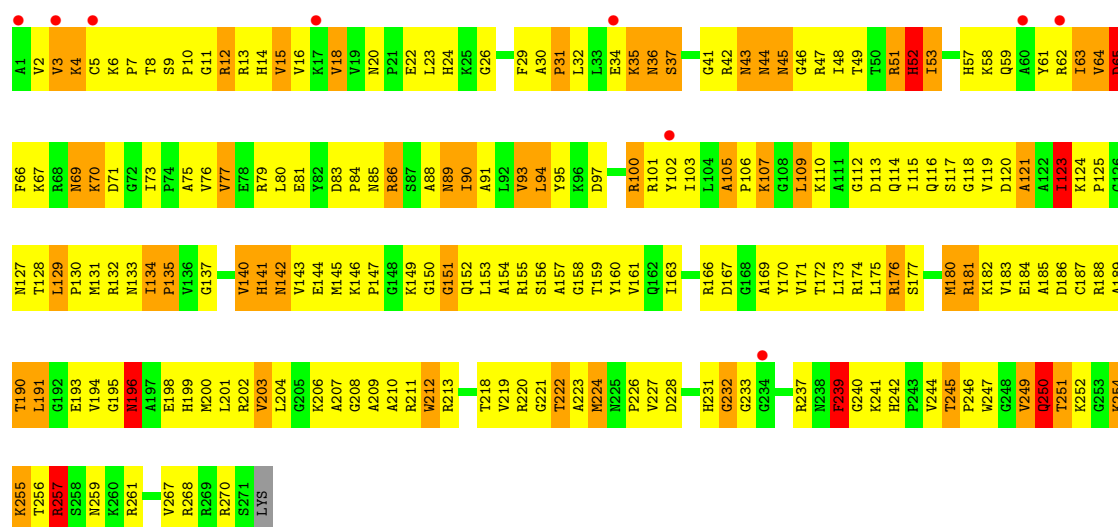


Chain DI:



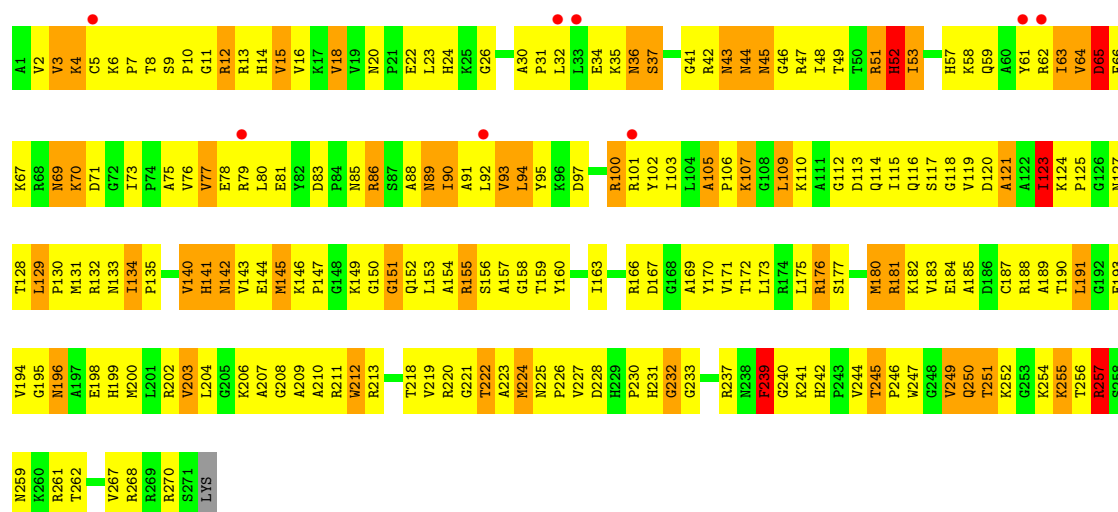
• Molecule 25: 50S ribosomal protein L2

Chain BC:



• Molecule 25: 50S ribosomal protein L2

Chain DC:



• Molecule 26: 50S ribosomal protein L3

G195	A196	T197	L201	L202	V203	K204	P205	A206	V207	K208	A209	D131	A132	T133	H134	G135	N136	S137	L138	S139	H140	R141	G142	P143	G144	S145	I146	G147	Q148	N149	Q150	T151	P152	G153	K154	K159	K160	M161	A162	G163	P164	M165	G166	N167	E168	R169	V170	Q173	S174	L175	D176	V177	L178	R179	V180	D181	A182	E183	R184	N185	L186	L187	L188	V189	K190	G191	A192	V193	P194	E64	H67	A69	K70	G71	G72	V73	E74	A75	G76	R77	L78	G79	N80	E81	F82	R83	L84	E88	F89	F90	T91	V92	G93	Q94	S95	I96	S97	V98	E99	L100	F101	V104	K105	K106	V107	D108	V109	T110	G111	T112	S113	L114	G115	K116	G117	F118	T121	V122	K123	R124	N125	V126	F127	M1	T2	G3	L4	V5	G6	K7	X8	V9	G10	M11	T12	R13	T14	F15	T16	E17	D18	G19	T22	P23	V24	T25	V26	T27	E28	V29	E30	A31	N32	R33	V34	T35	Q36	V37	K38	D39	L40	A41	N42	Y45	R46	A47	O49	V50	T51	T52	G53	A54	K55	V56	R56	A57	N58	T61	K62	R63
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain DD: 

V193	P194	G195	A196	T197	L201	I202	V203	K204	P205	A206	V207	K208	A209	E64	A65	G66	H67	F68	A69	K70	V73	G74	H75	G76	F77	G78	L79	H80	E81	F82	R83	L84	E88	P89	F90	V91	G92	G93	Q94	S95	I96	S97	V98	E99	L100	F101	V104	K105	K106	V107	D108	V109	T110	G111	T112	S113	L148	O149	V50	T51	T52	G53	A54	K55	R56	A57	N58	T61	F62
D131	A132	T133	H134	G135	N136	S137	L138	S139	H140	A141	V142	P143	G144	S145	I146	G147	Q148	N149	Q150	T151	P152	G153	K154	K159	K160	M161	A162	G163	Q164	M165	G166	N167	E168	P169	V170	T171	V172	Q173	S174	L175	D176	V177	V178	R179	V180	D181	A182	E183	R184	N185	L186	L187	V189	K190	G191	A192													

- Chain BK:

● Molecule 27: 50S ribosomal protein L14

Chain DK:

- WORLDWIDE  
 **PDB**  
PROTEIN DATA BANK



G68	G69	G70	G71	G72	G73	G74	G75	G76	G77	G78	G79	G80	G81	G82	G83	G84	G85	G86	G87	G88	G89	G90	G91	G92	G93	G94	G95	G96	G97	G98	G99	R100	R101	R102	T103	G104	G105	A106	A107	R108	E111	R112	L113	M114
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------

- Molecule 28: 50S ribosomal protein L19

V69  
E70  
R71  
F72  
F73  
Q74  
T75  
H76  
S77  
P78  
V79  
W80  
D81  
S82  
I83  
S84  
H85  
K86  
R87  
R88  
G89  
A90  
V91  
R92  
K93  
A94  
K95  
L96  
Y97  
Y98  
L99  
R100  
E101  
R102  
T103  
G104  
K105  
A106  
A107  
R108  
T109  
K110  
E111  
R112  
L113  
N114

- Molecule 29: 50S ribosomal protein L4

K194  
Q195  
V196  
E197

L200  
A201

- Molecule 29: 50S ribosomal protein L4

A192  
V193  
K194  
Q195  
V196  
E197  
A201

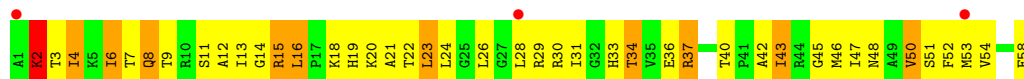
- Molecule 30: 50S ribosomal protein L30

Chain BY:



- Molecule 30: 50S ribosomal protein L30

Chain DY:



- Molecule 31: 50S ribosomal protein L32

Chain B0:



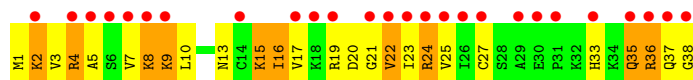
- Molecule 31: 50S ribosomal protein L32

Chain D0:



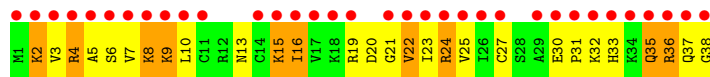
- Molecule 32: 50S ribosomal protein L36

Chain B4:



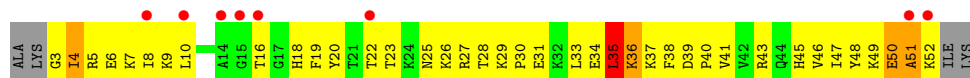
- Molecule 32: 50S ribosomal protein L36

Chain D4:



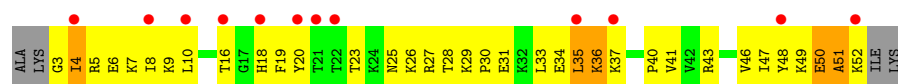
- Molecule 33: 50S ribosomal protein L33

Chain B1:



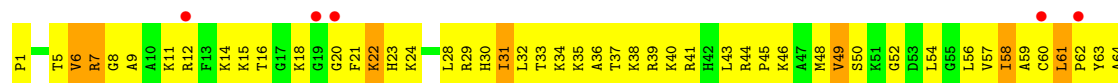
- Molecule 33: 50S ribosomal protein L33

Chain D1:



- Molecule 34: 50S ribosomal protein L35

Chain B3:



- Molecule 34: 50S ribosomal protein L35

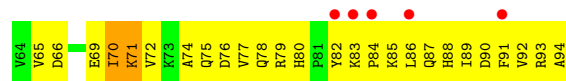
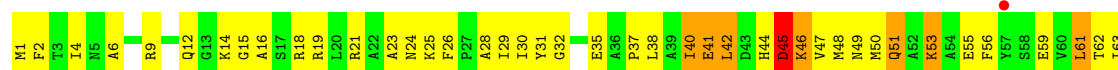
Chain D3:



P62  
Y63  
A64

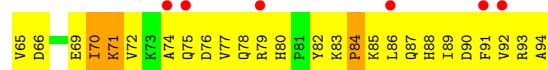
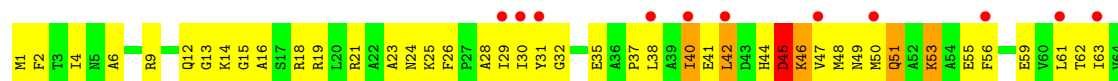
- Molecule 35: 50S ribosomal protein L25

Chain BV:



- Molecule 35: 50S ribosomal protein L25

Chain DV:



- Molecule 36: 50S ribosomal protein L34

Chain B2:



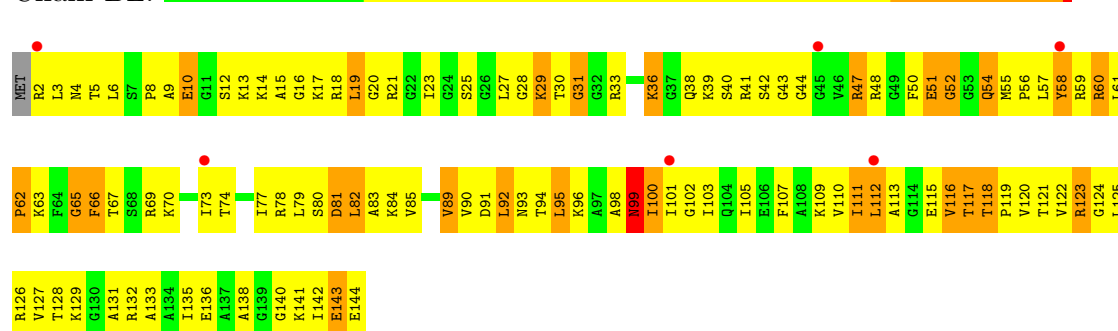
- Molecule 36: 50S ribosomal protein L34

Chain D2:



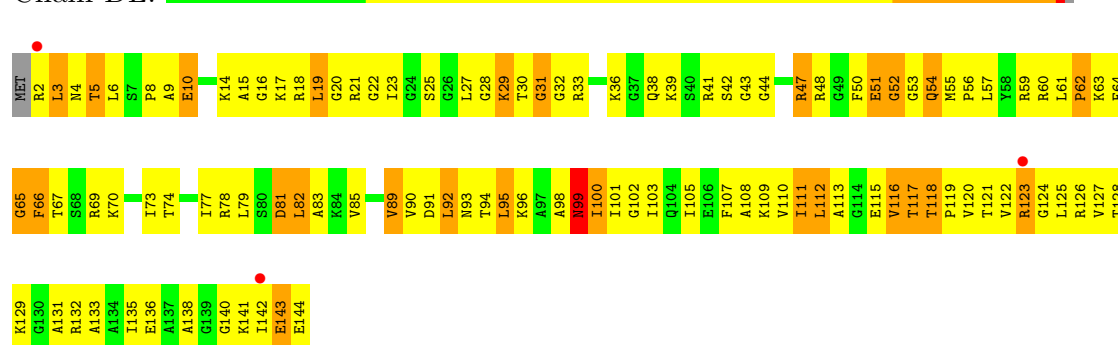
- Molecule 37: 50S ribosomal protein L15

Chain BL:



