



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:37 PM BST

PDB ID : 4V53  
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with gentamicin.  
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 : 2007-06-16  
Resolution : 3.54 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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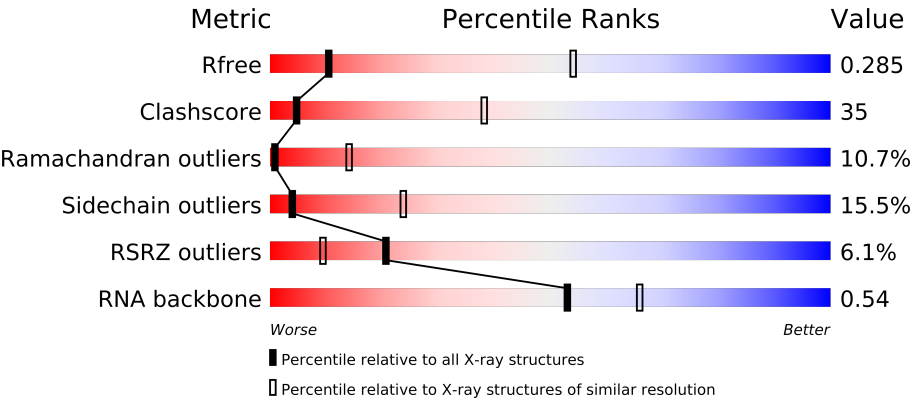
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.54 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	1270 (3.78-3.30)
Clashscore	79885	1033 (3.70-3.38)
Ramachandran outliers	78287	1067 (3.72-3.36)
Sidechain outliers	78261	1067 (3.72-3.36)
RSRZ outliers	66119	1270 (3.78-3.30)
RNA backbone	1838	1011 (4.30-2.76)

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	

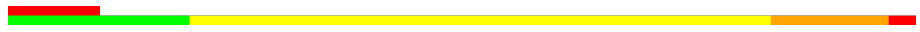
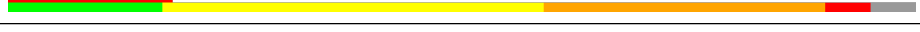
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Mol	Chain	Length	Quality of chain
28	BP	114	
28	DP	114	
29	BE	201	
29	DE	201	
30	BY	58	
30	DY	58	
31	B0	56	
31	D0	56	
32	B4	38	
32	D4	38	
33	B1	54	
33	D1	54	
34	B3	64	
34	D3	64	
35	BV	94	
35	DV	94	
36	B2	46	
36	D2	46	
37	BL	144	
37	DL	144	
38	BM	136	
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	

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

Mol	Type	Chain	Res	Geometry	Electron density
53	MG	AA	2002	-	X
53	MG	AA	2019	-	X
53	MG	AA	2022	-	X
53	MG	AA	2023	-	X
53	MG	AA	2024	-	X
53	MG	AA	2025	-	X
53	MG	AA	2032	-	X
53	MG	AA	2037	-	X
53	MG	AA	2047	-	X
53	MG	AA	2051	-	X
53	MG	AA	2056	-	X
53	MG	AA	2057	-	X
53	MG	AA	2059	-	X
53	MG	BB	3033	-	X
53	MG	BB	3043	-	X
53	MG	BB	3063	-	X
53	MG	BB	3084	-	X
53	MG	BB	3087	-	X
53	MG	BB	3093	-	X
53	MG	CA	2019	-	X
53	MG	CA	2020	-	X
53	MG	CA	2022	-	X
53	MG	CA	2026	-	X
53	MG	CA	2027	-	X
53	MG	CA	2029	-	X
53	MG	CA	2038	-	X
53	MG	CA	2045	-	X
53	MG	CA	2058	-	X
53	MG	DB	3052	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
53	MG	DB	3058	-	X
53	MG	DB	3083	-	X
53	MG	DB	3089	-	X
53	MG	DB	3091	-	X
53	MG	DB	3101	-	X
54	LLL	AA	2062	-	X
54	LLL	AA	2063	-	X
54	LLL	BB	3111	-	X
54	LLL	CA	2063	-	X
54	LLL	DB	3112	-	X

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 284252 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.

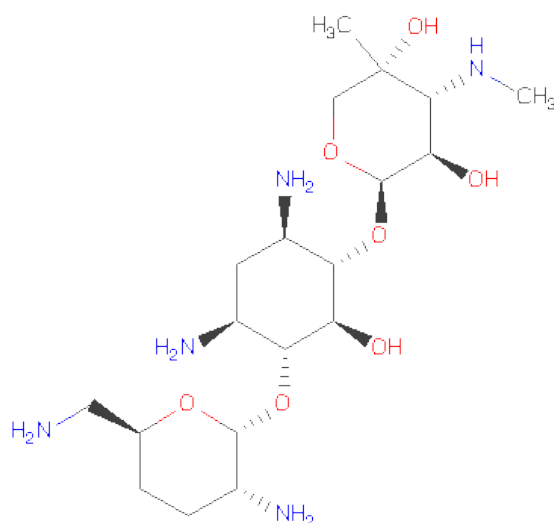
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
52	DW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



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

- Molecule 54 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-O-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C<sub>19</sub>H<sub>39</sub>N<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
54	AA	1	Total	C	N	O	0	0
			31	19	5	7		
54	AA	1	Total	C	N	O	0	0
			31	19	5	7		
54	AA	1	Total	C	N	O	0	0
			31	19	5	7		
54	BB	1	Total	C	N	O	0	0
			31	19	5	7		
54	CA	1	Total	C	N	O	0	0
			31	19	5	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
54	CA	1	Total	C	N	O	0	0
			31	19	5	7		
54	CA	1	Total	C	N	O	0	0
			31	19	5	7		
54	DB	1	Total	C	N	O	0	0
			31	19	5	7		

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	292	Total	O	0	0
			292	292		
56	AE	1	Total	O	0	0
			1	1		
56	AK	1	Total	O	0	0
			1	1		
56	AL	2	Total	O	0	0
			2	2		
56	AN	2	Total	O	0	0
			2	2		
56	AT	2	Total	O	0	0
			2	2		
56	BB	492	Total	O	0	0
			492	492		
56	BC	7	Total	O	0	0
			7	7		
56	BE	3	Total	O	0	0
			3	3		
56	B2	1	Total	O	0	0
			1	1		
56	BL	3	Total	O	0	0
			3	3		
56	BH	1	Total	O	0	0
			1	1		

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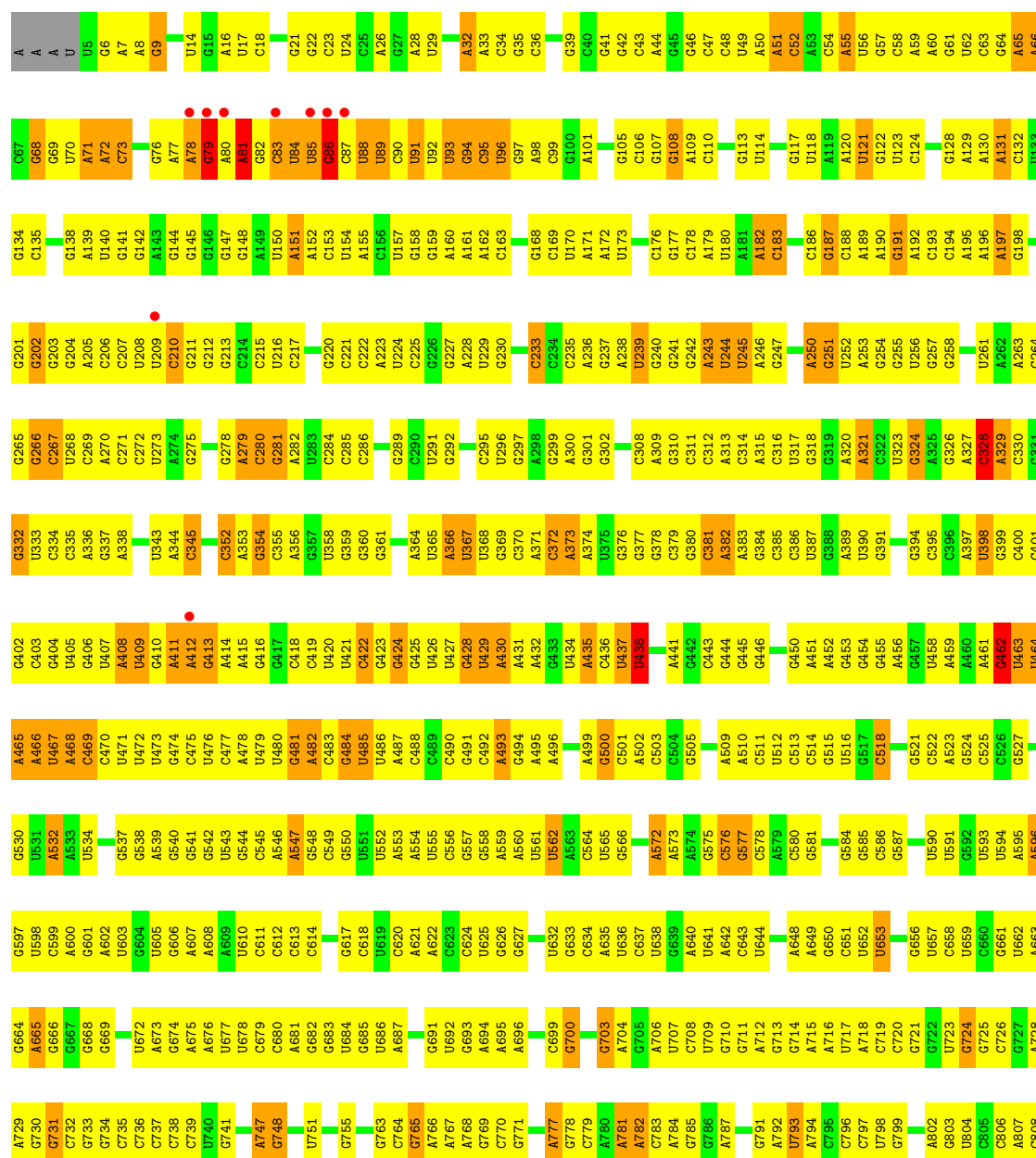
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CA	297	Total 297	O 297	0	0
56	CE	2	Total 2	O 2	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	2	Total 2	O 2	0	0
56	CN	4	Total 4	O 4	0	0
56	CT	2	Total 2	O 2	0	0
56	DB	502	Total 502	O 502	0	0
56	DC	4	Total 4	O 4	0	0
56	DE	2	Total 2	O 2	0	0
56	DL	4	Total 4	O 4	0	0

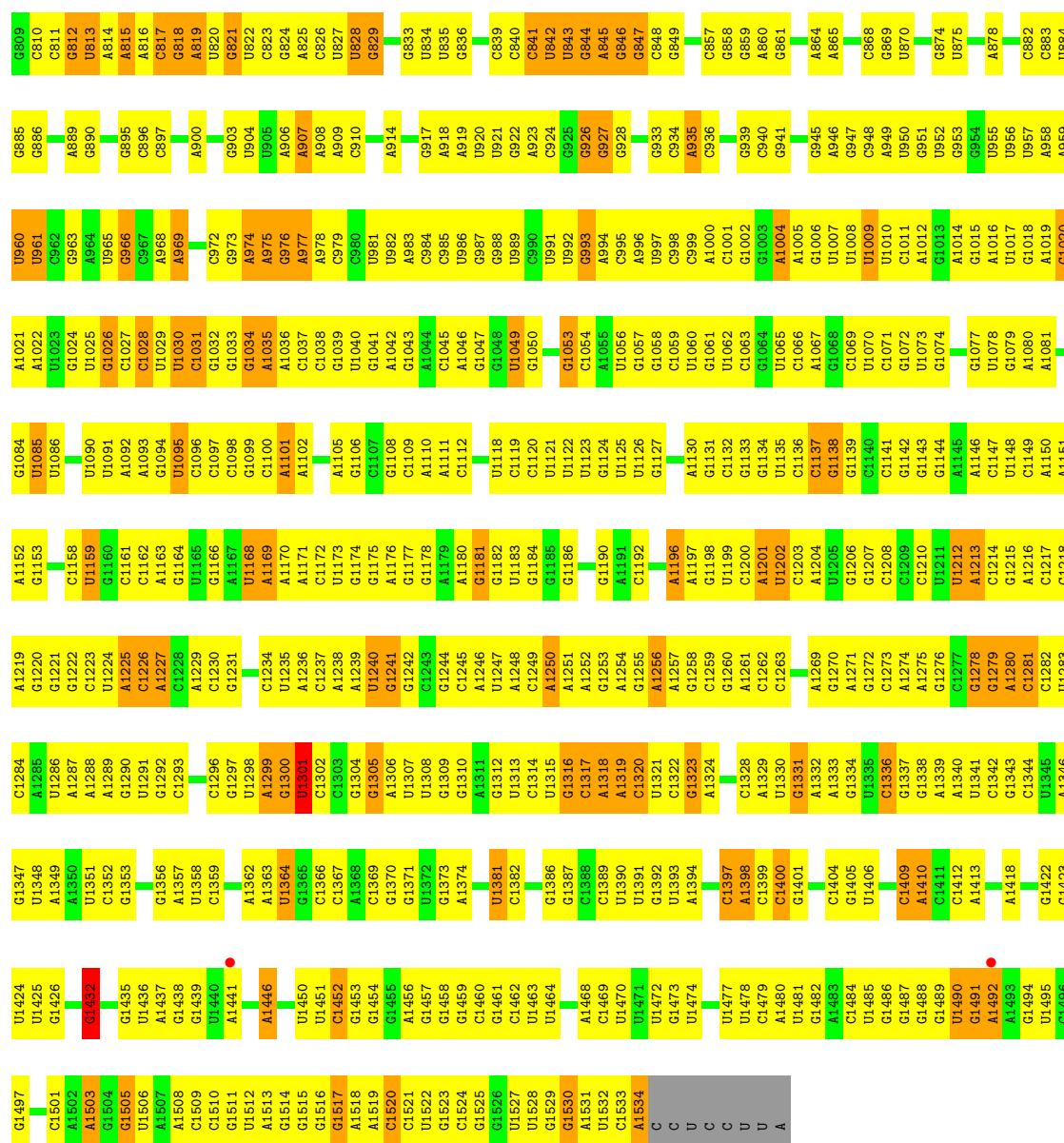
### 3 Residue-property plots

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.