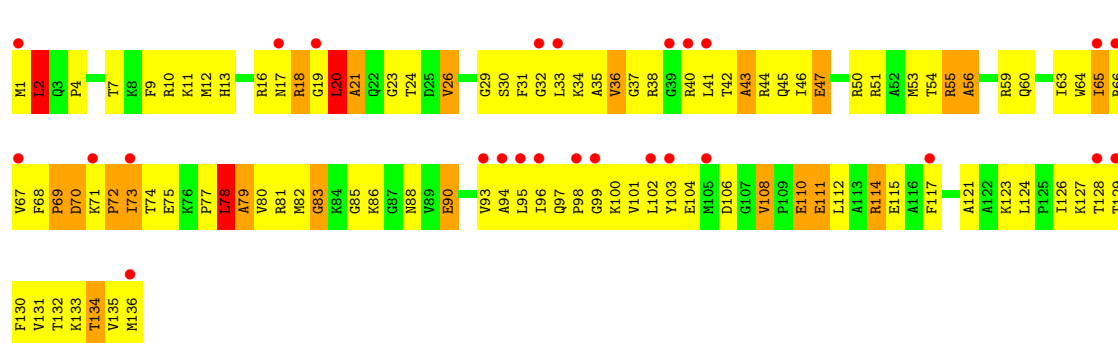
- Molecule 37: 50S ribosomal protein L15

Chain DL:



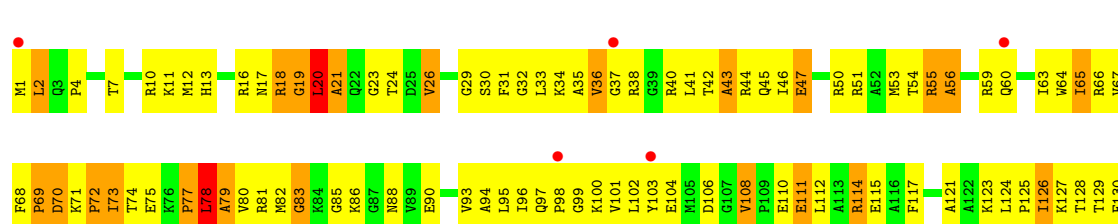
- Molecule 38: 50S ribosomal protein L16

Chain BM:



- Molecule 38: 50S ribosomal protein L16

Chain DM:



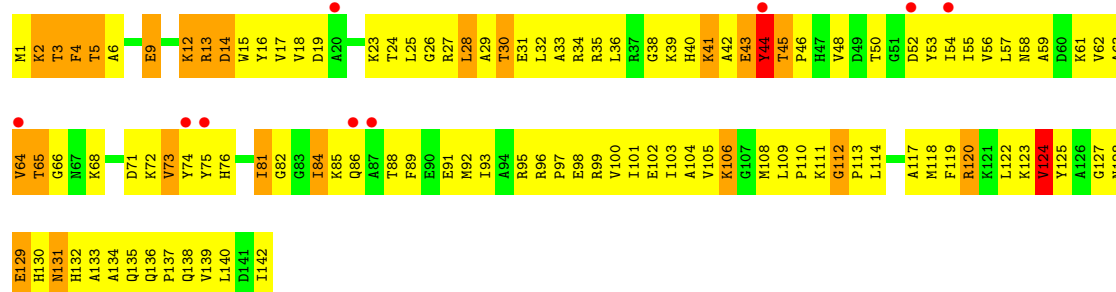


Chain BJ:



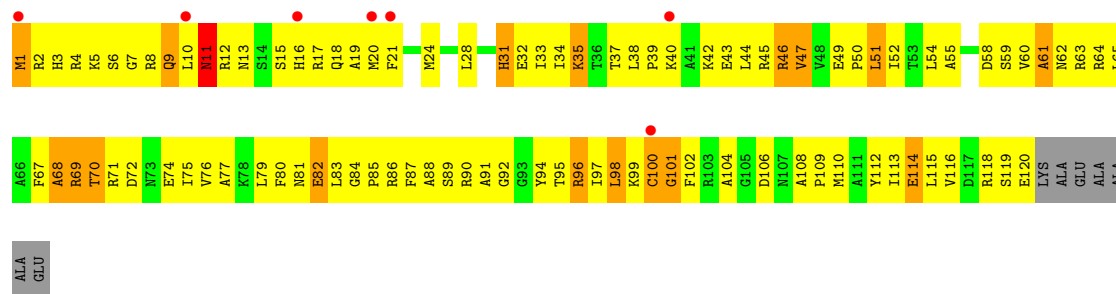
- Molecule 41: 50S ribosomal protein L13

Chain DJ:



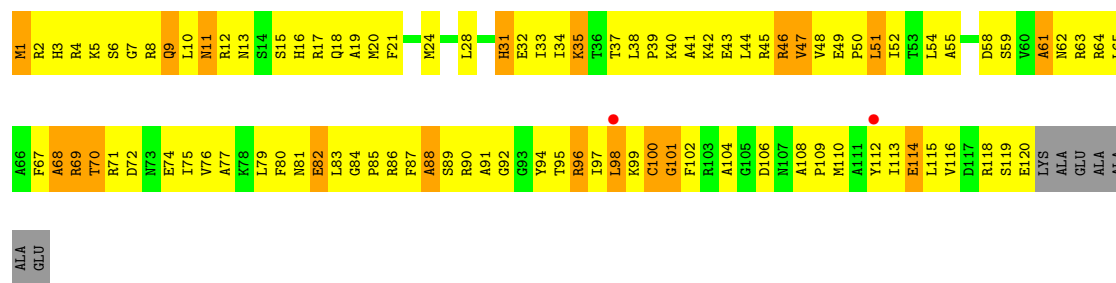
- Molecule 42: 50S ribosomal protein L17

Chain BN:



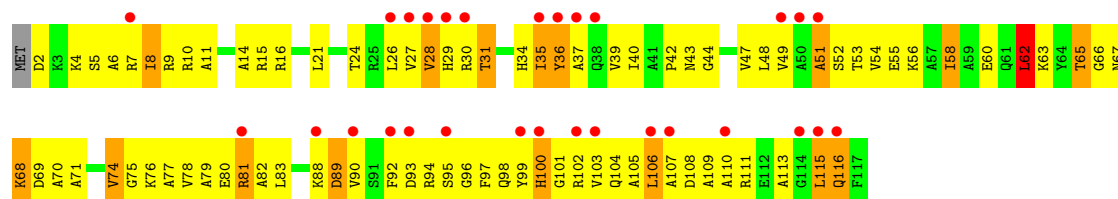
- Molecule 42: 50S ribosomal protein L17

Chain DN:



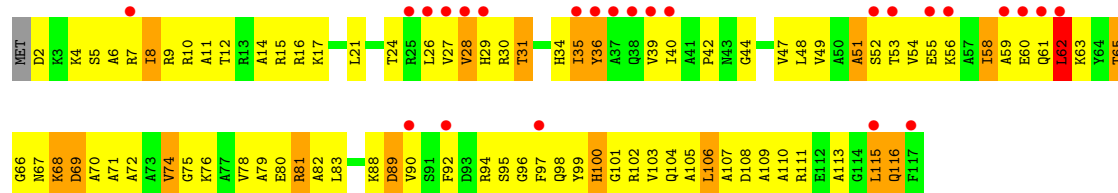
- Molecule 43: 50S ribosomal protein L18

Chain BO: 



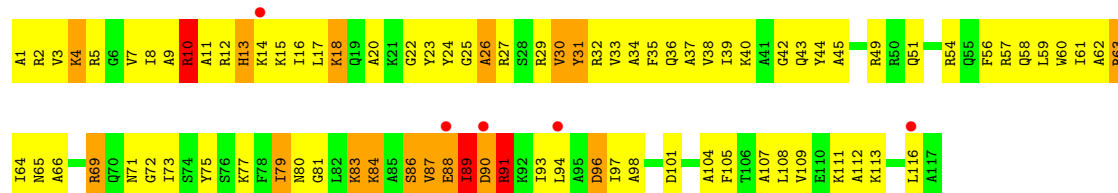
- Molecule 43: 50S ribosomal protein L18

Chain DO: 



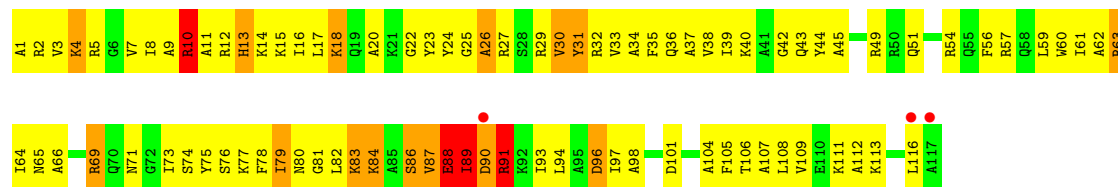
- Molecule 44: 50S ribosomal protein L20

Chain BQ: 



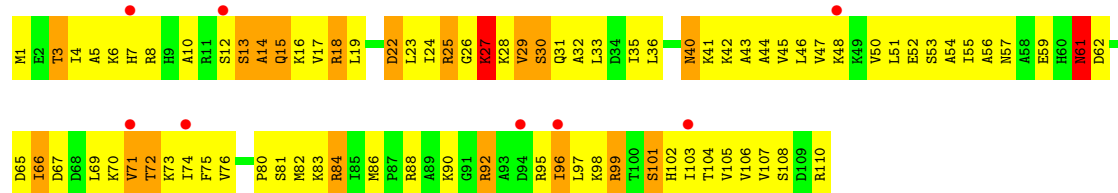
- Molecule 44: 50S ribosomal protein L20

Chain DQ: 



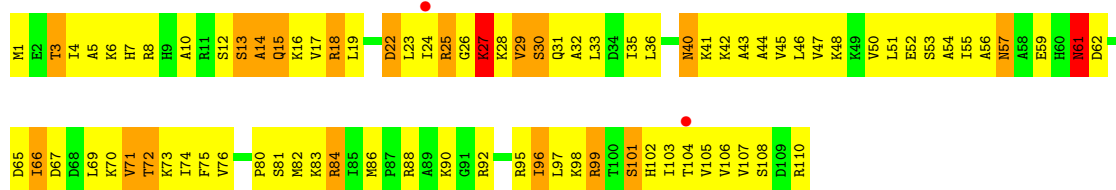
- Molecule 45: 50S ribosomal protein L22

Chain BS: 



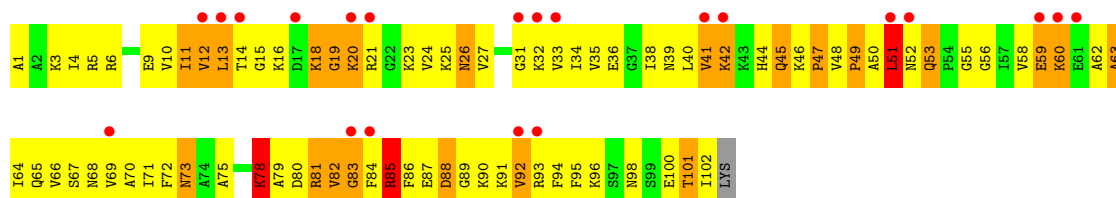
- Molecule 45: 50S ribosomal protein L22

Chain DS: 



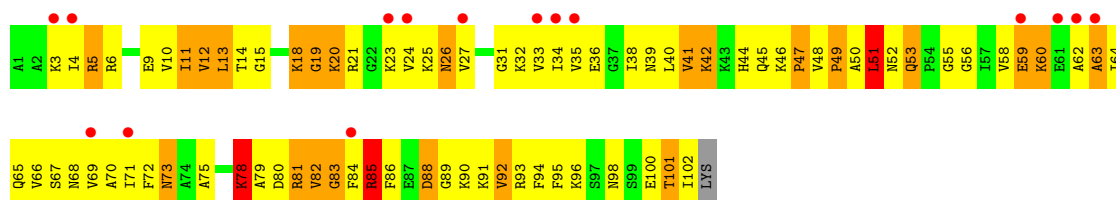
• Molecule 46: 50S ribosomal protein L24

Chain BU:



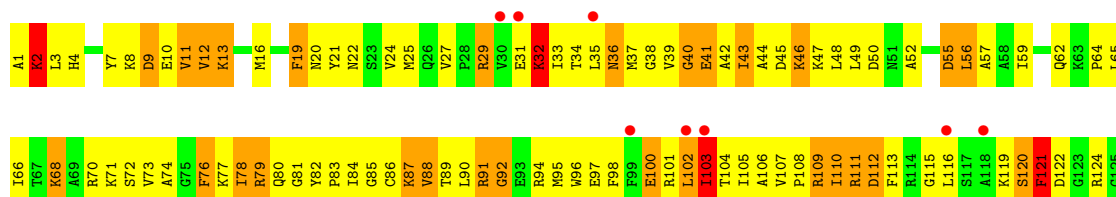
• Molecule 46: 50S ribosomal protein L24

Chain DU:



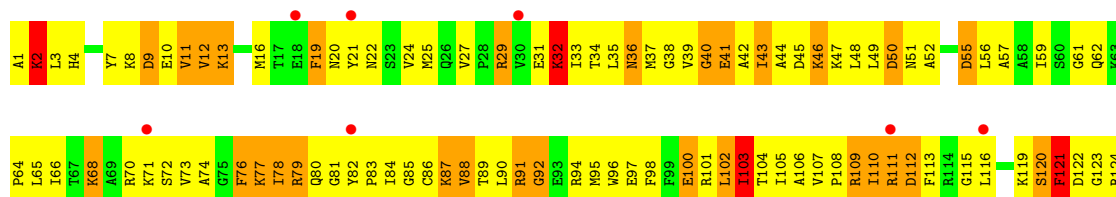
• Molecule 47: 50S ribosomal protein L5

Chain BF:

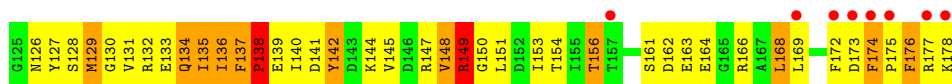


• Molecule 47: 50S ribosomal protein L5

Chain DF:

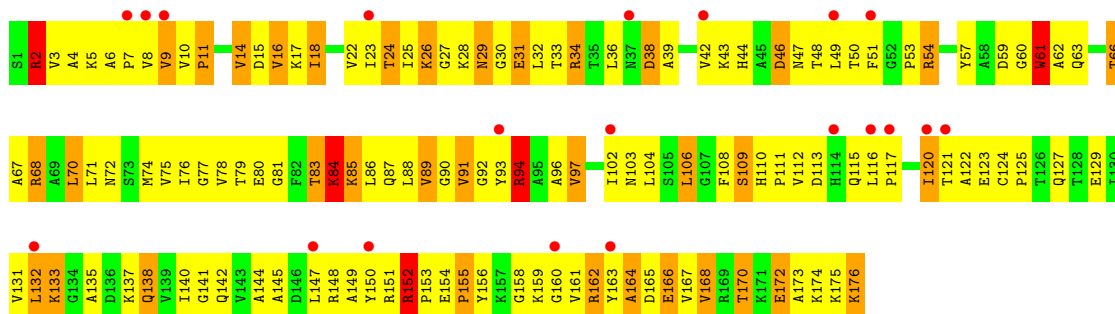






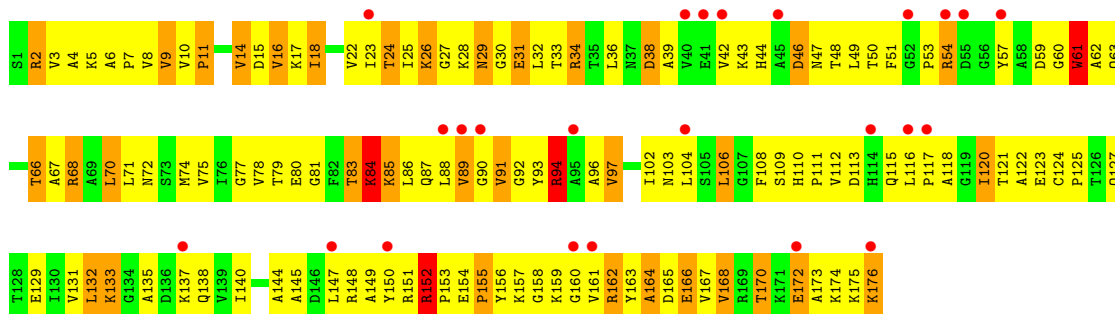
• Molecule 48: 50S ribosomal protein L6

Chain BG:



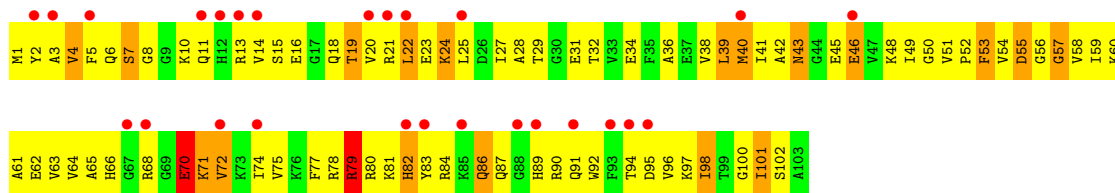
• Molecule 48: 50S ribosomal protein L6

Chain DG:



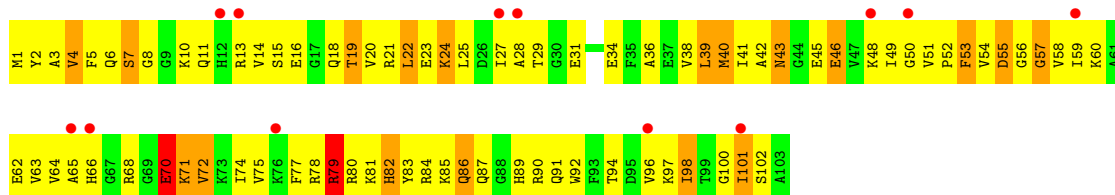
• Molecule 49: 50S ribosomal protein L21

Chain BR:



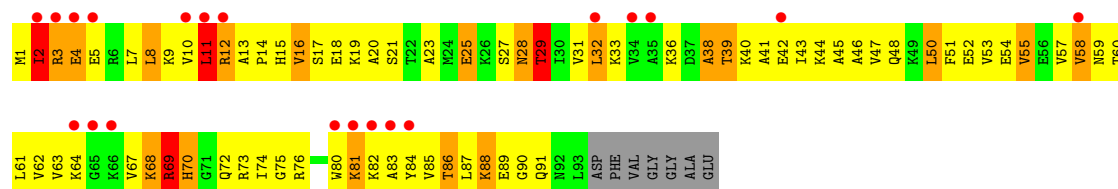
• Molecule 49: 50S ribosomal protein L21

Chain DR:



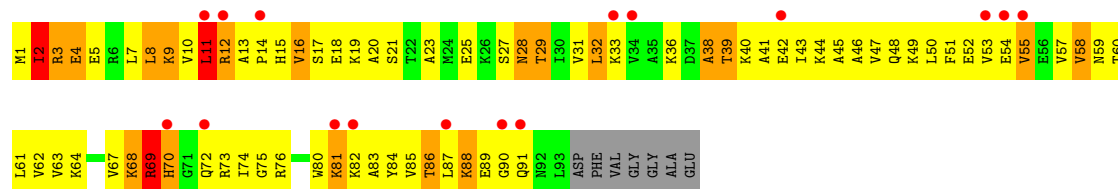
• Molecule 50: 50S ribosomal protein L23

Chain BT:



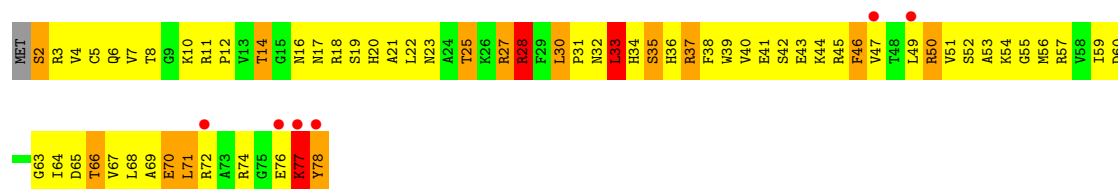
- Molecule 50: 50S ribosomal protein L23

Chain DT:



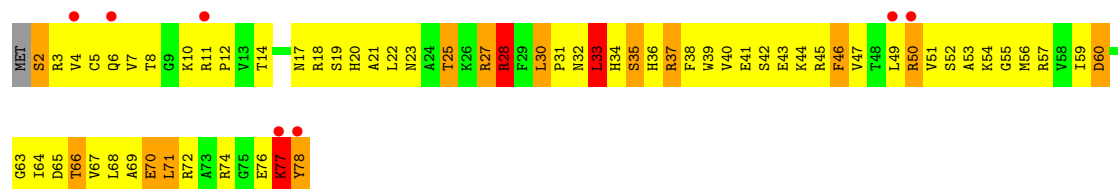
- Molecule 51: 50S ribosomal protein L28

Chain BZ:



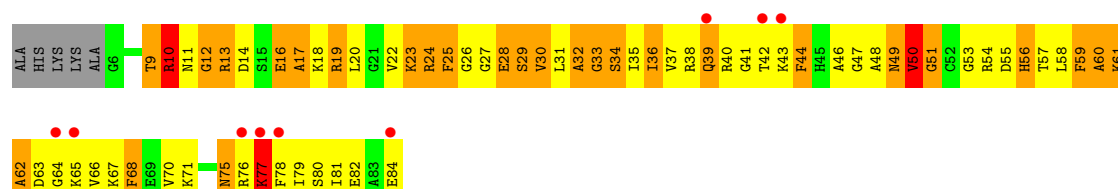
- Molecule 51: 50S ribosomal protein L28

Chain DZ:



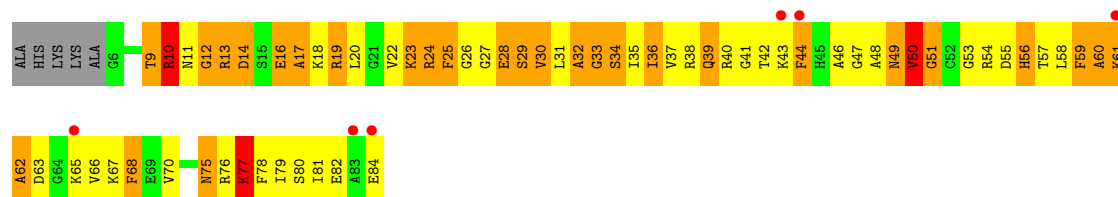
- Molecule 52: 50S ribosomal protein L27

Chain BW:



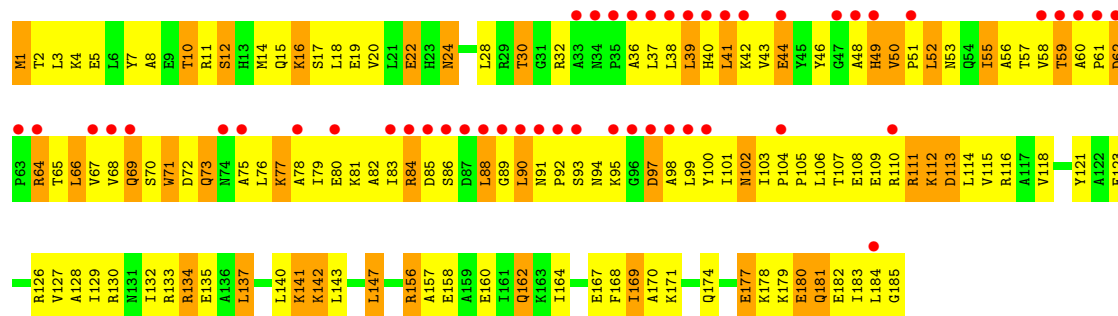
- Molecule 52: 50S ribosomal protein L27

Chain DW:



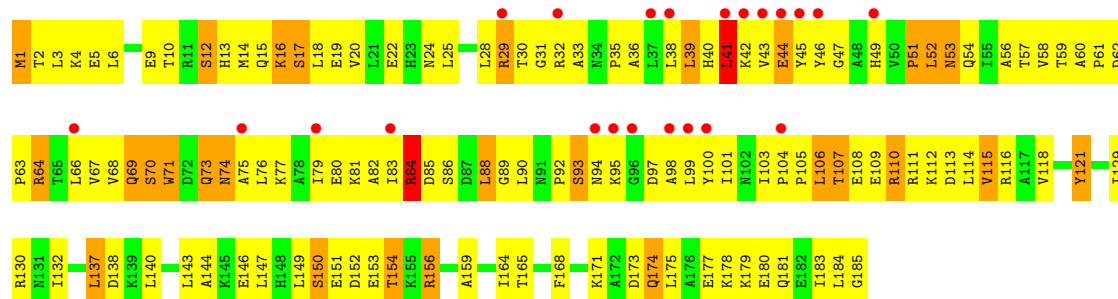
• Molecule 53: 50S ribosomal protein RRF

Chain B6:



• Molecule 53: 50S ribosomal protein RRF

Chain D6:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.87Å 378.75Å 738.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.45 69.15 – 4.45	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.00-4.45) 95.6 (69.15-4.45)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 4.46Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.263 , 0.309 0.246 , 0.280	Depositor DCC
$R_{free}$ test set	16978 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	150.5	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 18.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 341454 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	287128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, MG, PAR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AA	0.28	1/36762 (0.0%)	0.76	6/57350 (0.0%)
1	CA	0.28	1/36762 (0.0%)	0.76	10/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.44	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.44	0/2227
4	AE	0.23	0/1118	0.45	0/1504
4	CE	0.24	0/1118	0.45	0/1504
5	AF	0.24	0/835	0.45	0/1128
5	CF	0.24	0/835	0.45	0/1128
6	AG	0.23	0/1187	0.45	0/1591
6	CG	0.23	0/1211	0.45	0/1624
7	AH	0.23	0/989	0.44	0/1326
7	CH	0.23	0/989	0.44	0/1326
8	AI	0.24	0/1034	0.45	0/1375
8	CI	0.24	0/1034	0.45	0/1375
9	AJ	0.22	0/796	0.49	0/1077
9	CJ	0.22	0/796	0.48	0/1077
10	AK	0.24	0/893	0.46	0/1205
10	CK	0.24	0/893	0.46	0/1205
11	AL	0.22	0/969	0.48	0/1300
11	CL	0.22	0/969	0.48	0/1300
12	AM	0.21	0/892	0.45	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AN	0.24	0/785	0.46	0/1043
13	CN	0.24	0/785	0.46	0/1043
14	AO	0.23	0/722	0.47	0/964
14	CO	0.23	0/722	0.47	0/964
15	AP	0.25	0/659	0.46	0/884
15	CP	0.25	0/648	0.46	0/870
16	AQ	0.23	0/657	0.47	0/881
16	CQ	0.24	0/666	0.47	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AR	0.23	0/462	0.45	0/621
17	CR	0.23	0/462	0.45	0/621
18	AS	0.25	0/652	0.46	0/877
18	CS	0.25	0/660	0.47	0/888
19	AT	0.24	0/671	0.40	0/888
19	CT	0.24	0/671	0.40	0/888
20	AB	0.25	0/1735	0.45	0/2338
20	CB	0.25	0/1735	0.45	0/2338
21	AU	0.26	0/430	0.48	0/570
21	CU	0.26	0/430	0.47	0/570
22	BA	0.55	6/2803 (0.2%)	0.83	7/4371 (0.2%)
22	DA	0.56	6/2803 (0.2%)	0.83	7/4371 (0.2%)
23	BB	0.31	8/68314 (0.0%)	0.79	41/106569 (0.0%)
23	DB	0.31	7/68314 (0.0%)	0.79	38/106569 (0.0%)
24	BI	0.24	0/1046	0.47	0/1410
24	DI	0.25	0/1046	0.48	0/1410
25	BC	0.22	0/2121	0.48	0/2852
25	DC	0.22	0/2121	0.48	0/2852
26	BD	0.24	0/1586	0.48	0/2134
26	DD	0.24	0/1586	0.48	0/2134
27	BK	0.24	0/939	0.55	0/1258
27	DK	0.24	0/939	0.55	0/1258
28	BP	0.24	0/929	0.51	0/1242
28	DP	0.24	0/929	0.51	0/1242
29	BE	0.24	0/1571	0.50	0/2113
29	DE	0.24	0/1571	0.50	0/2113
30	BY	0.23	0/453	0.49	0/605
30	DY	0.23	0/453	0.49	0/605
31	B0	0.22	0/450	0.55	0/599
31	D0	0.22	0/450	0.55	0/599
32	B4	0.23	0/303	0.47	0/397
32	D4	0.23	0/303	0.47	0/397
33	B1	0.27	0/416	0.49	0/554
33	D1	0.27	0/416	0.49	0/554
34	B3	0.24	0/513	0.48	0/676
34	D3	0.24	0/513	0.48	0/676
35	BV	0.25	0/766	0.43	0/1025
35	DV	0.25	0/766	0.42	0/1025
36	B2	0.26	0/380	0.46	0/498
36	D2	0.26	0/380	0.46	0/498
37	BL	0.24	0/1054	0.48	0/1403
37	DL	0.23	0/1054	0.48	0/1403
38	BM	0.25	0/1093	0.48	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DM	0.25	0/1093	0.48	0/1460
39	BX	0.24	0/510	0.54	0/677
39	DX	0.24	0/510	0.54	0/677
40	BH	0.25	0/1122	0.47	0/1515
40	DH	0.25	0/1122	0.49	0/1515
41	BJ	0.24	0/1152	0.48	0/1551
41	DJ	0.24	0/1152	0.48	0/1551
42	BN	0.24	0/973	0.52	0/1301
42	DN	0.24	0/973	0.52	0/1301
43	BO	0.23	0/902	0.48	0/1209
43	DO	0.23	0/902	0.48	0/1209
44	BQ	0.25	0/960	0.49	0/1278
44	DQ	0.25	0/960	0.49	0/1278
45	BS	0.22	0/864	0.52	0/1156
45	DS	0.22	0/864	0.52	0/1156
46	BU	0.25	0/787	0.47	0/1051
46	DU	0.25	0/787	0.47	0/1051
47	BF	0.26	0/1444	0.51	0/1937
47	DF	0.26	0/1444	0.52	0/1937
48	BG	0.23	0/1343	0.46	0/1816
48	DG	0.23	0/1343	0.46	0/1816
49	BR	0.25	0/829	0.48	0/1107
49	DR	0.25	0/829	0.48	0/1107
50	BT	0.23	0/744	0.55	0/994
50	DT	0.23	0/744	0.55	0/994
51	BZ	0.25	0/635	0.52	0/848
51	DZ	0.25	0/635	0.52	0/848
52	BW	0.28	0/603	0.51	0/797
52	DW	0.27	0/603	0.51	0/797
53	B6	0.23	0/1497	0.48	0/2017
53	D6	0.24	0/1497	0.47	0/2017
All	All	0.29	29/309354 (0.0%)	0.71	109/462003 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	14
1	CA	0	12
22	BA	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	DA	0	2
23	BB	0	50
23	DB	0	48
All	All	0	128

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-16.24	1.26	1.41
23	DB	1086	A	C5-C6	-16.14	1.26	1.41
22	DA	28	C	C2-O2	-14.83	1.11	1.24
22	BA	28	C	C2-O2	-14.74	1.11	1.24
23	DB	2276	G	O3'-P	-14.11	1.44	1.61

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-29.74	75.02	110.70
23	BB	2204	G	O5'-P-OP2	-28.61	76.37	110.70
23	BB	2791	G	O5'-P-OP1	-27.22	78.03	110.70
23	DB	2791	G	O5'-P-OP2	-26.58	78.80	110.70
23	BB	2791	G	O5'-P-OP2	18.87	133.34	110.70

There are no chirality outliers.

5 of 128 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	78	A	Sidechain
1	AA	86	G	Sidechain

## 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	32831	0	16521	1250	0
1	CA	32831	0	16521	1242	0
2	AC	1624	0	1699	139	0
2	CC	1624	0	1699	141	0
3	AD	1643	0	1710	173	0
3	CD	1643	0	1710	170	0
4	AE	1105	0	1148	99	0
4	CE	1105	0	1148	104	0
5	AF	817	0	808	83	0
5	CF	817	0	808	80	0
6	AG	1174	0	1230	115	0
6	CG	1196	0	1246	98	0
7	AH	979	0	1034	94	0
7	CH	979	0	1034	90	0
8	AI	1022	0	1070	142	0
8	CI	1022	0	1070	134	0
9	AJ	786	0	828	79	0
9	CJ	786	0	828	85	0
10	AK	877	0	887	108	0
10	CK	877	0	887	99	0
11	AL	955	0	1019	82	0
11	CL	955	0	1019	82	0
12	AM	883	0	944	105	0
12	CM	876	0	937	108	0
13	AN	774	0	827	113	0
13	CN	774	0	827	117	0
14	AO	714	0	734	47	0
14	CO	714	0	734	48	0
15	AP	649	0	666	51	0
15	CP	638	0	656	53	0
16	AQ	648	0	691	58	0
16	CQ	657	0	702	61	0
17	AR	455	0	478	45	0
17	CR	455	0	478	49	0
18	AS	637	0	665	89	0
18	CS	644	0	675	88	0
19	AT	665	0	714	58	0
19	CT	665	0	714	55	0
20	AB	1704	0	1732	189	0
20	CB	1704	0	1732	206	0
21	AU	425	0	449	77	0
21	CU	425	0	449	70	0
22	BA	2507	0	1270	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	2507	0	1270	119	1
23	BB	60995	0	30679	2401	0
23	DB	60995	0	30677	2528	1
24	BI	1032	0	1088	117	0
24	DI	1032	0	1088	185	0
25	BC	2082	0	2157	254	0
25	DC	2082	0	2157	253	0
26	BD	1565	0	1616	196	0
26	DD	1565	0	1616	200	0
27	BK	930	0	1000	107	0
27	DK	930	0	1000	114	0
28	BP	917	0	965	102	0
28	DP	917	0	965	99	0
29	BE	1552	0	1619	211	0
29	DE	1552	0	1619	196	0
30	BY	449	0	491	51	0
30	DY	449	0	491	51	0
31	B0	444	0	461	56	0
31	D0	444	0	461	53	0
32	B4	302	0	340	34	0
32	D4	302	0	341	40	0
33	B1	409	0	440	48	0
33	D1	409	0	440	44	0
34	B3	504	0	574	51	0
34	D3	504	0	574	52	0
35	BV	753	0	780	90	0
35	DV	753	0	780	101	0
36	B2	377	0	418	36	0
36	D2	377	0	418	38	0
37	BL	1045	0	1117	163	0
37	DL	1045	0	1117	163	0
38	BM	1074	0	1157	117	0
38	DM	1074	0	1157	121	0
39	BX	509	0	543	70	0
39	DX	509	0	543	66	0
40	BH	1111	0	1148	207	0
40	DH	1111	0	1148	144	0
41	BJ	1129	0	1162	144	0
41	DJ	1129	0	1162	146	0
42	BN	960	0	1000	123	0
42	DN	960	0	1000	121	0
43	BO	892	0	923	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DO	892	0	923	113	0
44	BQ	947	0	1022	156	0
44	DQ	947	0	1022	160	0
45	BS	857	0	922	106	0
45	DS	857	0	922	109	0
46	BU	779	0	834	117	0
46	DU	779	0	834	116	0
47	BF	1420	0	1460	236	0
47	DF	1420	0	1460	248	0
48	BG	1323	0	1374	200	0
48	DG	1323	0	1374	195	0
49	BR	816	0	839	124	0
49	DR	816	0	839	127	0
50	BT	738	0	807	120	0
50	DT	738	0	807	116	0
51	BZ	625	0	652	77	0
51	DZ	625	0	652	71	0
52	BW	596	0	610	124	0
52	DW	596	0	610	130	0
53	B6	1478	0	1526	187	0
53	D6	1478	0	1526	166	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	61	0	0	0	0
54	CE	1	0	0	0	0
54	DB	111	0	0	0	0
55	AA	42	0	45	3	0
55	BB	42	0	45	1	0
55	CA	42	0	45	2	0
55	DB	42	0	45	1	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	291	0	0	5	0
57	AL	3	0	0	0	0
57	AN	4	0	0	0	0
57	AT	2	0	0	0	0
57	BB	495	0	0	8	0
57	BC	6	0	0	0	0
57	BD	1	0	0	0	0
57	BE	2	0	0	0	0
57	BL	1	0	0	0	0
57	BT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	CA	296	0	0	1	0
57	CE	3	0	0	0	0
57	CL	4	0	0	0	0
57	CN	4	0	0	0	0
57	CP	1	0	0	0	0
57	CT	1	0	0	0	0
57	DB	502	0	0	15	0
57	DC	4	0	0	0	0
57	DD	1	0	0	0	0
57	DE	1	0	0	0	0
57	DL	2	0	0	0	0
57	DQ	1	0	0	0	0
57	DR	1	0	0	0	0
All	All	287128	0	193895	17520	1

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 37.

The worst 5 of 17520 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:DB:1099:G:H8	24:DI:3:LYS:N	1.37	1.19
49:DR:60:LYS:H	49:DR:100:GLY:HA3	1.08	1.15
40:BH:31:VAL:HB	40:BH:32:PRO:HD2	1.28	1.15
2:CC:126:ARG:HH22	2:CC:190:THR:HG23	1.09	1.14
50:DT:5:GLU:HA	50:DT:8:LEU:HB2	1.30	1.13

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:DA:53:A:OP1	23:DB:1592:C:O2'[1.655]	2.08	0.12