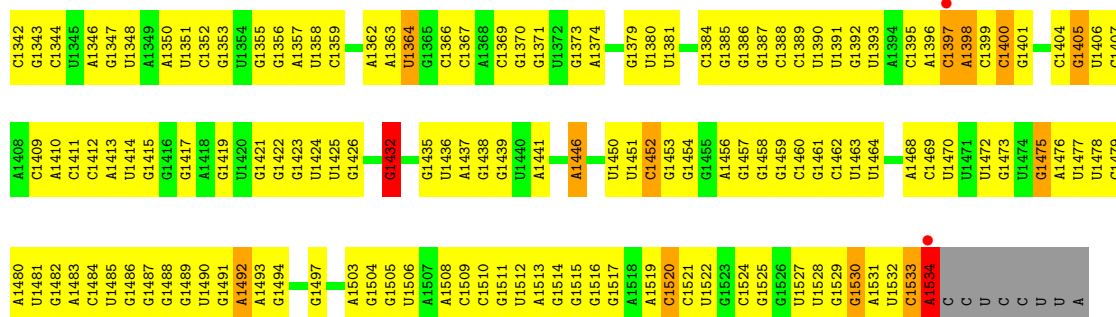
#### • Molecule 1: 16S rRNA

Chain AA: 



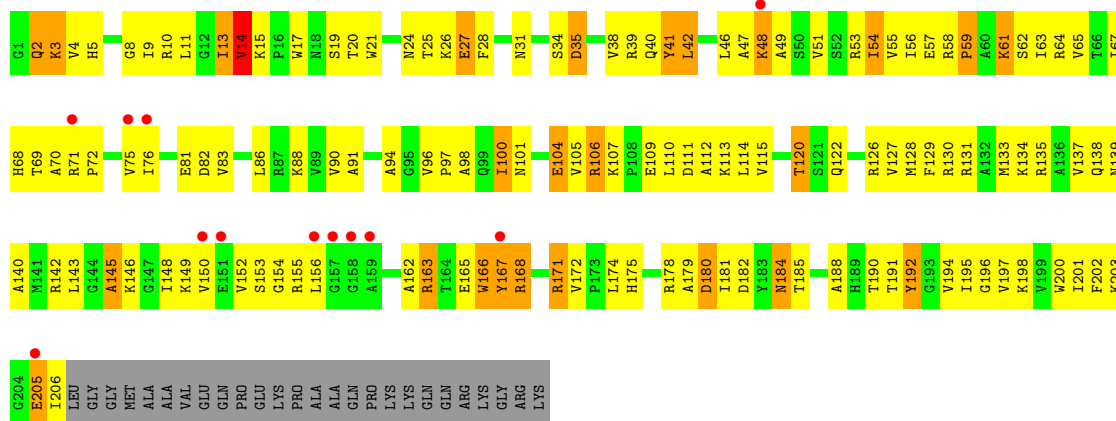


G1279	C1217	A1150	U1085	A1019	A958	A889	C811	G734	G601	U534	C469	G406	A336	U268
A1280	C1218	A1151	U1086	G1020	A959	G890	G812	C735	A602	U535	C470	U407	G337	C269
C1281	G1219	A1152	U1086	A1021	U960	G891	U813	C736	G603	G538	U471	U408	A338	A270
C1282	G1220	A1153	U1086	A1022	U961	G892	A814	C737	U604	G539	U472	U409	U343	C271
C1284	G1221	U1086	U1090	G1023	G962	C895	A815	C738	U605	G540	U473	U410	U344	C272
C1285	G1222	U1086	U1091	G1024	G963	C896	A816	C739	U606	G541	U474	U411	C345	U273
C1286	G1223	U1086	U1092	U1025	U964	C897	C817	U740	U607	G542	U475	U412	C346	C274
C1287	U1224	G1160	A1093	G1026	U965	A900	G818	G741	A608	G543	U476	U413	C352	G275
C1288	U1225	G1161	A1094	G1027	U966	A901	U820	G742	U609	U544	C477	A414	C353	G278
C1289	C1226	C1162	U1095	C1028	C967	G903	U821	A743	U610	G545	U478	A415	A354	A279
C1290	A1227	A1163	A968	U1029	A968	U904	U822	C744	C611	C546	U479	A416	C355	C280
C1291	C1228	G1164	A969	U1030	C970	U905	U823	A747	C612	A547	U480	G417	C356	G281
C1292	C1230	U1165	C970	C1031	C971	A906	G824	G748	C613	A548	U481	C418	A357	G282
C1293	G1231	G1166	G1099	G1032	G972	A907	G825	U751	C614	G548	U482	C419	C358	A282
C1296	U1234	A1167	C1100	G1033	C973	A908	A826	U752	G617	C549	U483	U420	U359	C285
C1297	U1235	U1168	A1101	G1034	A974	A909	U827	U753	C618	G550	U484	U421	G360	C286
C1298	A1236	A1169	A1102	A1035	A975	A910	U828	G754	U619	U552	U485	C422	G361	U287
C1299	C1237	A1170	C1103	A1036	G976	U911	G829	G755	C620	A553	U486	G423	A364	C288
C1300	C1238	C1171	G1104	C1037	A977	C912	G833	G763	A621	A554	U487	G424	U365	C290
C1301	U1240	U1172	U1105	G1038	A978	A913	U834	G764	C623	C556	U488	U425	U366	U291
C1302	G1241	G1173	G1106	G1039	C979	A914	U835	G765	C624	G557	U489	G428	U367	G292
C1303	U1242	G1174	G1107	G1040	C980	A915	U836	A766	U625	G558	U490	U429	U368	C295
C1304	G1243	A1175	C1109	A1042	U981	G917	G837	A767	U638	A559	U491	U430	C370	U296
C1305	U1244	G1176	A1110	G1043	U982	A918	C839	A768	U639	A560	U494	A431	A371	C299
C1306	G1245	G1177	C1112	A1044	A983	A919	C840	G769	G633	U562	U495	A432	C372	G301
C1307	U1246	A1180	U1118	C1045	C984	U920	C841	C770	C634	A573	U496	G433	A373	G302
C1308	A1246	A1181	U1119	A1046	C985	U921	U842	G771	U641	A574	U500	U434	A374	A303
C1309	U1247	G1182	C1119	G1047	U986	G922	U843	U772	U636	C564	U501	U435	U375	C308
C1310	C1248	A1183	G1120	U1049	C987	A923	U844	U773	U637	U565	U502	U436	G376	A309
C1311	C1249	G1184	U1121	G1050	U988	C924	A845	A777	U638	G566	U503	U437	G377	C312
C1312	A1250	U1185	U1122	C1051	C990	G925	A846	G778	U639	A575	U504	U438	G378	A313
C1313	A1251	G1186	U1123	G1052	U991	G927	G847	C779	A640	A576	U505	U439	G379	A314
C1314	U1252	U1187	C1124	C1053	U992	G928	C848	A780	U641	A577	U506	U440	C381	A315
C1315	G1253	U1188	U1125	A1055	C993	G929	C857	A781	U642	C578	U507	U441	C382	C316
C1316	A1254	A1191	U1126	U1056	A994	C930	G858	C783	U643	C579	U508	U442	C383	U317
C1317	G1255	C1192	G1127	G1057	C995	C931	G859	A784	U644	C580	U509	U443	C384	G318
C1318	U1256	U1193	C1128	C1058	A996	G932	U860	G785	A648	C581	U510	U444	A385	C319
C1319	A1257	A1194	U1129	G1059	U997	C933	A861	G786	U649	C582	U511	G449	C386	A320
C1320	G1258	A1195	C1130	U1060	C998	C934	G862	U787	A650	C583	U512	U450	C387	A321
C1321	C1259	A1196	G1131	G1061	C999	A935	U863	A788	C651	C584	U513	U451	U387	U322
C1322	U1260	U1199	C1132	U1062	A1000	C936	U864	A789	U652	C585	U514	U452	C388	U323
C1323	A1261	C1200	G1133	C1063	C1001	G939	A865	G791	U653	C586	U515	U453	C389	C330
C1324	C1262	A1201	G1134	U1064	G1002	C940	A866	A792	U654	C587	U516	U454	C400	G331
C1325	U1263	U1202	U1135	C1065	G1003	C941	C868	U793	U655	C588	U517	U455	C401	G332
C1326	U1264	C1203	C1136	U1066	A1004	G945	G869	A794	U656	C589	U518	U456	C402	G333
C1327	C1265	A1204	C1137	C1067	U1005	G946	U870	C796	U657	C590	U519	U457	C403	C334
C1328	U1266	U1205	G1138	U1068	G1006	C947	G874	U798	U658	C591	U520	U458	C404	U405
C1329	G1268	G1206	G1139	C1071	U1007	C948	U875	U799	U659	U590	U521	U459	C395	
C1330	A1269	U1207	C1140	G1072	U1008	C949	U876	G802	U660	U591	U522	U460	C396	G326
C1331	G1270	C1208	U1141	U1073	U1009	A949	A802	C726	U661	G592	U523	U461	C397	A327
C1332	A1271	C1209	G1142	U1074	U1010	U950	U877	G727	U662	U593	U524	U462	U398	C328
C1333	G1272	C1210	G1143	G1075	C1011	G951	A878	U803	U663	U594	U525	U463	U399	C329
C1334	C1273	U1211	U1144	U1076	A1012	U952	C882	C806	U664	A595	U526	U464	C400	C330
C1335	A1274	U1212	A1145	G1077	G1013	G953	C883	A807	U665	A596	U527	U465	C401	G331
C1336	C1275	U1213	A1146	U1078	A1014	G954	C884	U807	U666	C597	U528	U466	C402	G332
C1337	A1276	U1214	U1147	U1079	U1015	U955	U884	C808	U667	U598	U529	U467	C403	C333
C1338	C1277	G1215	U1148	A1080	U1017	U956	G885	G809	U668	C599	U530	U468	C404	C334
C1339	U1278	U1216	C1149	A1081	G1018	U957	C810	G733	U669	A600	U531	U469	C405	C335



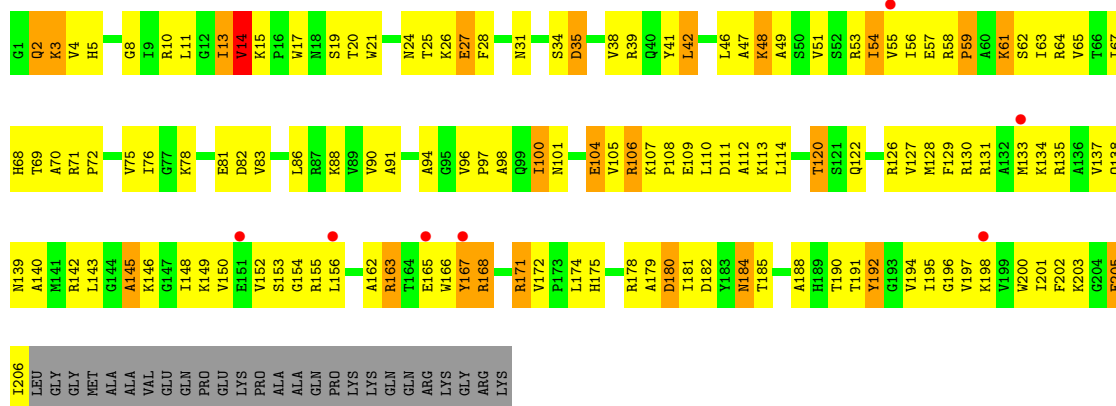
### • Molecule 2: 30S ribosomal protein S3

Chain AC:



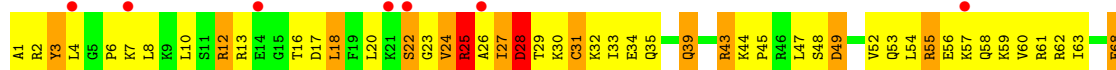
### • Molecule 2: 30S ribosomal protein S3