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	204/232 (88%)	150 (74%)	41 (20%)	13 (6%)	2	36
2	CC	204/232 (88%)	154 (76%)	36 (18%)	14 (7%)	2	33
3	AD	203/205 (99%)	151 (74%)	41 (20%)	11 (5%)	3	41
3	CD	203/205 (99%)	150 (74%)	41 (20%)	12 (6%)	2	38
4	AE	148/166 (89%)	113 (76%)	32 (22%)	3 (2%)	11	67
4	CE	148/166 (89%)	116 (78%)	28 (19%)	4 (3%)	8	60
5	AF	98/135 (73%)	66 (67%)	25 (26%)	7 (7%)	2	32
5	CF	98/135 (73%)	67 (68%)	24 (24%)	7 (7%)	2	32
6	AG	148/178 (83%)	121 (82%)	23 (16%)	4 (3%)	8	60
6	CG	150/178 (84%)	123 (82%)	23 (15%)	4 (3%)	8	60
7	AH	127/129 (98%)	96 (76%)	27 (21%)	4 (3%)	7	57
7	CH	127/129 (98%)	96 (76%)	28 (22%)	3 (2%)	9	63
8	AI	125/129 (97%)	96 (77%)	23 (18%)	6 (5%)	4	44
8	CI	125/129 (97%)	96 (77%)	22 (18%)	7 (6%)	3	40
9	AJ	96/103 (93%)	72 (75%)	16 (17%)	8 (8%)	1	27
9	CJ	96/103 (93%)	71 (74%)	17 (18%)	8 (8%)	1	27
10	AK	115/128 (90%)	86 (75%)	22 (19%)	7 (6%)	2	37
10	CK	115/128 (90%)	85 (74%)	23 (20%)	7 (6%)	2	37
11	AL	121/123 (98%)	76 (63%)	34 (28%)	11 (9%)	1	24
11	CL	121/123 (98%)	74 (61%)	36 (30%)	11 (9%)	1	24
12	AM	112/117 (96%)	77 (69%)	28 (25%)	7 (6%)	2	36
12	CM	111/117 (95%)	79 (71%)	25 (22%)	7 (6%)	2	36
13	AN	92/100 (92%)	58 (63%)	21 (23%)	13 (14%)	0	10
13	CN	92/100 (92%)	59 (64%)	21 (23%)	12 (13%)	0	13
14	AO	86/89 (97%)	66 (77%)	17 (20%)	3 (4%)	6	54
14	CO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	6	54
15	AP	80/82 (98%)	58 (72%)	18 (22%)	4 (5%)	3	43
15	CP	78/82 (95%)	56 (72%)	17 (22%)	5 (6%)	2	36
16	AQ	78/83 (94%)	58 (74%)	16 (20%)	4 (5%)	3	42
16	CQ	79/83 (95%)	59 (75%)	15 (19%)	5 (6%)	2	36
17	AR	53/74 (72%)	45 (85%)	8 (15%)	0	100	100
17	CR	53/74 (72%)	44 (83%)	9 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AS	77/91 (85%)	52 (68%)	24 (31%)	1 (1%)	18	75
18	CS	78/91 (86%)	53 (68%)	23 (30%)	2 (3%)	8	61
19	AT	83/86 (96%)	67 (81%)	13 (16%)	3 (4%)	5	53
19	CT	83/86 (96%)	67 (81%)	13 (16%)	3 (4%)	5	53
20	AB	216/240 (90%)	159 (74%)	36 (17%)	21 (10%)	1	21
20	CB	216/240 (90%)	156 (72%)	37 (17%)	23 (11%)	1	18
21	AU	49/70 (70%)	27 (55%)	14 (29%)	8 (16%)	0	7
21	CU	49/70 (70%)	26 (53%)	14 (29%)	9 (18%)	0	5
24	BI	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	5	53
24	DI	139/141 (99%)	114 (82%)	21 (15%)	4 (3%)	7	58
25	BC	269/272 (99%)	164 (61%)	63 (23%)	42 (16%)	0	8
25	DC	269/272 (99%)	161 (60%)	68 (25%)	40 (15%)	0	9
26	BD	207/209 (99%)	118 (57%)	55 (27%)	34 (16%)	0	7
26	DD	207/209 (99%)	115 (56%)	59 (28%)	33 (16%)	0	7
27	BK	119/123 (97%)	72 (60%)	30 (25%)	17 (14%)	0	10
27	DK	119/123 (97%)	71 (60%)	30 (25%)	18 (15%)	0	8
28	BP	112/114 (98%)	62 (55%)	37 (33%)	13 (12%)	1	15
28	DP	112/114 (98%)	63 (56%)	35 (31%)	14 (12%)	1	14
29	BE	199/201 (99%)	124 (62%)	56 (28%)	19 (10%)	1	22
29	DE	199/201 (99%)	121 (61%)	58 (29%)	20 (10%)	1	20
30	BY	56/58 (97%)	36 (64%)	15 (27%)	5 (9%)	1	24
30	DY	56/58 (97%)	37 (66%)	14 (25%)	5 (9%)	1	24
31	B0	54/56 (96%)	35 (65%)	13 (24%)	6 (11%)	1	17
31	D0	54/56 (96%)	36 (67%)	11 (20%)	7 (13%)	0	13
32	B4	36/38 (95%)	18 (50%)	11 (31%)	7 (19%)	0	4
32	D4	36/38 (95%)	18 (50%)	11 (31%)	7 (19%)	0	4
33	B1	48/54 (89%)	36 (75%)	7 (15%)	5 (10%)	1	18
33	D1	48/54 (89%)	36 (75%)	7 (15%)	5 (10%)	1	18
34	B3	62/64 (97%)	40 (64%)	16 (26%)	6 (10%)	1	21
34	D3	62/64 (97%)	41 (66%)	14 (23%)	7 (11%)	1	16
35	BV	92/94 (98%)	70 (76%)	16 (17%)	6 (6%)	2	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	DV	92/94 (98%)	69 (75%)	18 (20%)	5 (5%)	3	41
36	B2	44/46 (96%)	26 (59%)	15 (34%)	3 (7%)	2	33
36	D2	44/46 (96%)	26 (59%)	15 (34%)	3 (7%)	2	33
37	BL	141/144 (98%)	76 (54%)	42 (30%)	23 (16%)	0	7
37	DL	141/144 (98%)	76 (54%)	40 (28%)	25 (18%)	0	5
38	BM	134/136 (98%)	88 (66%)	31 (23%)	15 (11%)	1	16
38	DM	134/136 (98%)	89 (66%)	29 (22%)	16 (12%)	1	14
39	BX	61/63 (97%)	36 (59%)	18 (30%)	7 (12%)	1	15
39	DX	61/63 (97%)	37 (61%)	17 (28%)	7 (12%)	1	15
40	BH	147/149 (99%)	71 (48%)	49 (33%)	27 (18%)	0	5
40	DH	147/149 (99%)	96 (65%)	28 (19%)	23 (16%)	0	8
41	BJ	140/142 (99%)	89 (64%)	34 (24%)	17 (12%)	1	14
41	DJ	140/142 (99%)	88 (63%)	36 (26%)	16 (11%)	1	16
42	BN	118/127 (93%)	73 (62%)	34 (29%)	11 (9%)	1	23
42	DN	118/127 (93%)	71 (60%)	35 (30%)	12 (10%)	1	19
43	BO	114/117 (97%)	80 (70%)	25 (22%)	9 (8%)	1	28
43	DO	114/117 (97%)	79 (69%)	26 (23%)	9 (8%)	1	28
44	BQ	115/117 (98%)	70 (61%)	34 (30%)	11 (10%)	1	21
44	DQ	115/117 (98%)	69 (60%)	35 (30%)	11 (10%)	1	21
45	BS	108/110 (98%)	72 (67%)	22 (20%)	14 (13%)	0	13
45	DS	108/110 (98%)	70 (65%)	24 (22%)	14 (13%)	0	13
46	BU	100/103 (97%)	52 (52%)	28 (28%)	20 (20%)	0	4
46	DU	100/103 (97%)	50 (50%)	29 (29%)	21 (21%)	0	4
47	BF	176/178 (99%)	106 (60%)	43 (24%)	27 (15%)	0	8
47	DF	176/178 (99%)	107 (61%)	42 (24%)	27 (15%)	0	8
48	BG	174/176 (99%)	100 (58%)	49 (28%)	25 (14%)	0	10
48	DG	174/176 (99%)	99 (57%)	49 (28%)	26 (15%)	0	9
49	BR	101/103 (98%)	67 (66%)	21 (21%)	13 (13%)	0	13
49	DR	101/103 (98%)	68 (67%)	20 (20%)	13 (13%)	0	13
50	BT	91/100 (91%)	51 (56%)	26 (29%)	14 (15%)	0	8
50	DT	91/100 (91%)	50 (55%)	27 (30%)	14 (15%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	BZ	75/78 (96%)	51 (68%)	18 (24%)	6 (8%)	1	28
51	DZ	75/78 (96%)	51 (68%)	18 (24%)	6 (8%)	1	28
52	BW	77/84 (92%)	31 (40%)	21 (27%)	25 (32%)	0	0
52	DW	77/84 (92%)	31 (40%)	21 (27%)	25 (32%)	0	0
53	B6	183/185 (99%)	151 (82%)	25 (14%)	7 (4%)	5	51
53	D6	183/185 (99%)	132 (72%)	40 (22%)	11 (6%)	2	37
All	All	11607/12284 (94%)	7747 (67%)	2693 (23%)	1167 (10%)	1	20

5 of 1167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	54	ILE
2	AC	205	GLU
6	AG	6	ILE
8	AI	8	THR
9	AJ	36	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	170/189 (90%)	142 (84%)	28 (16%)	3	25
2	CC	170/189 (90%)	142 (84%)	28 (16%)	3	25
3	AD	172/172 (100%)	147 (86%)	25 (14%)	5	31
3	CD	172/172 (100%)	148 (86%)	24 (14%)	5	33
4	AE	113/125 (90%)	96 (85%)	17 (15%)	4	30
4	CE	113/125 (90%)	96 (85%)	17 (15%)	4	30
5	AF	87/116 (75%)	71 (82%)	16 (18%)	2	18
5	CF	87/116 (75%)	70 (80%)	17 (20%)	2	15
6	AG	123/146 (84%)	106 (86%)	17 (14%)	5	34
6	CG	125/146 (86%)	109 (87%)	16 (13%)	6	38
7	AH	104/104 (100%)	96 (92%)	8 (8%)	18	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	CH	104/104 (100%)	96 (92%)	8 (8%)	18	64
8	AI	105/106 (99%)	88 (84%)	17 (16%)	3	26
8	CI	105/106 (99%)	88 (84%)	17 (16%)	3	26
9	AJ	86/90 (96%)	73 (85%)	13 (15%)	4	29
9	CJ	86/90 (96%)	73 (85%)	13 (15%)	4	29
10	AK	90/98 (92%)	76 (84%)	14 (16%)	4	28
10	CK	90/98 (92%)	76 (84%)	14 (16%)	4	28
11	AL	103/103 (100%)	92 (89%)	11 (11%)	10	48
11	CL	103/103 (100%)	91 (88%)	12 (12%)	8	42
12	AM	92/95 (97%)	78 (85%)	14 (15%)	4	29
12	CM	91/95 (96%)	77 (85%)	14 (15%)	4	28
13	AN	79/83 (95%)	66 (84%)	13 (16%)	3	25
13	CN	79/83 (95%)	66 (84%)	13 (16%)	3	25
14	AO	76/77 (99%)	64 (84%)	12 (16%)	4	27
14	CO	76/77 (99%)	64 (84%)	12 (16%)	4	27
15	AP	65/65 (100%)	60 (92%)	5 (8%)	18	64
15	CP	65/65 (100%)	60 (92%)	5 (8%)	18	64
16	AQ	74/77 (96%)	66 (89%)	8 (11%)	9	47
16	CQ	75/77 (97%)	67 (89%)	8 (11%)	10	48
17	AR	48/64 (75%)	45 (94%)	3 (6%)	25	73
17	CR	48/64 (75%)	45 (94%)	3 (6%)	25	73
18	AS	70/78 (90%)	54 (77%)	16 (23%)	1	10
18	CS	71/78 (91%)	55 (78%)	16 (22%)	1	11
19	AT	65/65 (100%)	56 (86%)	9 (14%)	5	34
19	CT	65/65 (100%)	56 (86%)	9 (14%)	5	34
20	AB	180/198 (91%)	150 (83%)	30 (17%)	3	24
20	CB	180/198 (91%)	149 (83%)	31 (17%)	3	22
21	AU	44/60 (73%)	31 (70%)	13 (30%)	0	5
21	CU	44/60 (73%)	31 (70%)	13 (30%)	0	5
24	BI	109/109 (100%)	107 (98%)	2 (2%)	71	93
24	DI	109/109 (100%)	103 (94%)	6 (6%)	30	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	BC	216/217 (100%)	178 (82%)	38 (18%)	3	20
25	DC	216/217 (100%)	179 (83%)	37 (17%)	3	22
26	BD	164/164 (100%)	142 (87%)	22 (13%)	6	35
26	DD	164/164 (100%)	140 (85%)	24 (15%)	5	31
27	BK	102/104 (98%)	75 (74%)	27 (26%)	1	7
27	DK	102/104 (98%)	75 (74%)	27 (26%)	1	7
28	BP	99/99 (100%)	82 (83%)	17 (17%)	3	22
28	DP	99/99 (100%)	82 (83%)	17 (17%)	3	22
29	BE	165/165 (100%)	141 (86%)	24 (14%)	5	31
29	DE	165/165 (100%)	140 (85%)	25 (15%)	4	29
30	BY	48/48 (100%)	38 (79%)	10 (21%)	2	13
30	DY	48/48 (100%)	38 (79%)	10 (21%)	2	13
31	B0	47/47 (100%)	39 (83%)	8 (17%)	3	23
31	D0	47/47 (100%)	39 (83%)	8 (17%)	3	23
32	B4	34/34 (100%)	28 (82%)	6 (18%)	3	20
32	D4	34/34 (100%)	28 (82%)	6 (18%)	3	20
33	B1	45/48 (94%)	42 (93%)	3 (7%)	23	70
33	D1	45/48 (94%)	42 (93%)	3 (7%)	23	70
34	B3	51/51 (100%)	47 (92%)	4 (8%)	18	64
34	D3	51/51 (100%)	47 (92%)	4 (8%)	18	64
35	BV	78/78 (100%)	66 (85%)	12 (15%)	4	28
35	DV	78/78 (100%)	67 (86%)	11 (14%)	5	33
36	B2	38/38 (100%)	34 (90%)	4 (10%)	10	48
36	D2	38/38 (100%)	34 (90%)	4 (10%)	10	48
37	BL	102/103 (99%)	87 (85%)	15 (15%)	4	30
37	DL	102/103 (99%)	88 (86%)	14 (14%)	5	34
38	BM	109/109 (100%)	88 (81%)	21 (19%)	2	16
38	DM	109/109 (100%)	89 (82%)	20 (18%)	2	18
39	BX	55/55 (100%)	40 (73%)	15 (27%)	0	6
39	DX	55/55 (100%)	42 (76%)	13 (24%)	1	9
40	BH	114/114 (100%)	68 (60%)	46 (40%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	DH	114/114 (100%)	91 (80%)	23 (20%)	2	14
41	BJ	116/116 (100%)	99 (85%)	17 (15%)	4	30
41	DJ	116/116 (100%)	99 (85%)	17 (15%)	4	30
42	BN	100/103 (97%)	86 (86%)	14 (14%)	5	33
42	DN	100/103 (97%)	86 (86%)	14 (14%)	5	33
43	BO	86/87 (99%)	73 (85%)	13 (15%)	4	29
43	DO	86/87 (99%)	74 (86%)	12 (14%)	5	33
44	BQ	89/89 (100%)	76 (85%)	13 (15%)	5	31
44	DQ	89/89 (100%)	75 (84%)	14 (16%)	4	27
45	BS	93/93 (100%)	79 (85%)	14 (15%)	4	29
45	DS	93/93 (100%)	80 (86%)	13 (14%)	5	33
46	BU	83/84 (99%)	69 (83%)	14 (17%)	3	23
46	DU	83/84 (99%)	69 (83%)	14 (17%)	3	23
47	BF	149/149 (100%)	114 (76%)	35 (24%)	1	9
47	DF	149/149 (100%)	116 (78%)	33 (22%)	1	11
48	BG	137/137 (100%)	114 (83%)	23 (17%)	3	24
48	DG	137/137 (100%)	115 (84%)	22 (16%)	3	26
49	BR	84/84 (100%)	72 (86%)	12 (14%)	5	32
49	DR	84/84 (100%)	72 (86%)	12 (14%)	5	32
50	BT	80/84 (95%)	65 (81%)	15 (19%)	2	17
50	DT	80/84 (95%)	68 (85%)	12 (15%)	4	30
51	BZ	67/68 (98%)	53 (79%)	14 (21%)	1	13
51	DZ	67/68 (98%)	54 (81%)	13 (19%)	2	16
52	BW	59/62 (95%)	47 (80%)	12 (20%)	2	14
52	DW	59/62 (95%)	46 (78%)	13 (22%)	1	11
53	B6	157/157 (100%)	119 (76%)	38 (24%)	1	9
53	D6	157/157 (100%)	123 (78%)	34 (22%)	1	11
All	All	9647/10014 (96%)	8085 (84%)	1562 (16%)	3	26

5 of 1562 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	BR	4	VAL

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Mol	Chain	Res	Type
5	CF	61	LEU
47	DF	111	ARG
50	BT	50	LEU
53	B6	174	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 336 such sidechains are listed below:

Mol	Chain	Res	Type
49	BR	11	GLN
6	CG	67	ASN
46	DU	73	ASN
50	BT	91	GLN
2	CC	2	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	246 (16%)	16 (1%)
1	CA	1529/1542 (99%)	244 (15%)	16 (1%)
22	BA	116/120 (96%)	18 (15%)	0
22	DA	116/120 (96%)	18 (15%)	0
23	BB	2837/2904 (97%)	446 (15%)	14 (0%)
23	DB	2837/2904 (97%)	447 (15%)	16 (0%)
All	All	8964/9132 (98%)	1419 (15%)	62 (0%)

5 of 1419 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	14	U
1	AA	31	G
1	AA	32	A

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2832	U
1	CA	328	C
23	DB	2336	A

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Mol	Chain	Res	Type
1	CA	239	U
1	CA	372	C

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 349 ligands modelled in this entry, 345 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
55	PAR	AA	1661	-	45,45,45	1.70	10 (22%)	67,67,67	1.14	7 (10%)
55	PAR	BB	3111	-	45,45,45	1.79	11 (24%)	67,67,67	1.13	6 (8%)
55	PAR	CA	1662	-	45,45,45	1.79	11 (24%)	67,67,67	1.15	5 (7%)
55	PAR	DB	3112	-	45,45,45	1.83	12 (26%)	67,67,67	1.18	6 (8%)

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	PAR	AA	1661	-	-	0/18/94/94	0/4/4/4
55	PAR	BB	3111	-	-	0/18/94/94	0/4/4/4
55	PAR	CA	1662	-	-	0/18/94/94	0/4/4/4
55	PAR	DB	3112	-	-	0/18/94/94	0/4/4/4

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	CA	1662	PAR	O54-C14	4.65	1.53	1.41
55	BB	3111	PAR	O54-C14	4.52	1.53	1.41
55	DB	3112	PAR	O54-C14	4.50	1.53	1.41
55	AA	1661	PAR	O54-C14	4.42	1.53	1.41
55	CA	1662	PAR	C31-C21	4.38	1.59	1.53

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DB	3112	PAR	O52-C13-O43	3.58	115.04	111.57
55	DB	3112	PAR	O33-C14-C24	3.25	114.50	108.08
55	DB	3112	PAR	O54-C54-C64	3.18	112.02	105.97
55	AA	1661	PAR	O54-C54-C64	3.17	112.00	105.97
55	BB	3111	PAR	O33-C14-C24	3.11	114.23	108.08

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	1530/1542 (99%)	-0.13	20 (1%) 74 60	8, 88, 162, 180	0
1	CA	1530/1542 (99%)	-0.30	8 (0%) 88 79	5, 54, 146, 180	0
2	AC	206/232 (88%)	0.78	26 (12%) 4 7	9, 89, 158, 180	0
2	CC	206/232 (88%)	0.33	9 (4%) 33 29	9, 83, 141, 180	0
3	AD	205/205 (100%)	0.65	22 (10%) 6 10	5, 97, 172, 180	0
3	CD	205/205 (100%)	0.25	1 (0%) 88 79	5, 59, 151, 180	0
4	AE	150/166 (90%)	0.47	7 (4%) 30 27	5, 85, 159, 180	0
4	CE	150/166 (90%)	0.42	6 (4%) 36 32	5, 52, 137, 180	0
5	AF	100/135 (74%)	0.41	5 (5%) 28 26	8, 73, 146, 172	0
5	CF	100/135 (74%)	0.34	4 (4%) 36 32	5, 84, 153, 180	0
6	AG	150/178 (84%)	0.57	13 (8%) 10 14	10, 110, 170, 180	0
6	CG	152/178 (85%)	0.74	17 (11%) 6 10	28, 93, 162, 180	0
7	AH	129/129 (100%)	0.82	13 (10%) 7 12	15, 85, 159, 180	0
7	CH	129/129 (100%)	0.30	3 (2%) 57 45	5, 50, 128, 175	0
8	AI	127/129 (98%)	1.18	28 (22%) 1 3	5, 98, 163, 180	0
8	CI	127/129 (98%)	0.68	9 (7%) 16 18	5, 102, 180, 180	0
9	AJ	98/103 (95%)	0.80	13 (13%) 4 7	5, 105, 174, 180	0
9	CJ	98/103 (95%)	1.00	14 (14%) 3 6	10, 93, 158, 180	0
10	AK	117/128 (91%)	0.47	5 (4%) 34 30	9, 67, 129, 146	0
10	CK	117/128 (91%)	0.38	5 (4%) 34 30	5, 63, 134, 180	0
11	AL	123/123 (100%)	0.76	9 (7%) 15 17	19, 84, 158, 180	0
11	CL	123/123 (100%)	0.31	4 (3%) 44 37	5, 54, 113, 180	0
12	AM	114/117 (97%)	0.89	16 (14%) 3 6	55, 122, 180, 180	0
12	CM	113/117 (96%)	0.97	16 (14%) 3 6	31, 114, 180, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AN	96/100 (96%)	1.16	20 (20%) 1 3	5, 108, 170, 180	0
13	CN	96/100 (96%)	0.89	14 (14%) 3 6	6, 99, 162, 180	0
14	AO	88/89 (98%)	0.41	5 (5%) 23 23	7, 86, 156, 180	0
14	CO	88/89 (98%)	0.26	2 (2%) 57 45	5, 60, 132, 175	0
15	AP	82/82 (100%)	1.40	17 (20%) 1 3	35, 106, 173, 180	0
15	CP	80/82 (97%)	1.41	23 (28%) 1 3	5, 47, 142, 180	0
16	AQ	80/83 (96%)	1.18	19 (23%) 1 3	48, 104, 180, 180	0
16	CQ	81/83 (97%)	0.78	10 (12%) 5 8	5, 53, 140, 173	0
17	AR	55/74 (74%)	0.60	2 (3%) 41 35	5, 65, 143, 180	0
17	CR	55/74 (74%)	0.99	9 (16%) 2 5	13, 68, 130, 180	0
18	AS	79/91 (86%)	1.70	30 (37%) 1 2	55, 129, 180, 180	0
18	CS	80/91 (87%)	1.21	18 (22%) 1 3	46, 108, 180, 180	0
19	AT	85/86 (98%)	1.19	20 (23%) 1 3	44, 105, 154, 180	0
19	CT	85/86 (98%)	0.61	7 (8%) 12 15	5, 56, 117, 161	0
20	AB	218/240 (90%)	0.51	11 (5%) 28 26	7, 105, 171, 180	0
20	CB	218/240 (90%)	1.03	38 (17%) 2 4	23, 111, 172, 180	0
21	AU	51/70 (72%)	0.91	9 (17%) 2 4	23, 104, 180, 180	0
21	CU	51/70 (72%)	0.72	7 (13%) 4 6	24, 96, 173, 180	0
22	BA	117/120 (97%)	-0.36	1 (0%) 81 69	37, 82, 145, 178	0
22	DA	117/120 (97%)	-0.13	3 (2%) 53 43	18, 84, 143, 180	0
23	BB	2841/2904 (97%)	-0.23	32 (1%) 77 63	6, 58, 150, 180	0
23	DB	2841/2904 (97%)	-0.31	14 (0%) 88 79	5, 38, 149, 180	0
24	BI	141/141 (100%)	2.04	60 (42%) 1 2	63, 161, 180, 180	0
24	DI	141/141 (100%)	1.47	37 (26%) 1 3	65, 157, 180, 180	0
25	BC	271/272 (99%)	0.45	9 (3%) 44 37	5, 48, 108, 166	0
25	DC	271/272 (99%)	0.39	8 (2%) 48 39	5, 30, 102, 180	0
26	BD	209/209 (100%)	0.70	16 (7%) 13 16	5, 79, 148, 180	0
26	DD	209/209 (100%)	0.34	3 (1%) 72 58	5, 51, 123, 180	0
27	BK	121/123 (98%)	0.91	15 (12%) 5 8	5, 74, 149, 180	0
27	DK	121/123 (98%)	0.65	2 (1%) 67 54	5, 33, 106, 180	0
28	BP	114/114 (100%)	0.74	14 (12%) 5 8	18, 89, 153, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
28	DP	114/114 (100%)	0.51	3 (2%)	53	43	5, 48, 124, 180	0
29	BE	201/201 (100%)	0.50	9 (4%)	32	29	5, 67, 146, 180	0
29	DE	201/201 (100%)	0.38	6 (2%)	48	39	5, 67, 142, 177	0
30	BY	58/58 (100%)	0.89	7 (12%)	5	8	18, 82, 151, 171	0
30	DY	58/58 (100%)	0.66	3 (5%)	26	25	5, 68, 126, 162	0
31	B0	56/56 (100%)	0.58	3 (5%)	25	23	5, 73, 153, 164	0
31	D0	56/56 (100%)	0.53	6 (10%)	6	10	5, 56, 147, 180	0
32	B4	38/38 (100%)	3.03	26 (68%)	0	2	45, 115, 169, 180	0
32	D4	38/38 (100%)	3.60	34 (89%)	0	1	36, 110, 169, 180	0
33	B1	50/54 (92%)	1.19	8 (16%)	3	5	22, 95, 157, 180	0
33	D1	50/54 (92%)	1.32	12 (24%)	1	3	19, 73, 122, 161	0
34	B3	64/64 (100%)	0.81	5 (7%)	13	16	20, 63, 125, 145	0
34	D3	64/64 (100%)	0.67	5 (7%)	13	16	5, 35, 88, 129	0
35	BV	94/94 (100%)	0.61	6 (6%)	19	21	24, 96, 156, 180	0
35	DV	94/94 (100%)	0.85	17 (18%)	2	4	11, 93, 151, 180	0
36	B2	46/46 (100%)	0.46	2 (4%)	34	30	5, 75, 137, 180	0
36	D2	46/46 (100%)	0.40	0	100	100	5, 44, 101, 180	0
37	BL	143/144 (99%)	0.61	6 (4%)	35	30	5, 71, 133, 180	0
37	DL	143/144 (99%)	0.39	3 (2%)	60	48	5, 51, 116, 180	0
38	BM	136/136 (100%)	1.01	26 (19%)	2	4	9, 70, 149, 180	0
38	DM	136/136 (100%)	0.68	6 (4%)	33	29	5, 50, 131, 176	0
39	BX	63/63 (100%)	0.75	6 (9%)	8	13	7, 84, 165, 180	0
39	DX	63/63 (100%)	0.53	3 (4%)	29	27	47, 108, 173, 180	0
40	BH	149/149 (100%)	0.94	17 (11%)	6	9	5, 130, 180, 180	0
40	DH	149/149 (100%)	0.90	18 (12%)	5	8	12, 97, 172, 180	0
41	BJ	142/142 (100%)	0.70	15 (10%)	7	11	6, 81, 147, 180	0
41	DJ	142/142 (100%)	0.60	9 (6%)	19	21	5, 58, 135, 180	0
42	BN	120/127 (94%)	0.55	7 (5%)	22	22	5, 68, 139, 178	0
42	DN	120/127 (94%)	0.32	2 (1%)	67	54	5, 38, 101, 180	0
43	BO	116/117 (99%)	1.21	29 (25%)	1	3	21, 91, 147, 180	0
43	DO	116/117 (99%)	1.16	25 (21%)	1	3	8, 86, 164, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BQ	117/117 (100%)	0.39	5 (4%) 34 30	5, 66, 135, 176	0
44	DQ	117/117 (100%)	0.36	3 (2%) 53 43	5, 48, 134, 180	0
45	BS	110/110 (100%)	0.84	8 (7%) 15 17	6, 58, 139, 180	0
45	DS	110/110 (100%)	0.50	2 (1%) 65 52	5, 50, 121, 180	0
46	BU	102/103 (99%)	1.04	21 (20%) 1 3	5, 89, 144, 180	0
46	DU	102/103 (99%)	0.97	15 (14%) 3 6	24, 99, 159, 180	0
47	BF	178/178 (100%)	0.66	17 (9%) 8 12	36, 111, 174, 180	0
47	DF	178/178 (100%)	0.68	15 (8%) 11 15	8, 103, 177, 180	0
48	BG	176/176 (100%)	0.92	20 (11%) 6 9	9, 114, 179, 180	0
48	DG	176/176 (100%)	1.03	24 (13%) 4 7	15, 91, 167, 180	0
49	BR	103/103 (100%)	1.29	26 (25%) 1 3	16, 93, 157, 180	0
49	DR	103/103 (100%)	0.96	12 (11%) 5 9	5, 88, 145, 180	0
50	BT	93/100 (93%)	1.02	20 (21%) 1 3	5, 88, 180, 180	0
50	DT	93/100 (93%)	1.01	16 (17%) 2 4	7, 90, 180, 180	0
51	BZ	77/78 (98%)	0.77	6 (7%) 13 16	5, 52, 127, 154	0
51	DZ	77/78 (98%)	0.89	7 (9%) 9 14	5, 43, 95, 135	0
52	BW	79/84 (94%)	0.82	9 (11%) 6 9	10, 85, 145, 179	0
52	DW	79/84 (94%)	0.96	6 (7%) 14 16	5, 66, 152, 180	0
53	B6	185/185 (100%)	1.22	49 (26%) 1 3	5, 125, 180, 180	0
53	D6	185/185 (100%)	0.70	22 (11%) 5 9	5, 90, 180, 180	0
All	All	20787/21416 (97%)	0.32	1375 (6%) 18 20	5, 70, 162, 180	0

The worst 5 of 1375 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	BI	2	LYS	10.9
24	BI	5	GLN	10.3
32	D4	35	GLN	9.4
24	BI	1	ALA	8.9
23	BB	2147	A	8.6