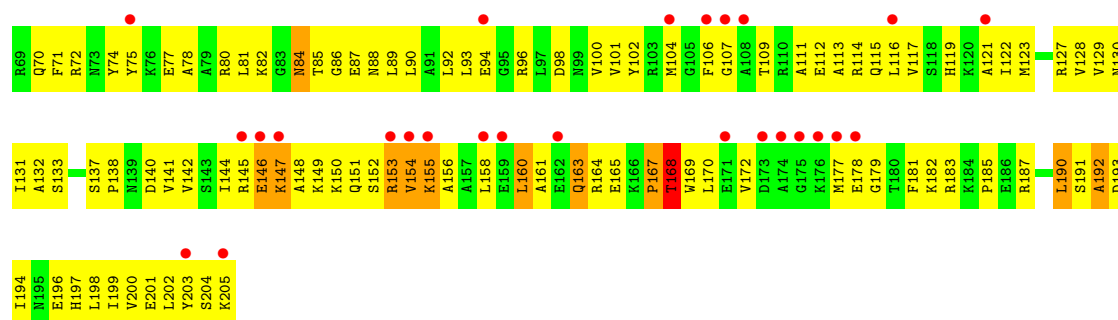
Chain CC:



### • Molecule 3: 30S ribosomal protein S4

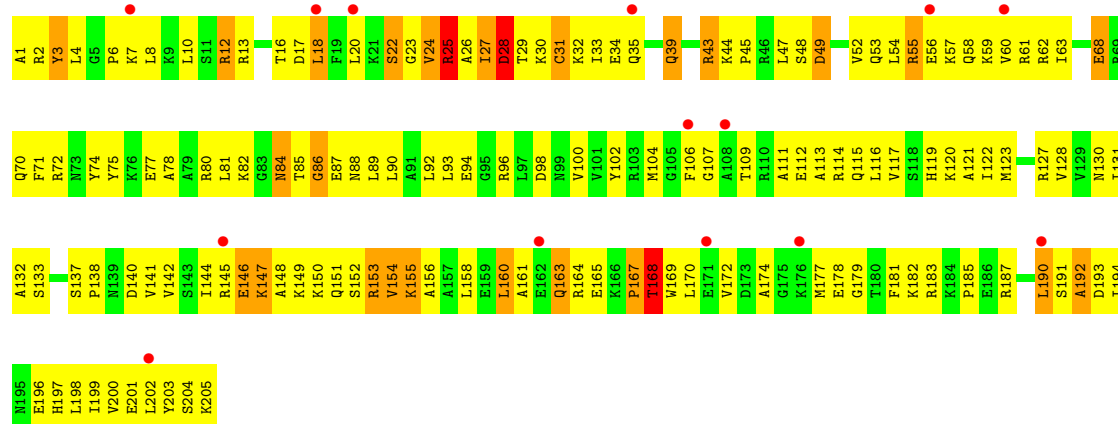
Chain AD:





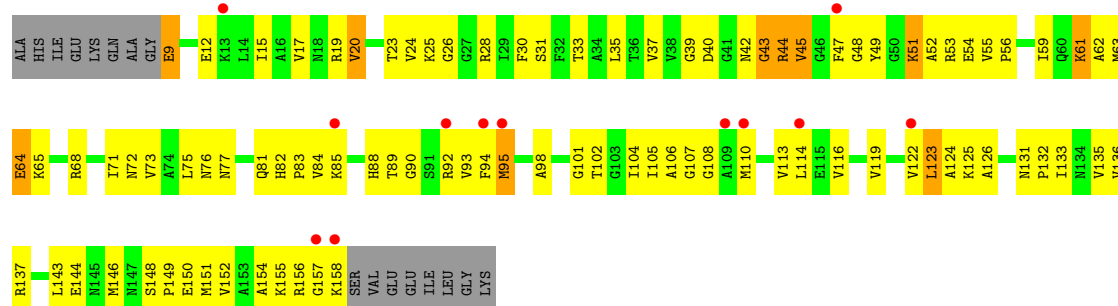
• Molecule 3: 30S ribosomal protein S4

Chain CD:



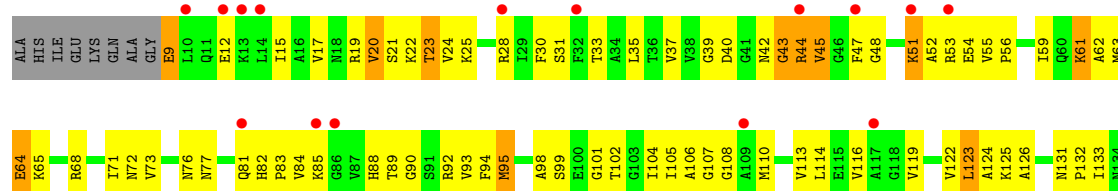
• Molecule 4: 30S ribosomal protein S5

Chain AE:



• Molecule 4: 30S ribosomal protein S5

Chain CE:

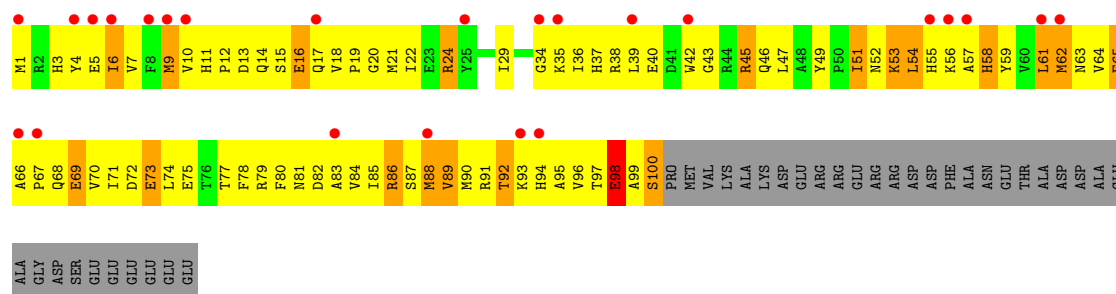






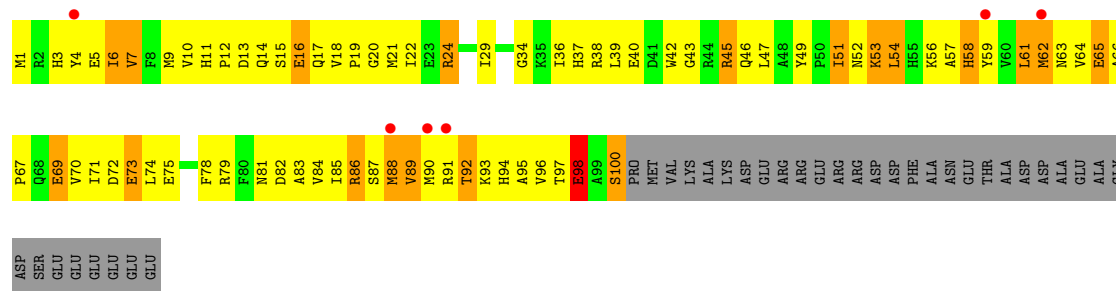
• Molecule 5: 30S ribosomal protein S6

Chain AF:



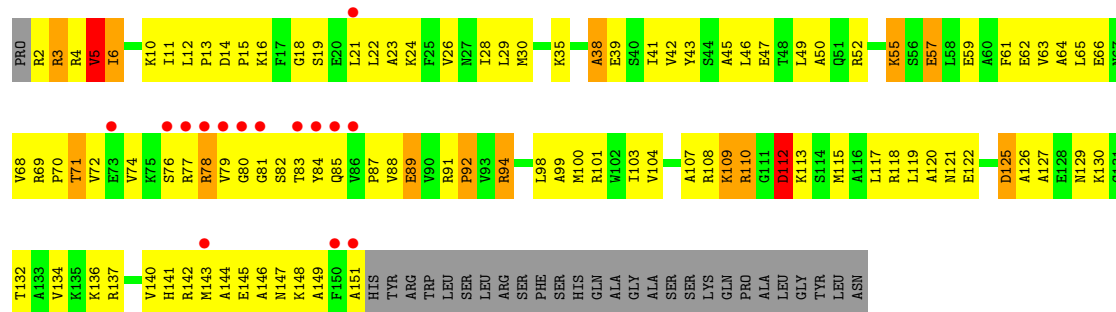
• Molecule 5: 30S ribosomal protein S6

Chain CF:



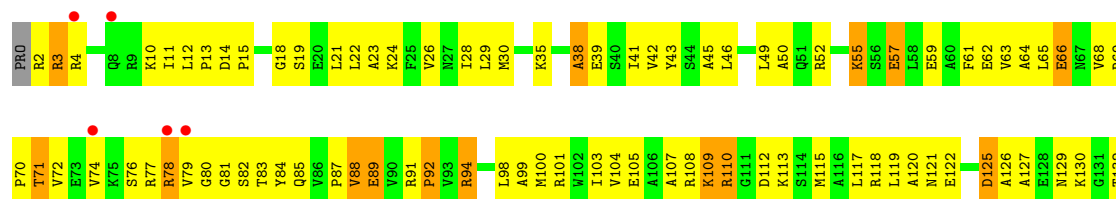
• Molecule 6: 30S ribosomal protein S7

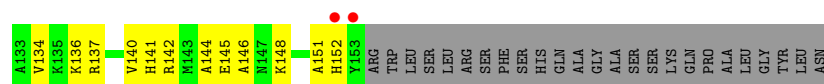
Chain AG:



• Molecule 6: 30S ribosomal protein S7

Chain CG:





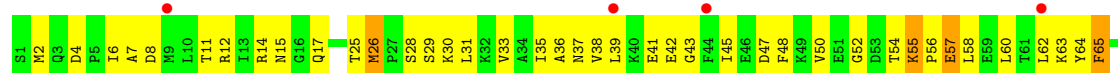
• Molecule 7: 30S ribosomal protein S8

Chain AH:



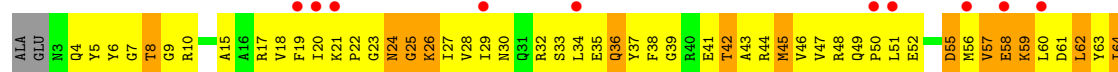
• Molecule 7: 30S ribosomal protein S8

Chain CH:



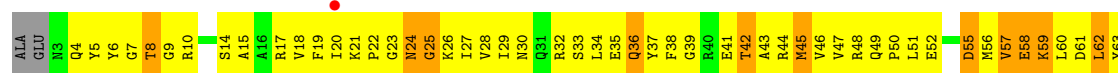
• Molecule 8: 30S ribosomal protein S9

Chain AI:



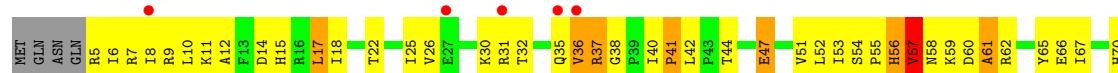
• Molecule 8: 30S ribosomal protein S9

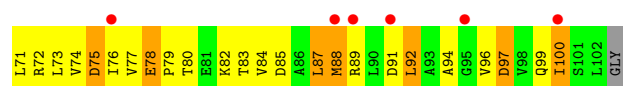
Chain CI:



• Molecule 9: 30S ribosomal protein S10

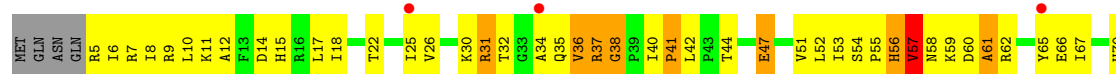
Chain AJ:





• 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:



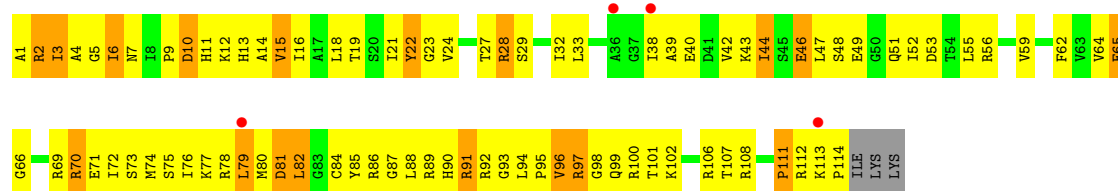
• Molecule 11: 30S ribosomal protein S12

Chain CL:



- Molecule 12: 30S ribosomal protein S13

Chain AM:



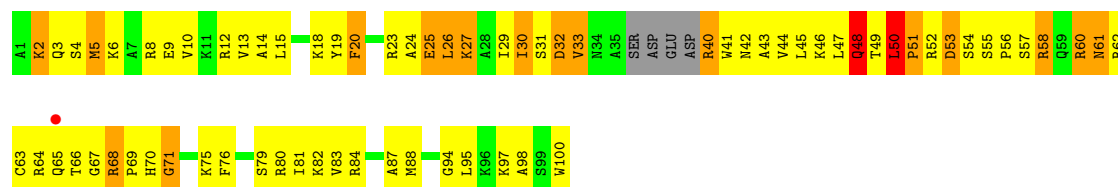
- Molecule 12: 30S ribosomal protein S13

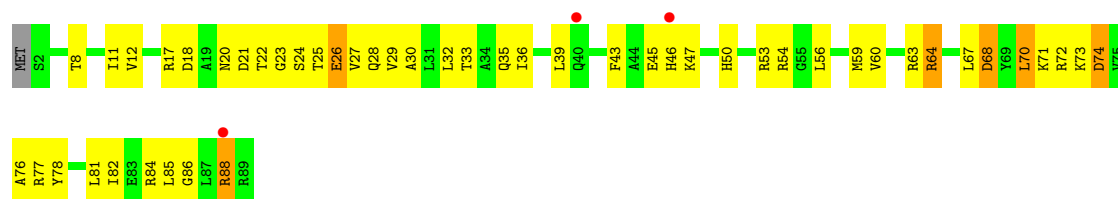
Chain CM:



- Molecule 13: 30S ribosomal protein S14

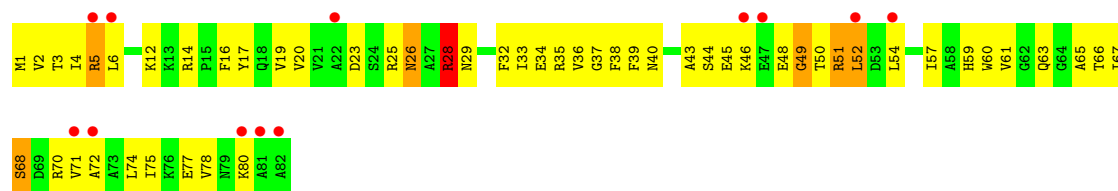
Chain AN:





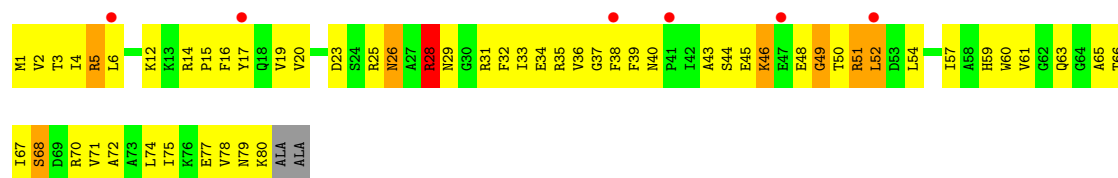
• Molecule 15: 30S ribosomal protein S16

Chain AP:



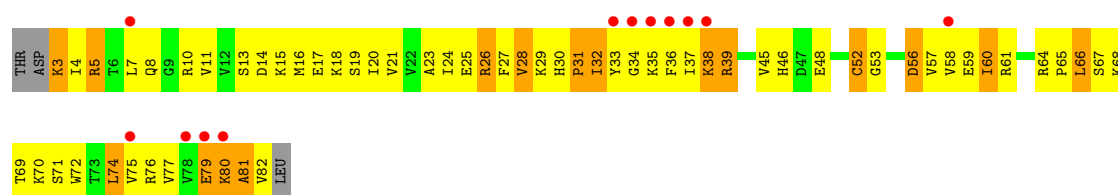
• Molecule 15: 30S ribosomal protein S16

Chain CP:



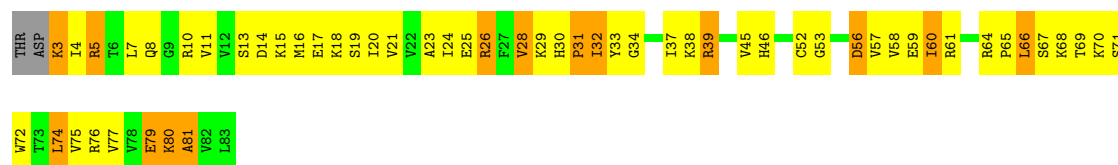
• Molecule 16: 30S ribosomal protein S17

Chain AQ:



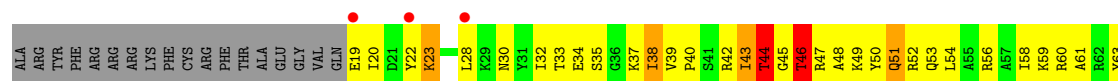
• Molecule 16: 30S ribosomal protein S17

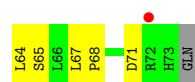
Chain CQ:



• Molecule 17: 30S ribosomal protein S18

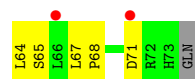
Chain AR:





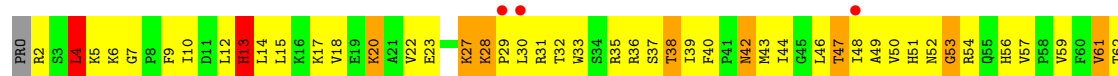
- Molecule 17: 30S ribosomal protein S18

Chain CR:



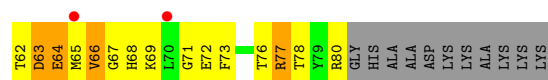
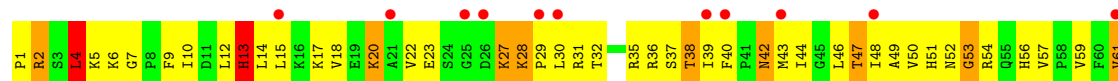
- Molecule 18: 30S ribosomal protein S19

Chain AS:



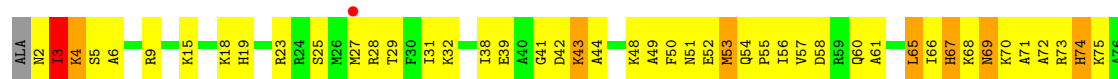
- Molecule 18: 30S ribosomal protein S19

Chain CS:



- Molecule 19: 30S ribosomal protein S20

Chain AT:



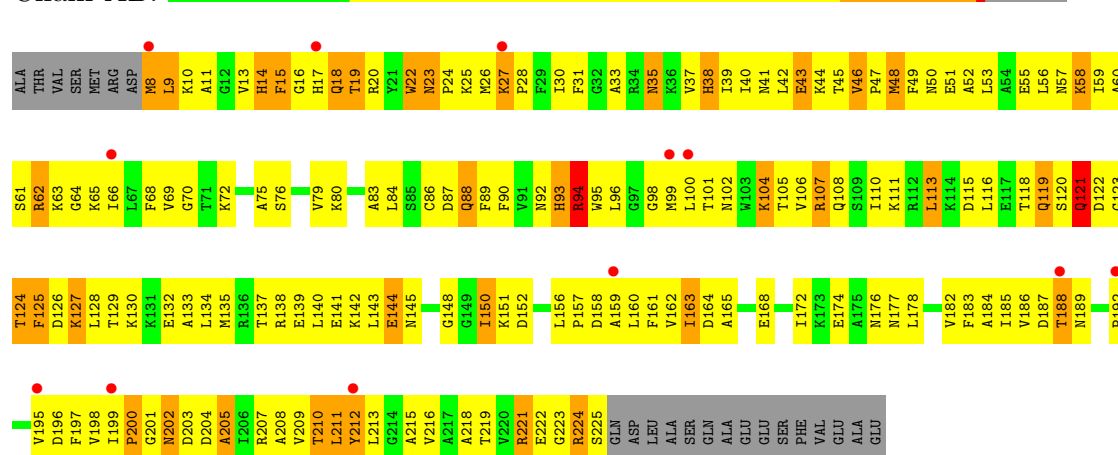
- Molecule 19: 30S ribosomal protein S20

Chain CT:



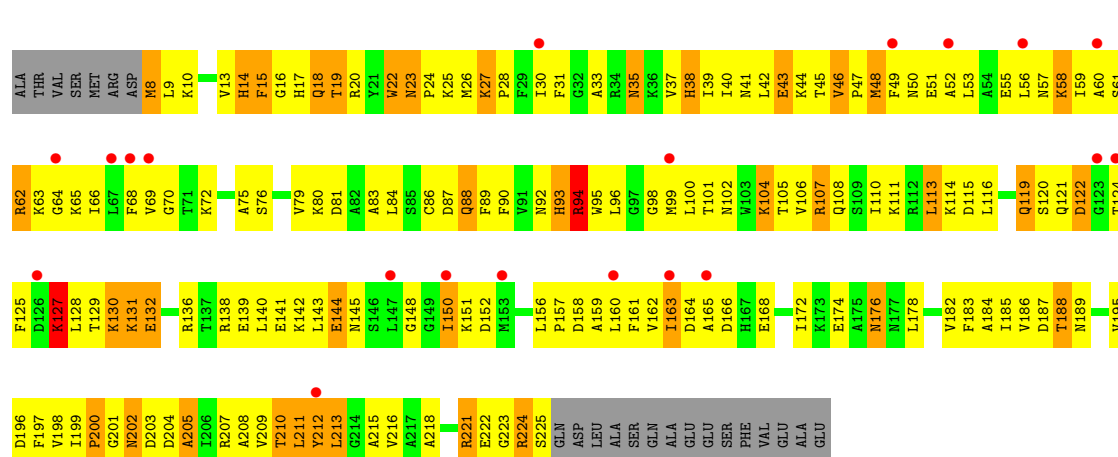
- Molecule 20: 30S ribosomal protein S2

Chain AB:



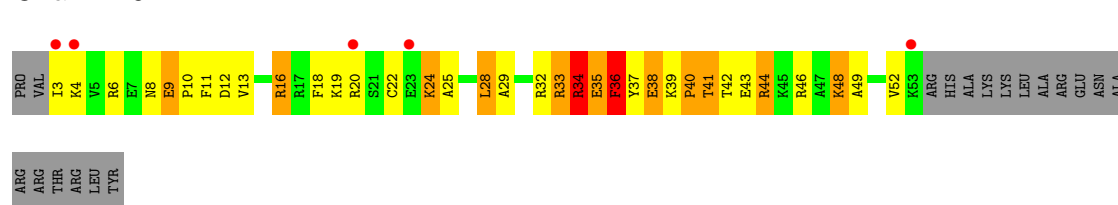
- Molecule 20: 30S ribosomal protein S2

Chain CB:



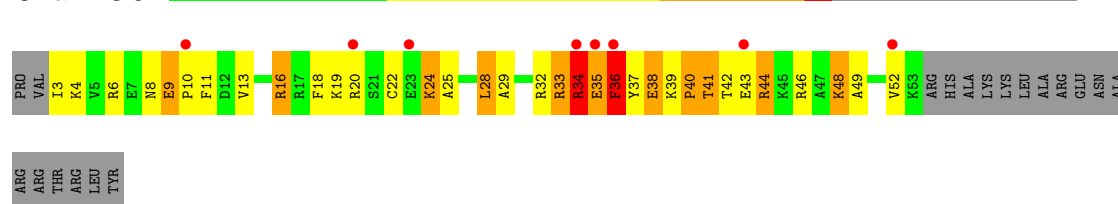
- Molecule 21: 30S ribosomal protein S21

Chain AU:



- Molecule 21: 30S ribosomal protein S21

Chain CU:



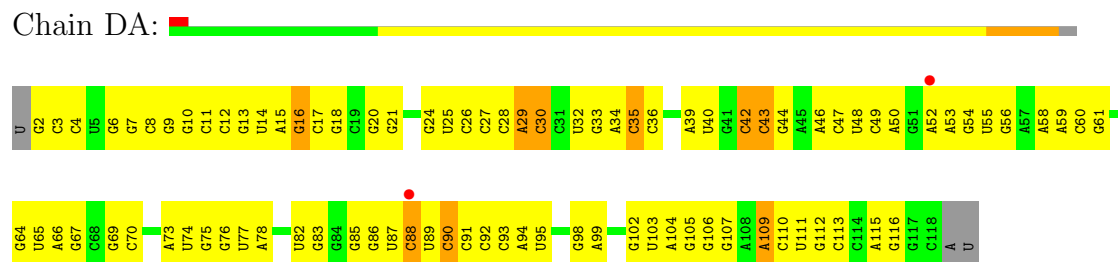
- Molecule 22: 5S rRNA

Chain BA:



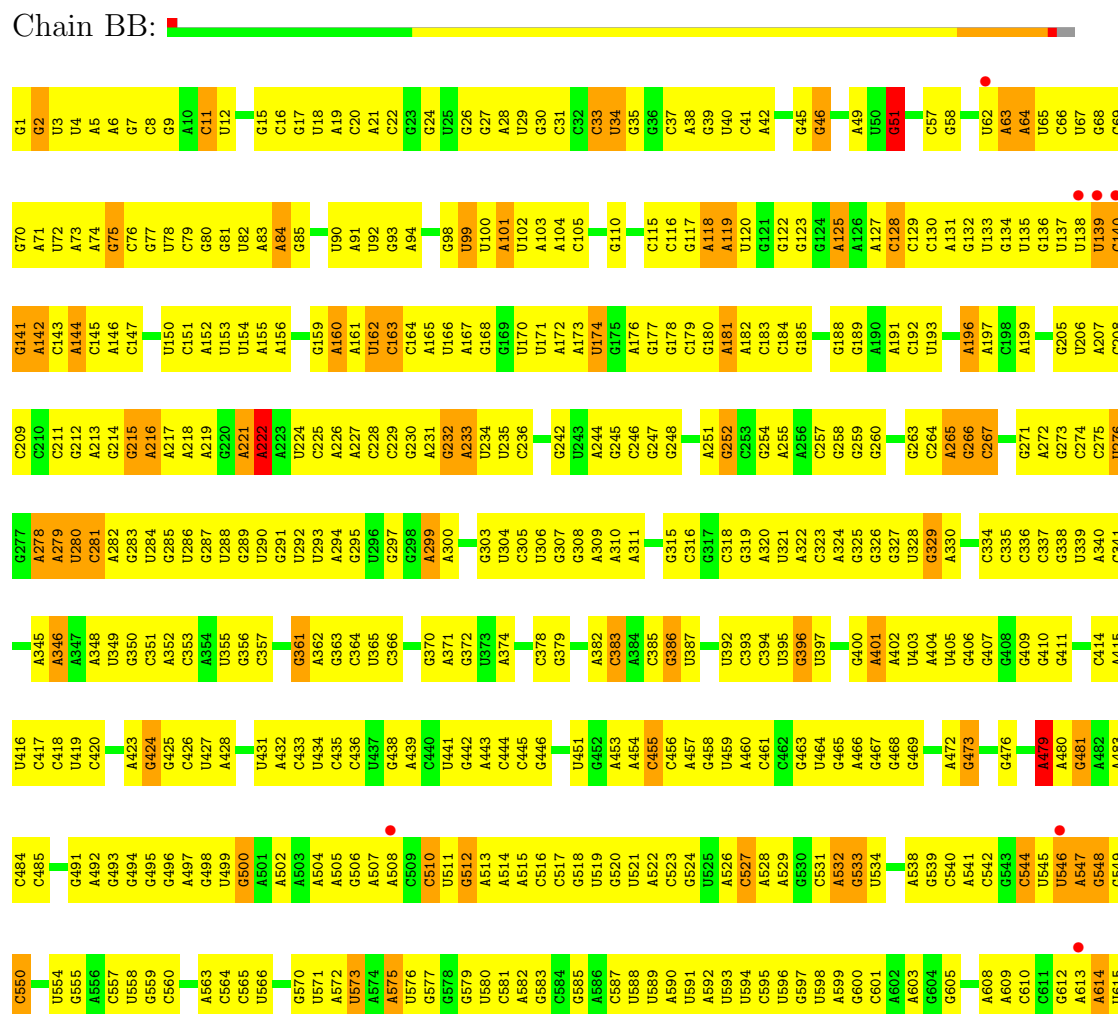
- Molecule 22: 5S rRNA

Chain DA:



- Molecule 23: 23S rRNA

Chain BB:







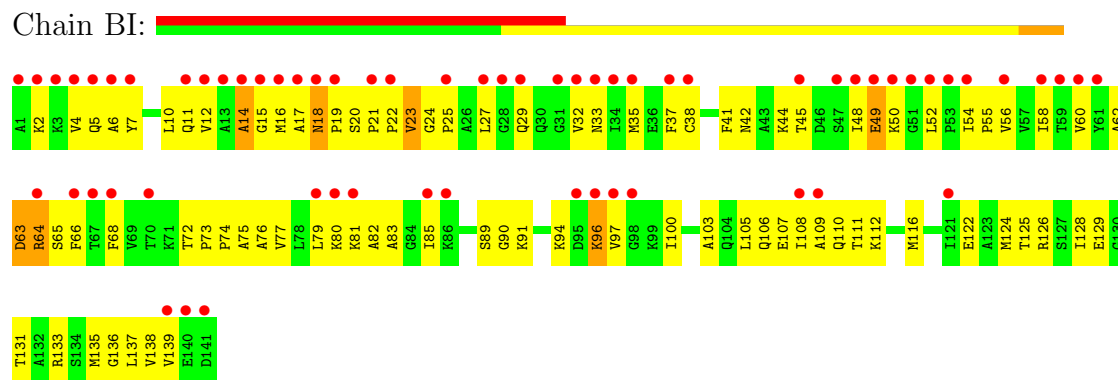




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G1843	C1843	C1844	C1771	G1702	U1563	A1495	G1429	A1368	G1296	G1223	A1088	G1017	C951	A	A821
G1844	C1844	C1845	A1772	C1703	C1564	A1496	G1430	G1369	C1297	U1224	A1089	U1018	G952	U	G822
G1845	C1845	C1846	A1773	C1704	C1565		A1431	C1370	C1298		A1090	U1019	G953	C	C823
G1846	C1846	C1847	A1774	C1705	U1566	G1501	G1432	C1371	C1299	G1228	G1091	A1020	G954	C	U824
G1847	C1847	C1848	U1775	C1706	G1567	A1502	G1433	U1372	G1300	A1237	G1092	A1021	U955	C	A825
G1848	C1848	C1849	G1776	G1707	G1568	A1503	A1434	U1373	G1301	U1231	G1093	G1022	G956	G	U826
G1849	C1849	C1850	U1777	C1708	A1569	A1504		A1376	A1301		U1094	U1023	C957	A	U827
G1850	C1850	C1851	G1778	U1709	U1570	A1505	C1437	A1377	A1302	G1235		G1024	U958	C	U828
G1851	C1851	C1852	U1779	C1710	A1571	A1506	U1438	U1374	G1303	A1236	U1097	G1025	A959	U	
G1852	C1852	C1853	U1780	G1711	U1572	U1507	A1439	U1375	A1304	G1237	A1098	A1027	A960	U	G831
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G1854	C1854	C1855	A1783	C1713	U1574	A1509	G1441	G1377	C1306	G1239	G1100	U1029	C961	A	U833
U1855	C1855	C1856	A1784	U1714	G1575	G1510	U1442	A1378	U1307		U1101	A1030	G962	C	G834
U1856	C1856	C1857	A1785	G1715	U1576	G1511	U1443	U1379	A1308	U1240	C1102	C1031		C898	
U1857	C1857	C1858	A1786	U1716	C1577	C1512	U1444	G1380	G1309	A1241	G1103	G1032	G965	A899	
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U1859	C1859	C1860	C1788	G1718	A1579	G1514	G1446	G1382	G1311	C1243	U1105		G967	C903	
U1860	C1860	C1861	C1789	U1719	A1580	A1515	G1447	A1383	G1312	U1244	G1106	U1033	C968	C838	
G1861	C1861	C1862	A1790	G1720	G1581	G1516	G1448	A1384	U1312	A1245	G1107	G1036	U970	A905	
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G1863	C1863	C1864	U1792	G1722	U1583	C1518	G1450	C1386	C1315	A1247	G1110	G1038	A972	C908	
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G1868	C1868	C1869	U1797	C1727		G1527	C1455	U1391	C1320	G1252	C1117	C1043	G976	A912	
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C1870	C1870	C1871	G1799	G1730	C1592	G1529	G1457	A1393	C1322	U1258	C1119	C1045	A979	C917	
A1871	C1871	C1872	C1800	G1731	A1593	G1530	U1458	U1394	C1323	G1259	G1120	A1046	A980	A917	
A1872	C1872	C1873	A1801	C1732	U1594	C1531	G1459	A1395	G1324	G1266	G1125	G1047	A981	A918	
C1873	C1873	C1874	A1802	G1733	C1595	A1532	U1460	U1396	U1325	U1268	A982		A982	A919	
G1875	C1875	C1876	A1803	G1734	A1596	C1533	C1461	U1397	U1326	G1269	A983	A1050	A984	A920	
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G1884	C1884	C1885	G1817	G1743	A1608	G1543	G1471	U1406	C1339	A1269	C992	G1062	C865	U929	
			A1818	A1744	A1609	A1544		U1407	U1340	G1270	G993	G1063	C866	U930	
			U1819	G1745	A1610	A1545	G1475	U1408	G1341	G1271	C994	C1064	C867	U931	
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A1889	C1889	C1890	A1821		G1613	C1547	U1477	G1410	G1346	A1272	A996		C869	A933	
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C1893	C1893	C1894	G1755		A1616	A1549	G1478	U1412	C1348	A1274	U934	U1069	U871	A877	
			G1756		C1617	A1550	G1479	A1413	C1349	A1275	C998	A1069	U872	A878	
C1894	C1894	C1895	A1757		C1617	A1551		A1413	C1350	A1276	U999	A1070	C873	A936	
			U1758		G1622	A1552	G1482	G1415	C1351	G1277	C1145	C1076	C874	C937	
			U1759		G1623	A1553	G1483	G1417	U1352	G1277		A1001	G875	G938	
			A1760		G1624	U1554	U1484	G1418	U1353	G1283	G1146	A1077	C876		
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			G1634		G1635	C1558	U1488	G1422	C1357	A1287		U1083	C880	C946	
			U1635		G1636	C1559	U1489	G1425	G1358	G1288		A1084	C881	A947	
			G1637		G1638	U1560	U1490	G1426	C1359	G1289		A1085	C882	C948	
			A1698		G1639	C1561	U1491	A1427	C1362	G1291		A1086	C883	G949	
			U1699		G1640	C1562	U1492						C884		
			A1700		G1641	C1563	U1493						C885		
					G1642	C1564	U1494						C886		
					G1643	C1565	U1495						C887		
					G1644	C1566	U1496						C888		
					G1645	C1567	U1497						C889		
					G1646	C1568	U1498						C890		
					G1647	C1569	U1499						C891		
					G1648	C1570	U1500						C892		
					G1649	C1571	U1501						C893		
					G1650	C1572	U1502						C894		
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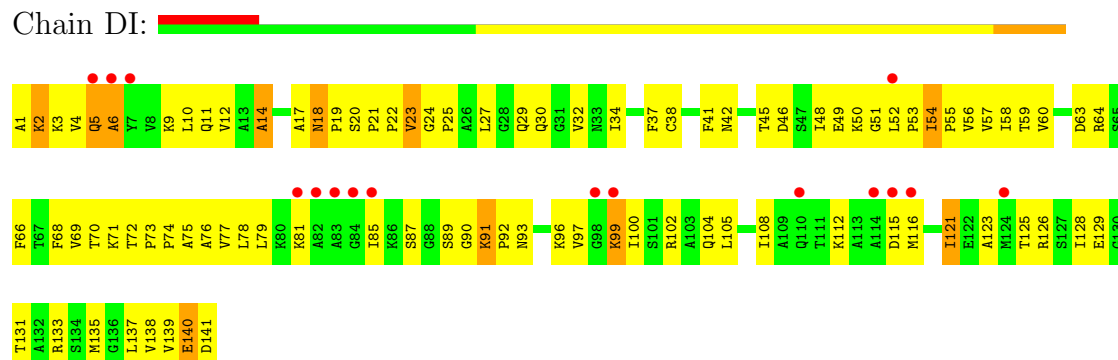
- Molecule 24: 50S ribosomal protein L11

Chain BI:



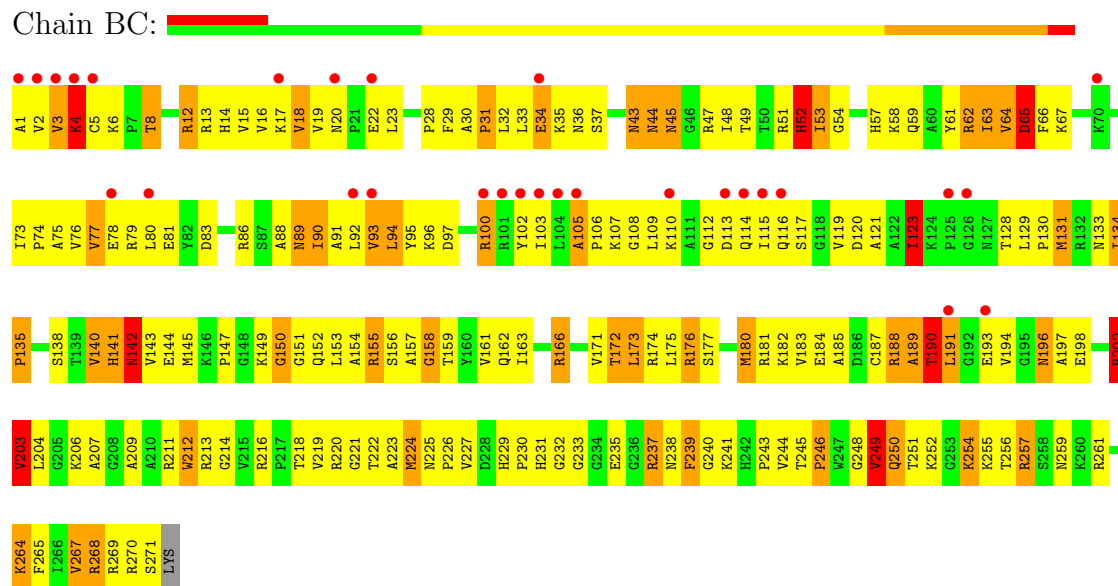
- Molecule 24: 50S ribosomal protein L11

Chain DI:



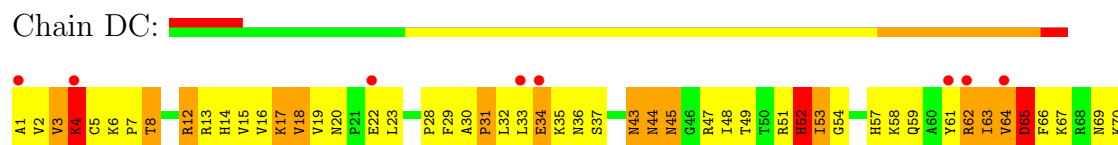
- Molecule 25: 50S ribosomal protein L2

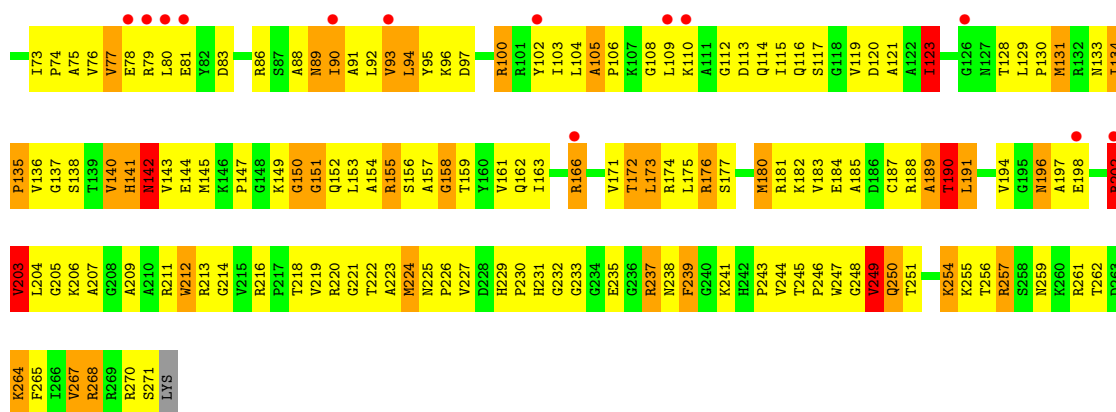
Chain BC:



- Molecule 25: 50S ribosomal protein L2

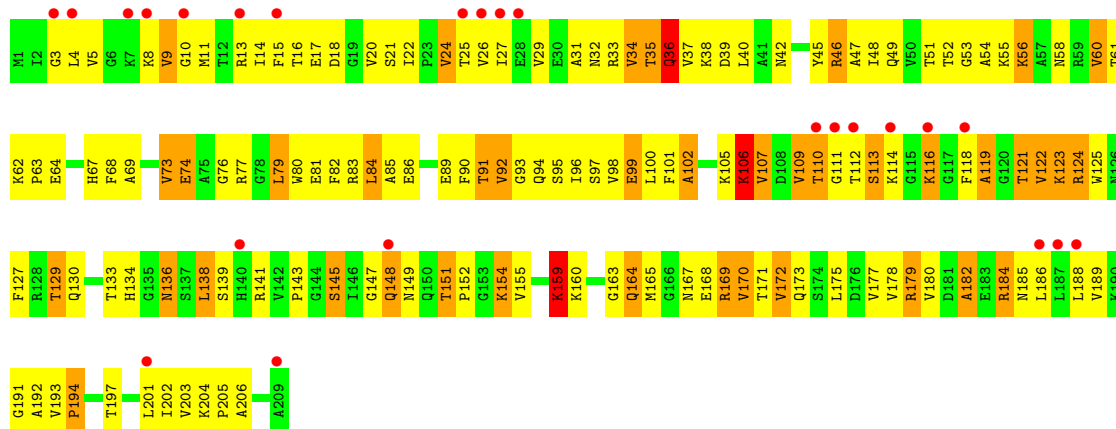
Chain DC:





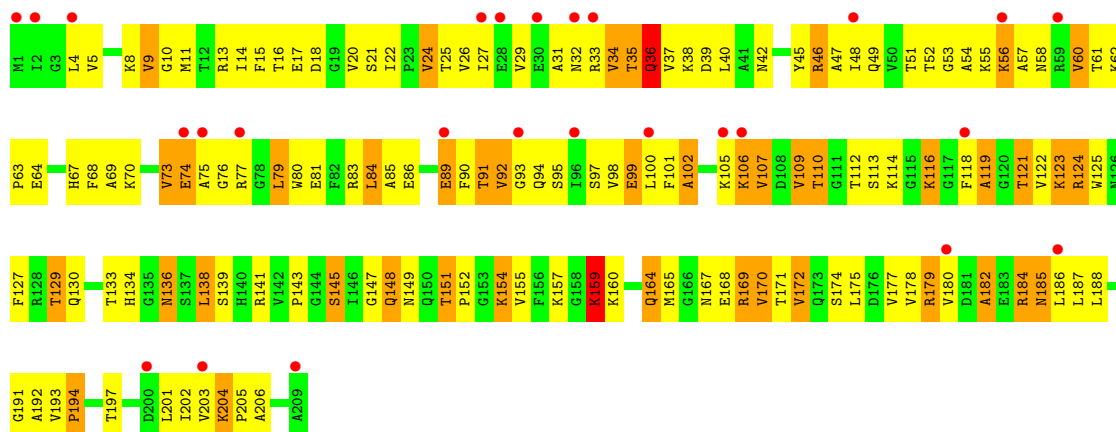
• Molecule 26: 50S ribosomal protein L3

Chain BD:



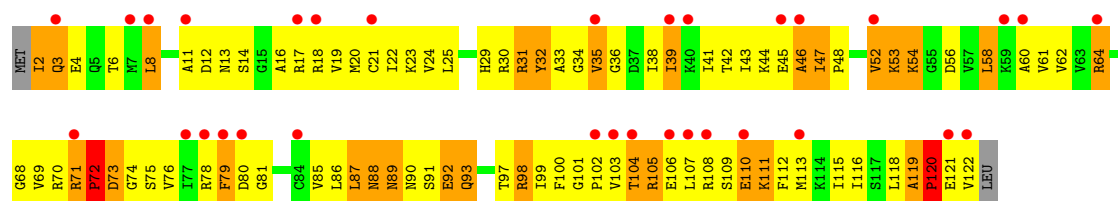
• Molecule 26: 50S ribosomal protein L3

Chain DD:



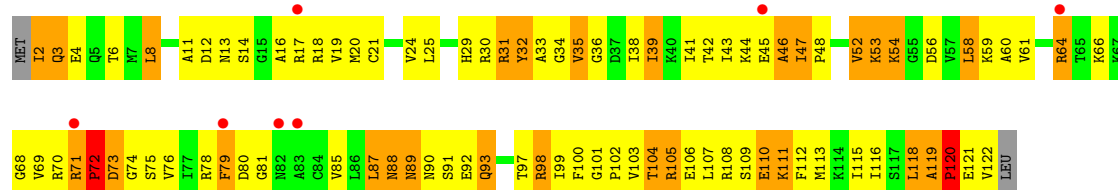
• Molecule 27: 50S ribosomal protein L14

Chain BK:



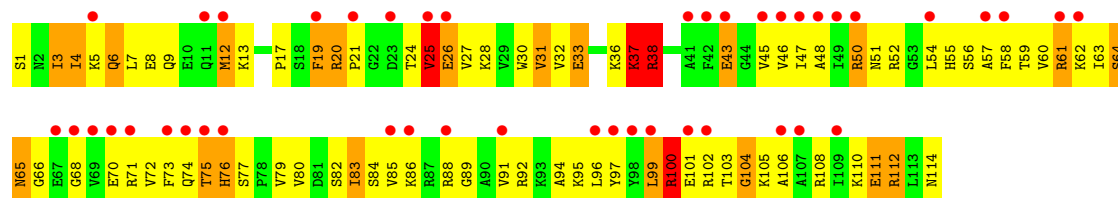
• Molecule 27: 50S ribosomal protein L14

Chain DK:



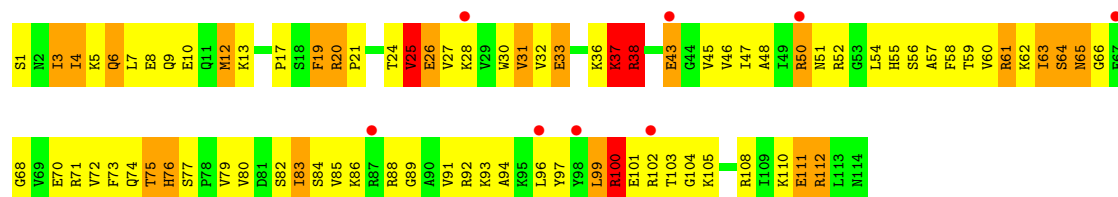
• Molecule 28: 50S ribosomal protein L19

Chain BP:



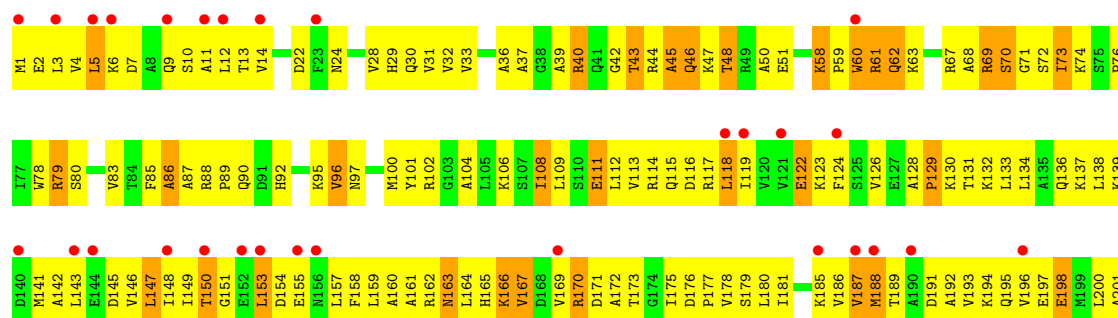
• Molecule 28: 50S ribosomal protein L19

Chain DP:



• Molecule 29: 50S ribosomal protein L4

Chain BE:



• Molecule 29: 50S ribosomal protein L4



A142	I73	M1
A143	K74	E2
E144	S75	L3
D145	P76	V4
V146	I77	L5
L147	W78	K6
I148	R79	D7
I149		A8
G150	V83	Q9
E151	T84	S10
E152	F85	A11
L153	A86	L12
D154	A87	T13
E155	R88	V14
N156	P89	
L157	Q90	D22
F158	D91	F23
L159	H92	N24
A160		
A161	K95	V28
R162	V96	H29
N163	N97	Q30
L164		V31
H165	M100	V32
K166	Y101	V33
V167		A34
D168	A104	V35
V169	L105	A36
R170	K106	A37
D171	S107	G38
A172	I108	A39
T173	L109	R40
G174	E110	Q41
I175	S111	G42
D176	L112	T43
P177	V113	R44
V178	R114	A45
S179	Q115	Q46
L180	D116	K47
I181	R117	T48
	L118	R49
K185	I119	A50
V186		E51
V187	E122	G56
T188	K123	K57
T189	F124	X58
A190		P59
D191	P129	W60
A192	K130	R61
V193	T131	Q62
K194	K132	Q63
V195	L133	K63
Q196	L134	G64
E197	A135	
E198	K136	R67
L200	T137	A68
A201	L138	R69
	K139	S70
	D140	G71
	M141	S72

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- A1  
 K2  
 T3  
 R4  
 K5  
 K6  
 L6  
 T7  
 Q8  
 T9  
 R10  
 S11  
 A12  
 I13  
 G14  
 R15  
 L16  
 P17  
 K18  
 H19  
 K20  
 A21  
 T22  
 L23  
 L24  
 G25  
 L26  
 G27  
 L28  
 R29  
 R30  
 I31  
 G32  
 G33  
 T34  
 V35  
 E36  
 R37  
 T40  
 P41  
 A42  
 I43  
 M46  
 I47  
 V50  
 S51  
 F52  
 M53  
 V54  
 K55  
 V56  
 E57  
 C58

- |     |     |     |     |     |
|-----|-----|-----|-----|-----|
| A1  | V2  | Q3  | Q4  | N6  |
| P7  | T8  | R9  | K11 | R15 |
| H18 | L21 | T22 | A23 | T25 |
| S26 | L27 | S28 | V29 | D30 |
| K31 | T32 | S33 | D30 | K31 |
| G34 | E35 | K36 | H37 | L38 |
| R39 | R39 | H40 | H40 | H40 |
| H41 | I42 | T43 | T43 | A44 |
| D45 | G46 | Y47 | Y48 | R49 |
| K52 | F53 | I54 | A55 | A55 |
| R51 | G50 | R51 | R51 | R51 |

- |    |    |    |    |    |    |    |    |    |     |     |  |     |  |     |  |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |  |     |     |     |     |     |     |     |     |     |     |     |     |     |
|----|----|----|----|----|----|----|----|----|-----|-----|--|-----|--|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| A1 | V2 | Q3 | Q4 | K5 | K6 | P7 | T8 | R9 | S10 | K11 |  | R15 |  | H18 |  | L21 | T22 | A23 | V24 | T25 | S26 | S28 | V29 | D30 | K31 | T32 | S33 | G34 | E35 | K36 | H37 | L38 | R39 | H40 | H41 | I42 | T43 |  | A44 | D45 | G46 | Y47 | Y48 | R49 | G50 | R51 | K52 | V53 | I54 | A55 | Y56 |
|----|----|----|----|----|----|----|----|----|-----|-----|--|-----|--|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- 
- | Category | Value |
|----------|-------|
| M1       | 1     |
| M2       | 1     |
| M3       | 1     |
| M4       | 1     |
| M5       | 1     |
| M6       | 1     |
| M7       | 1     |
| M8       | 1     |
| M9       | 1     |
| M10      | 1     |
| M11      | 1     |
| M12      | 1     |
| M13      | 1     |
| M14      | 1     |
| M15      | 1     |
| M16      | 1     |
| M17      | 1     |
| M18      | 1     |
| M19      | 1     |
| M20      | 1     |
| M21      | 1     |
| M22      | 1     |
| M23      | 1     |
| M24      | 1     |
| M25      | 1     |
| M26      | 1     |
| M27      | 1     |
| M28      | 1     |
| M29      | 1     |
| M30      | 1     |
| M31      | 1     |
| M32      | 1     |

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|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | K2 | V3 | R4 | A5 | S6 | V7 | K8 | R9 | L10 | C11 | R12 | N13 | G14 | K15 | L16 | V17 | K18 | R19 | D20 | G21 | V22 | I23 | R24 | V25 | I26 | C27 | S28 | A29 | H33 | K34 | Q35 | R36 | Q37 | G38 |
|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

Chain B1: 



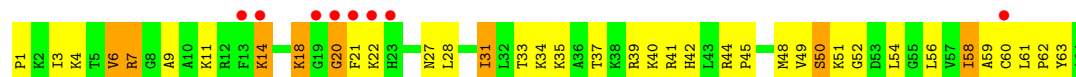
- Molecule 33: 50S ribosomal protein L33

Chain D1: 