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
54	MG	CA	1623	1/1	0.61	108.00	180,180,180,180	0
54	MG	AA	1657	1/1	1.39	61.65	155,155,155,155	0
54	MG	AA	1626	1/1	0.81	45.62	28,28,28,28	1
54	MG	BB	3057	1/1	0.47	43.00	65,65,65,65	0
54	MG	AA	1619	1/1	1.30	33.94	180,180,180,180	0
54	MG	CA	1657	1/1	0.48	31.19	97,97,97,97	0
54	MG	AA	1658	1/1	0.19	29.67	97,97,97,97	0
54	MG	AA	1647	1/1	0.92	27.19	180,180,180,180	0
54	MG	AA	1637	1/1	1.05	22.34	146,146,146,146	0
54	MG	CE	201	1/1	0.80	17.42	145,145,145,145	0
54	MG	DB	3036	1/1	0.45	14.83	51,51,51,51	0
54	MG	AA	1623	1/1	0.67	14.63	33,33,33,33	1
54	MG	CA	1615	1/1	0.26	14.22	180,180,180,180	0
54	MG	CA	1658	1/1	0.34	11.40	70,70,70,70	0
54	MG	CA	1628	1/1	0.32	10.92	82,82,82,82	0
54	MG	CA	1608	1/1	0.53	10.71	178,178,178,178	0
54	MG	CA	1627	1/1	0.36	10.42	35,35,35,35	1
54	MG	CA	1641	1/1	0.27	9.47	76,76,76,76	0
54	MG	DB	3083	1/1	0.38	9.21	72,72,72,72	0
54	MG	DB	3086	1/1	0.23	8.82	25,25,25,25	0
54	MG	AA	1621	1/1	0.31	8.71	27,27,27,27	0
54	MG	DB	3058	1/1	0.50	8.12	157,157,157,157	0
54	MG	DB	3028	1/1	0.28	7.54	33,33,33,33	0
54	MG	BB	3108	1/1	0.33	6.81	88,88,88,88	0
54	MG	AA	1639	1/1	2.26	6.72	126,126,126,126	0
54	MG	DB	3065	1/1	0.21	6.37	68,68,68,68	0
55	PAR	BB	3111	42/42	0.40	6.27	100,100,100,100	42
54	MG	BB	3047	1/1	0.24	5.97	92,92,92,92	0
54	MG	AA	1633	1/1	0.42	5.85	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	AA	1608	1/1	0.43	5.85	136,136,136,136	0
54	MG	BB	3036	1/1	0.30	5.77	68,68,68,68	0
54	MG	CA	1620	1/1	0.23	5.73	104,104,104,104	0
54	MG	DB	3052	1/1	0.28	5.70	166,166,166,166	0
55	PAR	DB	3112	42/42	0.39	5.57	55,55,55,55	42
54	MG	AA	1632	1/1	0.45	5.57	80,80,80,80	0
54	MG	AA	1617	1/1	0.25	5.34	138,138,138,138	0
54	MG	BB	3020	1/1	0.37	5.31	23,23,23,23	0
54	MG	BB	3064	1/1	0.24	5.10	78,78,78,78	0
54	MG	BB	3097	1/1	0.24	5.08	95,95,95,95	0
54	MG	BB	3080	1/1	0.32	4.89	131,131,131,131	0
54	MG	CA	1621	1/1	0.34	4.66	67,67,67,67	0
54	MG	AA	1627	1/1	0.22	4.10	46,46,46,46	0
54	MG	AA	1622	1/1	0.27	4.09	111,111,111,111	0
54	MG	AA	1659	1/1	0.59	3.93	127,127,127,127	0
54	MG	DB	3030	1/1	0.25	3.91	30,30,30,30	0
54	MG	AA	1652	1/1	0.25	3.79	126,126,126,126	0
54	MG	AA	1656	1/1	0.23	3.71	50,50,50,50	0
54	MG	BB	3051	1/1	0.26	3.54	75,75,75,75	0
54	MG	BB	3033	1/1	0.18	3.50	125,125,125,125	0
54	MG	BB	3093	1/1	0.31	3.39	98,98,98,98	0
54	MG	BB	3028	1/1	0.24	3.19	95,95,95,95	0
54	MG	BB	3018	1/1	0.26	2.99	32,32,32,32	0
54	MG	BB	3078	1/1	0.26	2.96	92,92,92,92	0
54	MG	DB	3108	1/1	0.33	2.84	13,13,13,13	0
54	MG	AA	1651	1/1	0.22	2.79	55,55,55,55	0
54	MG	DB	3068	1/1	0.26	2.70	16,16,16,16	0
54	MG	BB	3055	1/1	0.25	2.67	78,78,78,78	0
54	MG	AA	1624	1/1	0.30	2.57	76,76,76,76	0
54	MG	DB	3101	1/1	0.28	2.46	7,7,7,7	0
54	MG	CA	1626	1/1	0.22	2.41	23,23,23,23	1
54	MG	CA	1646	1/1	0.23	2.32	78,78,78,78	0
54	MG	AA	1614	1/1	0.24	2.31	131,131,131,131	0
54	MG	AA	1625	1/1	0.20	2.29	144,144,144,144	1
54	MG	CA	1625	1/1	0.18	2.25	46,46,46,46	0
54	MG	BB	3017	1/1	0.20	2.25	46,46,46,46	0
54	MG	BB	3100	1/1	0.21	2.03	109,109,109,109	0
54	MG	DB	3111	1/1	0.26	2.01	68,68,68,68	0
54	MG	BB	3059	1/1	0.26	2.01	39,39,39,39	0
54	MG	CA	1629	1/1	0.28	1.96	96,96,96,96	1
54	MG	AA	1650	1/1	0.16	1.92	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	CA	1632	1/1	0.23	1.82	34,34,34,34	0
54	MG	CA	1636	1/1	0.33	1.64	90,90,90,90	0
54	MG	DB	3066	1/1	0.13	1.60	123,123,123,123	0
54	MG	DB	3013	1/1	0.21	1.56	35,35,35,35	0
54	MG	DB	3004	1/1	0.25	1.51	40,40,40,40	0
54	MG	BB	3075	1/1	0.21	1.49	55,55,55,55	0
54	MG	BB	3082	1/1	0.31	1.44	22,22,22,22	0
54	MG	BB	3013	1/1	0.19	1.40	86,86,86,86	0
54	MG	DB	3061	1/1	0.16	1.37	95,95,95,95	0
54	MG	AA	1610	1/1	0.29	1.34	82,82,82,82	0
54	MG	AA	1612	1/1	0.20	1.28	96,96,96,96	0
54	MG	CA	1649	1/1	0.33	1.20	134,134,134,134	0
54	MG	BB	3048	1/1	0.28	1.17	8,8,8,8	0
54	MG	DB	3089	1/1	0.23	1.15	75,75,75,75	0
55	PAR	AA	1661	42/42	0.29	1.12	62,62,62,62	0
54	MG	BB	3003	1/1	0.16	0.87	60,60,60,60	0
54	MG	CA	1652	1/1	0.26	0.83	58,58,58,58	0
54	MG	BB	3011	1/1	0.20	0.77	68,68,68,68	0
54	MG	CA	1651	1/1	0.17	0.64	37,37,37,37	0
54	MG	AA	1615	1/1	0.36	0.57	171,171,171,171	0
54	MG	CA	1624	1/1	0.13	0.54	48,48,48,48	0
54	MG	CA	1634	1/1	0.15	0.53	30,30,30,30	0
54	MG	DB	3011	1/1	0.16	0.52	22,22,22,22	0
54	MG	BB	3037	1/1	0.19	0.37	63,63,63,63	0
54	MG	DB	3046	1/1	0.15	0.36	38,38,38,38	0
54	MG	CA	1614	1/1	0.32	0.36	85,85,85,85	0
54	MG	BB	3038	1/1	0.14	0.32	157,157,157,157	0
54	MG	DB	3032	1/1	0.18	0.28	21,21,21,21	0
54	MG	AA	1636	1/1	0.18	0.27	38,38,38,38	0
54	MG	DB	3085	1/1	0.21	0.26	49,49,49,49	0
54	MG	AA	1635	1/1	0.19	0.21	120,120,120,120	0
54	MG	CA	1603	1/1	0.17	0.18	37,37,37,37	0
54	MG	DB	3096	1/1	0.16	0.16	37,37,37,37	0
54	MG	BB	3019	1/1	0.17	0.16	56,56,56,56	0
54	MG	BB	3014	1/1	0.15	0.16	46,46,46,46	0
55	PAR	CA	1662	42/42	0.21	0.12	45,45,45,45	0
54	MG	CA	1633	1/1	0.19	0.11	106,106,106,106	0
54	MG	BB	3071	1/1	0.19	0.09	63,63,63,63	0
54	MG	BB	3012	1/1	0.20	0.08	71,71,71,71	0
54	MG	CA	1613	1/1	0.18	0.02	24,24,24,24	0
54	MG	DB	3048	1/1	0.14	-0.00	8,8,8,8	0
54	MG	DB	3074	1/1	0.17	-0.01	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BB	3101	1/1	0.23	-0.07	64,64,64,64	0
54	MG	DB	3087	1/1	0.18	-0.08	67,67,67,67	0
54	MG	DB	3022	1/1	0.15	-0.09	85,85,85,85	0
54	MG	DB	3027	1/1	0.20	-0.09	11,11,11,11	0
54	MG	BB	3087	1/1	0.18	-0.14	102,102,102,102	0
54	MG	CA	1616	1/1	0.27	-0.16	94,94,94,94	0
54	MG	DB	3090	1/1	0.20	-0.19	35,35,35,35	0
54	MG	BB	3098	1/1	0.15	-0.19	10,10,10,10	0
54	MG	CA	1605	1/1	0.20	-0.26	5,5,5,5	0
54	MG	DB	3037	1/1	0.12	-0.29	45,45,45,45	0
54	MG	AA	1607	1/1	0.23	-0.30	35,35,35,35	0
54	MG	DB	3008	1/1	0.19	-0.33	11,11,11,11	0
54	MG	CA	1619	1/1	0.21	-0.34	78,78,78,78	0
54	MG	DB	3003	1/1	0.19	-0.36	5,5,5,5	0
54	MG	CA	1654	1/1	0.14	-0.37	72,72,72,72	0
54	MG	DB	3018	1/1	0.17	-0.40	17,17,17,17	0
54	MG	BB	3105	1/1	0.15	-0.42	21,21,21,21	0
54	MG	CA	1647	1/1	0.14	-0.42	58,58,58,58	0
54	MG	DB	3014	1/1	0.18	-0.42	39,39,39,39	0
54	MG	DB	3099	1/1	0.17	-0.43	21,21,21,21	0
54	MG	BB	3049	1/1	0.17	-0.44	25,25,25,25	0
54	MG	DB	3102	1/1	0.21	-0.46	20,20,20,20	0
54	MG	DB	3059	1/1	0.13	-0.46	152,152,152,152	0
54	MG	DB	3049	1/1	0.16	-0.49	11,11,11,11	0
54	MG	CA	1661	1/1	0.11	-0.49	40,40,40,40	0
54	MG	DB	3060	1/1	0.13	-0.50	160,160,160,160	0
54	MG	BB	3027	1/1	0.14	-0.51	83,83,83,83	0
54	MG	CA	1622	1/1	0.14	-0.52	38,38,38,38	0
54	MG	AA	1628	1/1	0.18	-0.53	49,49,49,49	0
54	MG	CA	1659	1/1	0.11	-0.55	70,70,70,70	0
54	MG	AA	1655	1/1	0.20	-0.59	83,83,83,83	0
54	MG	BB	3041	1/1	0.14	-0.62	15,15,15,15	0
54	MG	DB	3094	1/1	0.11	-0.62	81,81,81,81	0
54	MG	BB	3021	1/1	0.11	-0.66	62,62,62,62	0
54	MG	BB	3077	1/1	0.17	-0.68	64,64,64,64	0
54	MG	CA	1639	1/1	0.16	-0.69	5,5,5,5	0
54	MG	DB	3110	1/1	0.14	-0.70	44,44,44,44	0
54	MG	AA	1640	1/1	0.10	-0.71	77,77,77,77	0
54	MG	BB	3009	1/1	0.11	-0.72	76,76,76,76	0
54	MG	DB	3075	1/1	0.14	-0.72	10,10,10,10	0
54	MG	DB	3026	1/1	0.19	-0.72	54,54,54,54	0
54	MG	BB	3043	1/1	0.15	-0.75	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1642	1/1	0.15	-0.75	63,63,63,63	0
54	MG	DB	3073	1/1	0.13	-0.76	25,25,25,25	0
54	MG	AA	1649	1/1	0.11	-0.78	93,93,93,93	0
54	MG	DB	3079	1/1	0.15	-0.79	30,30,30,30	0
54	MG	DB	3109	1/1	0.17	-0.79	27,27,27,27	0
54	MG	AA	1602	1/1	0.17	-0.80	105,105,105,105	0
54	MG	DB	3050	1/1	0.12	-0.83	118,118,118,118	0
54	MG	DB	3023	1/1	0.10	-0.85	35,35,35,35	0
54	MG	DB	3100	1/1	0.16	-0.86	22,22,22,22	0
54	MG	BB	3083	1/1	0.17	-0.89	51,51,51,51	0
54	MG	CA	1637	1/1	0.13	-0.90	116,116,116,116	0
54	MG	DB	3007	1/1	0.16	-0.91	27,27,27,27	0
54	MG	CA	1642	1/1	0.09	-0.92	85,85,85,85	0
54	MG	BB	3026	1/1	0.14	-0.93	44,44,44,44	0
54	MG	BB	3023	1/1	0.13	-0.94	6,6,6,6	0
54	MG	CA	1612	1/1	0.12	-0.96	97,97,97,97	0
54	MG	AA	1613	1/1	0.19	-0.96	82,82,82,82	0
54	MG	BB	3029	1/1	0.11	-0.96	12,12,12,12	0
54	MG	CA	1606	1/1	0.19	-1.04	103,103,103,103	0
54	MG	BB	3104	1/1	0.16	-1.04	43,43,43,43	0
54	MG	BB	3034	1/1	0.14	-1.05	41,41,41,41	0
54	MG	BB	3092	1/1	0.08	-1.05	60,60,60,60	0
54	MG	DB	3051	1/1	0.14	-1.06	20,20,20,20	0
54	MG	DB	3015	1/1	0.10	-1.07	39,39,39,39	0
54	MG	BB	3001	1/1	0.10	-1.07	14,14,14,14	0
54	MG	DB	3045	1/1	0.12	-1.10	108,108,108,108	0
54	MG	BB	3099	1/1	0.10	-1.11	40,40,40,40	0
54	MG	CA	1653	1/1	0.05	-1.13	43,43,43,43	0
54	MG	BB	3062	1/1	0.16	-1.13	5,5,5,5	0
54	MG	BB	3065	1/1	0.14	-1.13	30,30,30,30	0
54	MG	CA	1660	1/1	0.12	-1.16	58,58,58,58	0
54	MG	BB	3046	1/1	0.20	-1.19	64,64,64,64	0
54	MG	BB	3006	1/1	0.08	-1.19	37,37,37,37	0
54	MG	CA	1602	1/1	0.17	-1.23	16,16,16,16	0
54	MG	BB	3109	1/1	0.11	-1.23	49,49,49,49	0
54	MG	AA	1603	1/1	0.17	-1.23	38,38,38,38	0
54	MG	BB	3040	1/1	0.12	-1.23	47,47,47,47	0
54	MG	BB	3106	1/1	0.13	-1.24	45,45,45,45	0
54	MG	BB	3039	1/1	0.12	-1.25	12,12,12,12	0
54	MG	BB	3096	1/1	0.16	-1.28	69,69,69,69	0
54	MG	DB	3097	1/1	0.15	-1.28	32,32,32,32	0
54	MG	DB	3024	1/1	0.18	-1.29	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DB	3010	1/1	0.15	-1.29	5,5,5,5	0
54	MG	DB	3019	1/1	0.15	-1.29	8,8,8,8	0
54	MG	BB	3090	1/1	0.13	-1.33	115,115,115,115	0
54	MG	CA	1617	1/1	0.10	-1.33	12,12,12,12	0
54	MG	BB	3067	1/1	0.11	-1.34	25,25,25,25	0
54	MG	DB	3025	1/1	0.10	-1.34	18,18,18,18	0
54	MG	AA	1648	1/1	0.10	-1.36	5,5,5,5	0
54	MG	BB	3005	1/1	0.11	-1.44	9,9,9,9	0
54	MG	DB	3035	1/1	0.13	-1.45	52,52,52,52	0
54	MG	BB	3079	1/1	0.17	-1.48	43,43,43,43	0
54	MG	AA	1660	1/1	0.12	-1.48	75,75,75,75	0
54	MG	BB	3025	1/1	0.11	-1.49	22,22,22,22	0
54	MG	DB	3078	1/1	0.08	-1.51	31,31,31,31	0
54	MG	DB	3106	1/1	0.12	-1.53	17,17,17,17	0
54	MG	BB	3060	1/1	0.15	-1.53	43,43,43,43	0
54	MG	BB	3053	1/1	0.11	-1.53	38,38,38,38	0
54	MG	DB	3069	1/1	0.18	-1.54	5,5,5,5	0
54	MG	BB	3094	1/1	0.12	-1.55	55,55,55,55	0
54	MG	BB	3008	1/1	0.16	-1.56	81,81,81,81	0
54	MG	DB	3064	1/1	0.12	-1.56	23,23,23,23	0
54	MG	CA	1643	1/1	0.13	-1.57	11,11,11,11	0
54	MG	BB	3042	1/1	0.07	-1.59	100,100,100,100	0
54	MG	CA	1618	1/1	0.12	-1.66	23,23,23,23	0
54	MG	DB	3088	1/1	0.14	-1.67	31,31,31,31	0
54	MG	AA	1645	1/1	0.12	-1.69	138,138,138,138	0
54	MG	DB	3055	1/1	0.14	-1.71	26,26,26,26	0
54	MG	BB	3007	1/1	0.15	-1.73	103,103,103,103	0
54	MG	BB	3110	1/1	0.15	-1.73	41,41,41,41	0
54	MG	AA	1611	1/1	0.09	-1.78	75,75,75,75	0
54	MG	CA	1650	1/1	0.05	-1.86	5,5,5,5	0
54	MG	AA	1638	1/1	0.15	-1.87	45,45,45,45	0
54	MG	DB	3095	1/1	0.13	-1.89	62,62,62,62	0
56	ZN	B4	101	1/1	0.23	-1.91	68,68,68,68	0
54	MG	CA	1644	1/1	0.12	-1.92	69,69,69,69	0
54	MG	CA	1604	1/1	0.10	-1.93	11,11,11,11	0
54	MG	CA	1630	1/1	0.12	-1.93	65,65,65,65	0
54	MG	BB	3010	1/1	0.11	-1.95	38,38,38,38	0
54	MG	DB	3084	1/1	0.16	-1.95	14,14,14,14	0
54	MG	BB	3086	1/1	0.11	-1.96	5,5,5,5	0
54	MG	DB	3047	1/1	0.16	-1.96	31,31,31,31	0
54	MG	AA	1618	1/1	0.06	-1.96	105,105,105,105	0
54	MG	CA	1638	1/1	0.10	-1.99	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BB	3052	1/1	0.10	-2.04	59,59,59,59	0
54	MG	BB	3004	1/1	0.19	-2.06	44,44,44,44	0
54	MG	BB	3024	1/1	0.07	-2.07	76,76,76,76	0
54	MG	BB	3002	1/1	0.10	-2.09	18,18,18,18	0
54	MG	CA	1607	1/1	0.05	-2.10	20,20,20,20	0
54	MG	DB	3063	1/1	0.08	-2.10	23,23,23,23	0
54	MG	DB	3005	1/1	0.12	-2.11	52,52,52,52	0
54	MG	BB	3045	1/1	0.09	-2.12	32,32,32,32	0
54	MG	BB	3091	1/1	0.10	-2.14	81,81,81,81	0
54	MG	AA	1634	1/1	0.11	-2.17	79,79,79,79	0
56	ZN	D4	101	1/1	0.44	-2.17	96,96,96,96	0
54	MG	DB	3057	1/1	0.05	-2.20	17,17,17,17	0
54	MG	AA	1644	1/1	0.09	-2.20	69,69,69,69	0
54	MG	DB	3040	1/1	0.12	-2.34	5,5,5,5	0
54	MG	DB	3098	1/1	0.11	-2.36	69,69,69,69	0
54	MG	CA	1610	1/1	0.09	-2.38	65,65,65,65	0
54	MG	DB	3033	1/1	0.22	-2.39	20,20,20,20	0
54	MG	AA	1653	1/1	0.08	-2.39	51,51,51,51	0
54	MG	DB	3104	1/1	0.13	-2.41	21,21,21,21	0
54	MG	BB	3031	1/1	0.14	-2.41	44,44,44,44	0
54	MG	DB	3043	1/1	0.12	-2.45	7,7,7,7	0
54	MG	AA	1601	1/1	0.12	-2.45	10,10,10,10	0
54	MG	DB	3105	1/1	0.07	-2.45	24,24,24,24	0
54	MG	DB	3092	1/1	0.10	-2.45	60,60,60,60	0
54	MG	BB	3068	1/1	0.16	-2.48	102,102,102,102	0
54	MG	AA	1630	1/1	0.11	-2.49	118,118,118,118	0
54	MG	CA	1601	1/1	0.13	-2.52	9,9,9,9	0
54	MG	AA	1654	1/1	0.08	-2.53	52,52,52,52	0
54	MG	BB	3072	1/1	0.12	-2.53	64,64,64,64	0
54	MG	DB	3093	1/1	0.14	-2.53	9,9,9,9	0
54	MG	DB	3076	1/1	0.12	-2.61	27,27,27,27	0
54	MG	BB	3081	1/1	0.15	-2.61	31,31,31,31	0
54	MG	AA	1609	1/1	0.08	-2.63	11,11,11,11	0
54	MG	BB	3073	1/1	0.12	-2.68	70,70,70,70	0
54	MG	BB	3107	1/1	0.06	-2.68	13,13,13,13	0
54	MG	DB	3012	1/1	0.13	-2.68	8,8,8,8	0
54	MG	AA	1616	1/1	0.08	-2.75	15,15,15,15	0
54	MG	DB	3053	1/1	0.11	-2.77	65,65,65,65	0
54	MG	DB	3067	1/1	0.14	-2.78	13,13,13,13	0
54	MG	CA	1656	1/1	0.05	-2.83	7,7,7,7	0
54	MG	BB	3070	1/1	0.12	-2.86	40,40,40,40	0
54	MG	DB	3002	1/1	0.10	-2.88	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BB	3016	1/1	0.10	-2.89	94,94,94,94	0
54	MG	DB	3001	1/1	0.10	-2.92	5,5,5,5	0
54	MG	BB	3054	1/1	0.08	-2.95	55,55,55,55	0
54	MG	AA	1631	1/1	0.07	-2.98	61,61,61,61	0
54	MG	DB	3091	1/1	0.10	-3.01	11,11,11,11	0
54	MG	BB	3061	1/1	0.09	-3.02	46,46,46,46	0
54	MG	DB	3016	1/1	0.11	-3.03	5,5,5,5	0
54	MG	DB	3103	1/1	0.09	-3.04	37,37,37,37	0
54	MG	BB	3085	1/1	0.11	-3.05	76,76,76,76	0
54	MG	BB	3088	1/1	0.06	-3.05	11,11,11,11	0
54	MG	DB	3021	1/1	0.14	-3.09	18,18,18,18	0
54	MG	BB	3035	1/1	0.15	-3.10	60,60,60,60	0
54	MG	DB	3070	1/1	0.09	-3.12	28,28,28,28	0
54	MG	DB	3042	1/1	0.07	-3.16	36,36,36,36	0
54	MG	DB	3031	1/1	0.10	-3.16	29,29,29,29	0
54	MG	AA	1620	1/1	0.05	-3.17	95,95,95,95	0
54	MG	DB	3017	1/1	0.13	-3.23	23,23,23,23	0
54	MG	AA	1606	1/1	0.05	-3.29	73,73,73,73	0
54	MG	BB	3066	1/1	0.06	-3.30	34,34,34,34	0
54	MG	DB	3077	1/1	0.10	-3.30	17,17,17,17	0
54	MG	DB	3044	1/1	0.11	-3.32	16,16,16,16	0
54	MG	DB	3039	1/1	0.07	-3.34	34,34,34,34	0
54	MG	CA	1640	1/1	0.14	-3.38	35,35,35,35	0
54	MG	CA	1648	1/1	0.14	-3.40	17,17,17,17	0
54	MG	BB	3032	1/1	0.11	-3.58	31,31,31,31	0
54	MG	BB	3050	1/1	0.09	-3.60	16,16,16,16	0
54	MG	AA	1641	1/1	0.05	-3.60	32,32,32,32	0
54	MG	BB	3076	1/1	0.08	-3.65	48,48,48,48	0
54	MG	DB	3071	1/1	0.09	-3.70	41,41,41,41	0
54	MG	CA	1611	1/1	0.09	-3.73	114,114,114,114	0
54	MG	DB	3080	1/1	0.12	-3.92	13,13,13,13	0
54	MG	AA	1646	1/1	0.09	-3.92	98,98,98,98	0
54	MG	DB	3020	1/1	0.10	-3.93	5,5,5,5	0
54	MG	BB	3074	1/1	0.07	-3.96	7,7,7,7	0
54	MG	AA	1629	1/1	0.12	-3.99	44,44,44,44	0
54	MG	CA	1635	1/1	0.09	-4.00	105,105,105,105	0
54	MG	BB	3103	1/1	0.09	-4.17	20,20,20,20	0
54	MG	BB	3056	1/1	0.06	-4.21	61,61,61,61	0
54	MG	BB	3058	1/1	0.08	-4.29	17,17,17,17	0
54	MG	DB	3081	1/1	0.08	-4.33	20,20,20,20	0
54	MG	DB	3041	1/1	0.09	-4.34	9,9,9,9	0
54	MG	BB	3102	1/1	0.12	-4.42	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DB	3056	1/1	0.15	-4.45	16,16,16,16	0
54	MG	BB	3022	1/1	0.05	-4.46	34,34,34,34	0
54	MG	AA	1643	1/1	0.09	-4.59	118,118,118,118	0
54	MG	BB	3044	1/1	0.06	-4.69	29,29,29,29	0
54	MG	BB	3084	1/1	0.09	-4.69	60,60,60,60	0
54	MG	DB	3072	1/1	0.07	-4.76	48,48,48,48	0
54	MG	DB	3006	1/1	0.07	-4.76	15,15,15,15	0
54	MG	BB	3030	1/1	0.05	-4.87	83,83,83,83	0
54	MG	BB	3069	1/1	0.07	-4.94	5,5,5,5	0
54	MG	CA	1655	1/1	0.08	-5.01	22,22,22,22	0
54	MG	AA	1604	1/1	0.10	-5.30	37,37,37,37	0
54	MG	BB	3089	1/1	0.06	-5.43	30,30,30,30	0
54	MG	DB	3038	1/1	0.11	-5.54	23,23,23,23	0
54	MG	AA	1605	1/1	0.11	-5.55	54,54,54,54	0
54	MG	BB	3095	1/1	0.11	-5.61	65,65,65,65	0
54	MG	DB	3009	1/1	0.09	-5.97	22,22,22,22	0
54	MG	DB	3034	1/1	0.11	-6.08	52,52,52,52	0
54	MG	DB	3062	1/1	0.06	-6.57	44,44,44,44	0
54	MG	CA	1609	1/1	0.13	-6.73	81,81,81,81	0
54	MG	BB	3063	1/1	0.09	-7.12	5,5,5,5	0
54	MG	BB	3015	1/1	0.08	-8.97	9,9,9,9	0
54	MG	DB	3082	1/1	0.07	-9.09	37,37,37,37	0
54	MG	CA	1631	1/1	0.10	-9.82	55,55,55,55	0
54	MG	CA	1645	1/1	0.07	-10.22	82,82,82,82	0
54	MG	DB	3107	1/1	0.08	-14.40	51,51,51,51	0
54	MG	DB	3054	1/1	0.13	-33.00	69,69,69,69	0
54	MG	DB	3029	1/1	0.18	-	70,70,70,70	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.