- Molecule 34: 50S ribosomal protein L35

Chain B3: 



- Molecule 34: 50S ribosomal protein L35

Chain D3: 



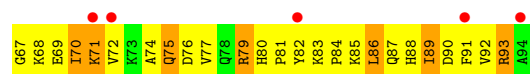
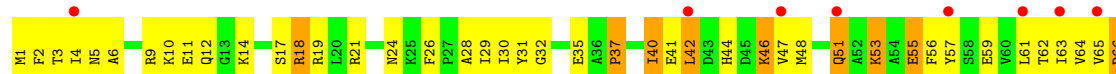
- Molecule 35: 50S ribosomal protein L25

Chain BV: 



- Molecule 35: 50S ribosomal protein L25

Chain DV: 



- Molecule 36: 50S ribosomal protein L34

Chain B2: 



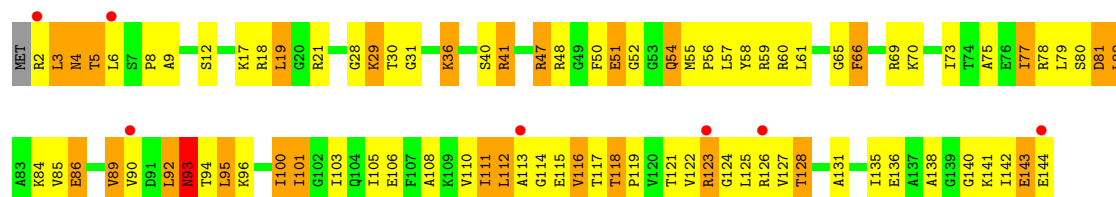
- Molecule 36: 50S ribosomal protein L34

Chain D2: 



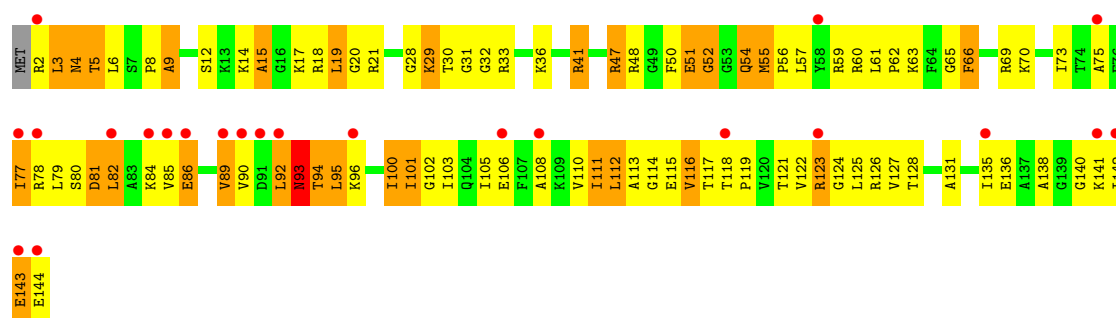
- Molecule 37: 50S ribosomal protein L15

Chain BL: 



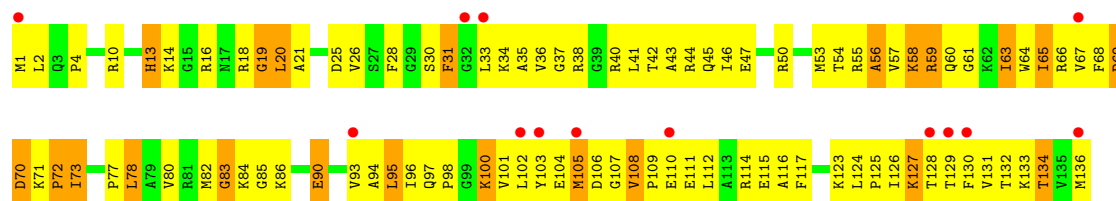
- Molecule 37: 50S ribosomal protein L15

Chain DL: 



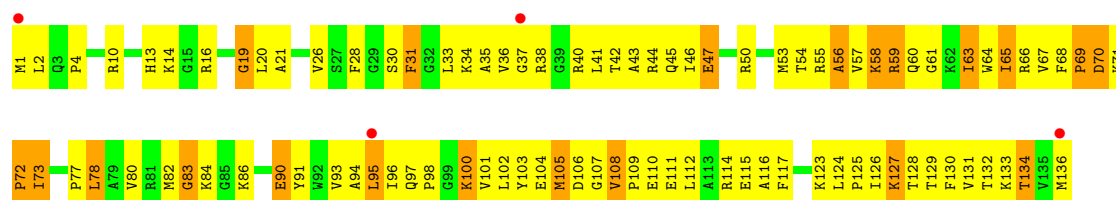
- Molecule 38: 50S ribosomal protein L16

Chain BM: 



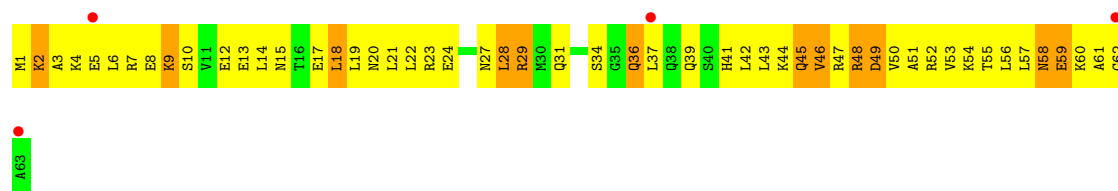
- Molecule 38: 50S ribosomal protein L16

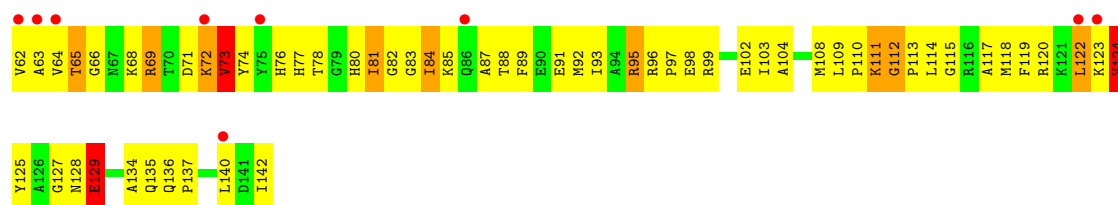
Chain DM: 



- Molecule 39: 50S ribosomal protein L29

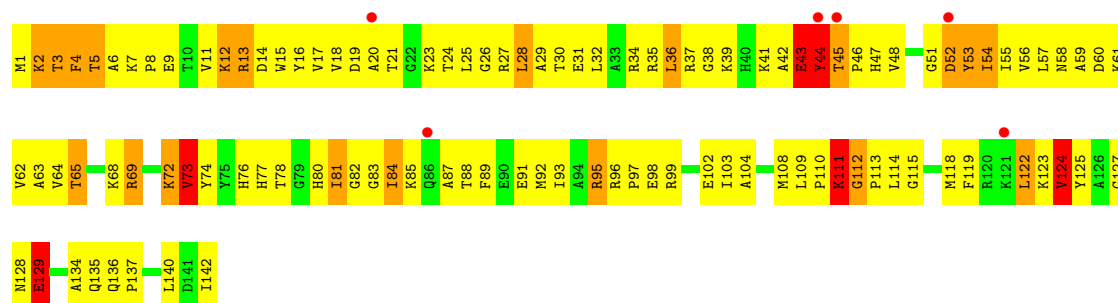
Chain BX: 





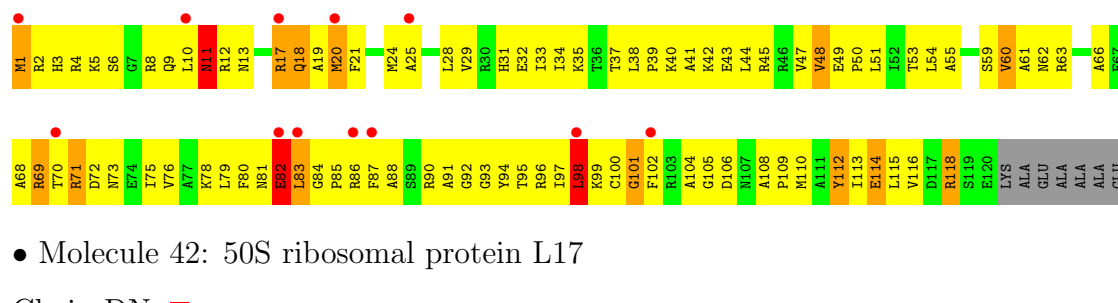
• Molecule 41: 50S ribosomal protein L13

Chain DJ:



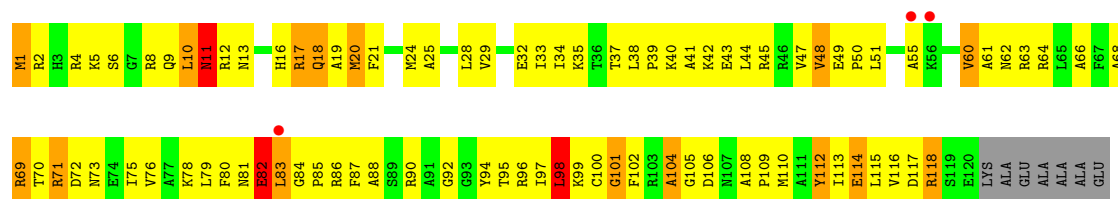
• Molecule 42: 50S ribosomal protein L17

Chain BN:



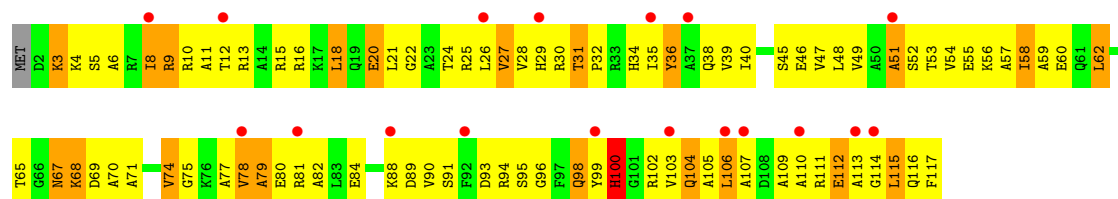
• Molecule 42: 50S ribosomal protein L17

Chain DN:



• Molecule 43: 50S ribosomal protein L18

Chain BO:



• Molecule 43: 50S ribosomal protein L18

MET
D2
K3
K4
S5
A6
R7
T8
R9
R10
A11
T12
R13
A14
R15
R16
K17
L18
Q19
E20
L21
G22
A23
T24
R25
L26
V27
V28
H29
R30
T31
R33
H34
I35
X36
A37
Q38
V39
L40
S45
E46
V47
L48
V49
A50
A51
S52
T53
V54
E55
X56
A57
L58
A59
E60
O61
L62

T65	G66	I67	K68	D69	A70	A71	V74	G75	K76	A77	V78	A79	E80	R81	A82	L83	E84	I87	K88	D89	V90	S91	F92	D93	R94	S95	G96	F97	Q98	Y99	H100	G101	R102	V103	Q104	A105	L106	A107	D108	A109	A110	R111	E112	A113	G114	L115	Q116	F117
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- Chain BQ: 

A66	A67	A68	A69	A70	A71	A72	A73	A74	A75	A76	A77	A78	A79	A80	A81	A82	A83	A84	A85	A86	A87	A88	A89	A90	A91	A92	A93	A94	A95	A96	A97	A98	A99	A100	A101	A102	A103	A104	A105	A106	A107	A108	A109	A110	A111	A112	A113	A114	A115	A116	A117	A118	A119	A120	A121	A122	A123	A124	A125	A126	A127	A128	A129	A130	A131	A132	A133	A134	A135	A136	A137	A138	A139	A140	A141	A142	A143	A144	A145	A146	A147	A148	A149	A150	A151	A152	A153	A154	A155	A156	A157	A158	A159	A160	A161	A162	A163	A164	A165	A166	A167	A168	A169	A170	A171	A172	A173	A174	A175	A176	A177	A178	A179	A180	A181	A182	A183	A184	A185	A186	A187	A188	A189	A190	A191	A192	A193	A194	A195	A196	A197	A198	A199	A200	A201	A202	A203	A204	A205	A206	A207	A208	A209	A210	A211	A212	A213	A214	A215	A216	A217	A218	A219	A220	A221	A222	A223	A224	A225	A226	A227	A228	A229	A230	A231	A232	A233	A234	A235	A236	A237	A238	A239	A240	A241	A242	A243	A244	A245	A246	A247	A248	A249	A250	A251	A252	A253	A254	A255	A256	A257	A258	A259	A260	A261	A262	A263	A264	A265	A266	A267	A268	A269	A270	A271	A272	A273	A274	A275	A276	A277	A278	A279	A280	A281	A282	A283	A284	A285	A286	A287	A288	A289	A290	A291	A292	A293	A294	A295	A296	A297	A298	A299	A300	A301	A302	A303	A304	A305	A306	A307	A308	A309	A310	A311	A312	A313	A314	A315	A316	A317	A318	A319	A320	A321	A322	A323	A324	A325	A326	A327	A328	A329	A330	A331	A332	A333	A334	A335	A336	A337	A338	A339	A340	A341	A342	A343	A344	A345	A346	A347	A348	A349	A350	A351	A352	A353	A354	A355	A356	A357	A358	A359	A360	A361	A362	A363	A364	A365	A366	A367	A368	A369	A370	A371	A372	A373	A374	A375	A376	A377	A378	A379	A380	A381	A382	A383	A384	A385	A386	A387	A388	A389	A390	A391	A392	A393	A394	A395	A396	A397	A398	A399	A400	A401	A402	A403	A404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581</
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- Chain DQ:

R69	Q70	I73	R74	Y75	S76	K77	F78	I79	N80	G81	L82	K83	K84	A85	S86	V87	E88	I89	D90	R91	K92	I93	L94	A95	D96	I97	A98	V103	A104	F105	T106	A107	L108	V109	E110	K111	A117	R49	S50	Q51	R52	K53	S54	Q55	F56	R57	Q58	L59	W60	I61	A62	R63	I64	N65	A66
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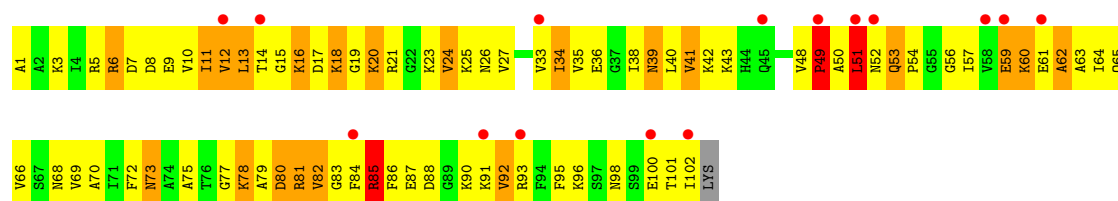
- Chain BS:

D62	D63	A64	D65	I66	L69	K70	V71	T72	K73	I74	F75	V76	D77	P80	S81	M82	K83	R84	I85	M86	F87	R88	A89	K90	G91	R92	A93	D94	R95	I96	L97	K98	R99	T100	S101	H102	I103	V104	I105	V106	I107	S108	D109	R110	D62	D63	A64	D65	I66	L69	K70	V71	T72	K73	I74	F75	V76	D77	P80	S81	M82	K83	R84	I85	M86	F87	R88	A89	K90	G91	R92	A93	D94	R95	I96	L97	K98	R99	T100	S101	H102	I103	V104	I105	V106	I107	S108	D109	R110	D62	D63	A64	D65	I66	L69	K70	V71	T72	K73	I74	F75	V76	D77	P80	S81	M82	K83	R84	I85	M86	F87	R88	A89	K90	G91	R92	A93	D94	R95	I96	L97	K98	R99	T100	S101	H102	I103	V104	I105	V106	I107	S108	D109	R110
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- Chain DS: 

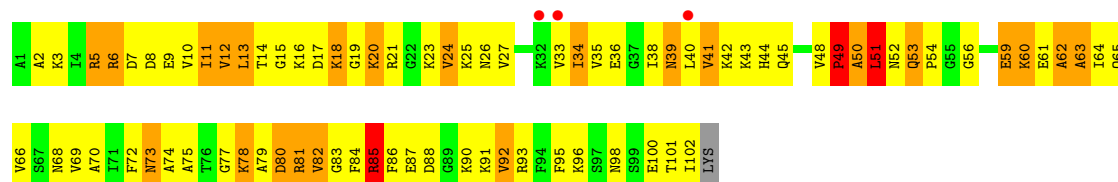
Category	Item	Value	Color
A	A64	100	Green
	D65	100	Red
	I66	100	Blue
	L69	100	Red
	K70	100	Green
	V71	100	Blue
	T72	100	Red
	K73	100	Green
	I74	100	Blue
	T75	100	Red
B	V76	100	Green
	D77	100	Blue
	P80	100	Green
	S81	100	Blue
	M82	100	Red
	K83	100	Green
	R84	100	Blue
	I85	100	Red
	M86	100	Green
	P87	100	Blue
C	R88	100	Red
	A89	100	Green
	G91	100	Blue
	K90	100	Red
	R92	100	Green
	R95	100	Blue
	I96	100	Red
	L97	100	Green
	K98	100	Blue
	R99	100	Red
D	T100	100	Green
	S101	100	Blue
	H102	100	Red
	I103	100	Green
	T104	100	Blue
	V105	100	Red
	V106	100	Green
	V107	100	Blue
	S108	100	Red
	D109	100	Green
E	R110	100	Blue
	A11	100	Red
	E12	100	Green
	T13	100	Blue
	I14	100	Red
	A15	100	Green
	K16	100	Blue
	H17	100	Red
	T18	100	Green
	K19	100	Blue
F	A10	100	Red
	S11	100	Green
	S12	100	Blue
	S13	100	Red
	A14	100	Green
	Q15	100	Blue
	K16	100	Red
	V17	100	Green
	A18	100	Blue
	L19	100	Red
V20	100	Green	
G	A21	100	Blue
	D22	100	Red
	L23	100	Green
	T24	100	Blue
	R25	100	Red
	G26	100	Green
	K27	100	Blue
	K28	100	Red
	V29	100	Green
	S30	100	Blue
H	Q31	100	Red
	A32	100	Green
	L33	100	Blue
	D34	100	Red
	I35	100	Green
	L36	100	Blue
	N40	100	Red
	K41	100	Green
	K42	100	Blue
	A43	100	Red
I	A44	100	Green
	V45	100	Blue
	L46	100	Red
	V47	100	Green
	K48	100	Blue
	K49	100	Red
	V50	100	Green
	L51	100	Blue
	E52	100	Red
	S53	100	Green
J	A54	100	Blue
	I55	100	Red
	A58	100	Green
	E59	100	Blue
	H60	100	Red
	N61	100	Green
	D62	100	Blue
	C63	100	Red

- Chain BU:



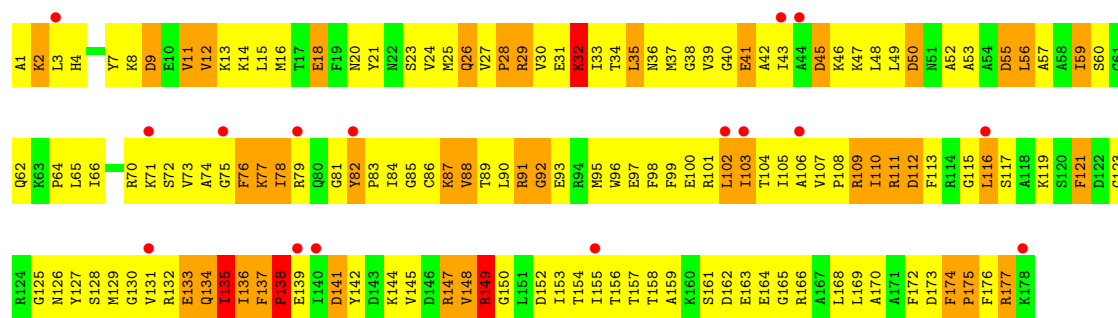
• Molecule 46: 50S ribosomal protein L24

Chain DU:



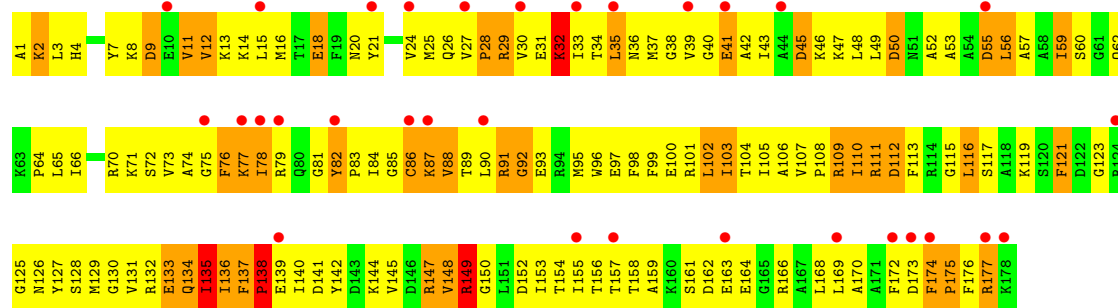
• Molecule 47: 50S ribosomal protein L5

Chain BF:



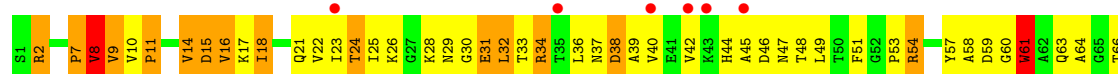
• Molecule 47: 50S ribosomal protein L5

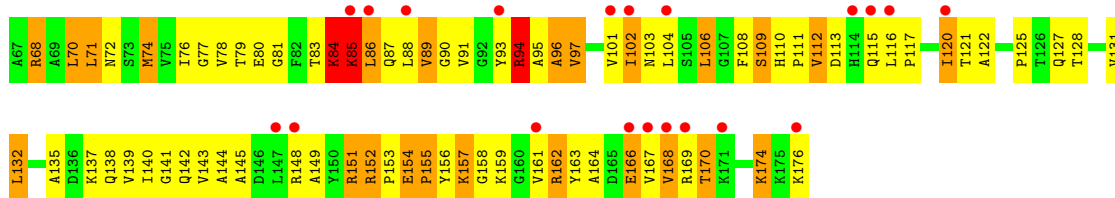
Chain DF:



• Molecule 48: 50S ribosomal protein L6

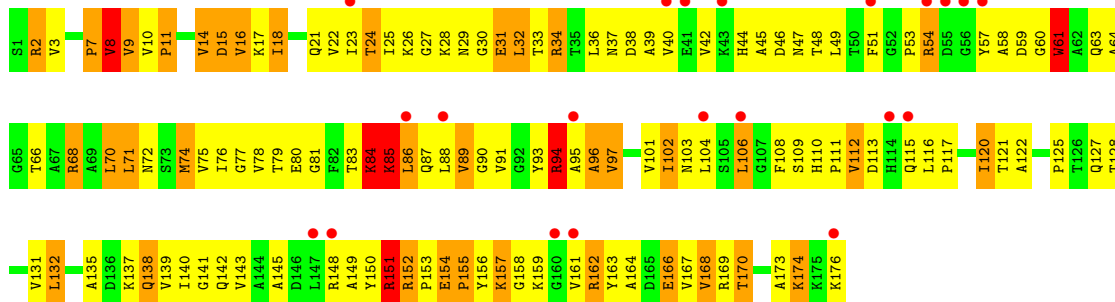
Chain BG:





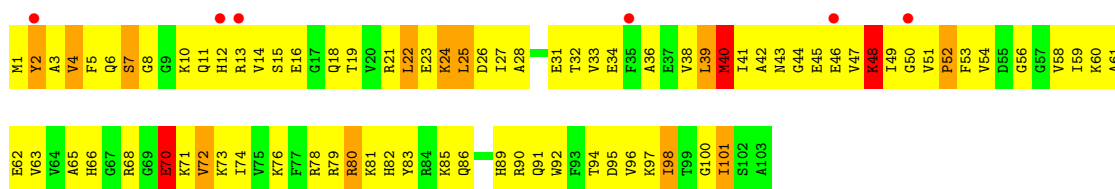
• Molecule 48: 50S ribosomal protein L6

Chain DG:



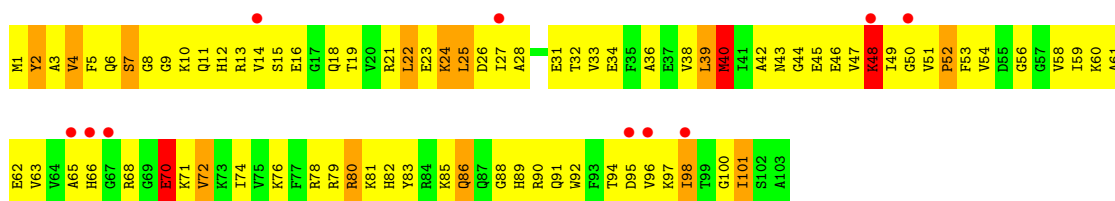
• Molecule 49: 50S ribosomal protein L21

Chain BR:



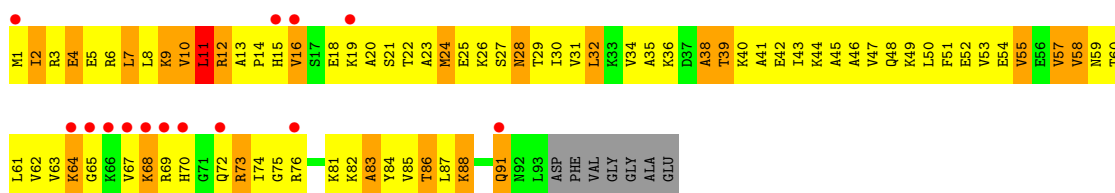
• Molecule 49: 50S ribosomal protein L21

Chain DR:



• Molecule 50: 50S ribosomal protein L23

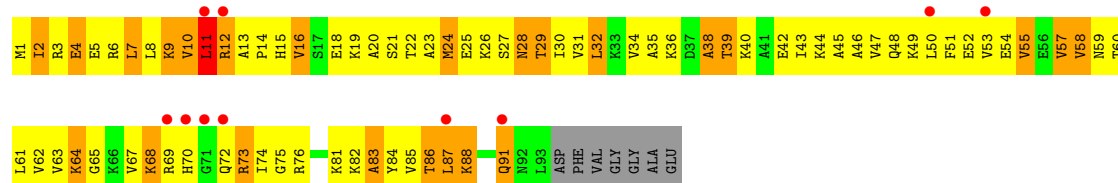
Chain BT:



• Molecule 50: 50S ribosomal protein L23

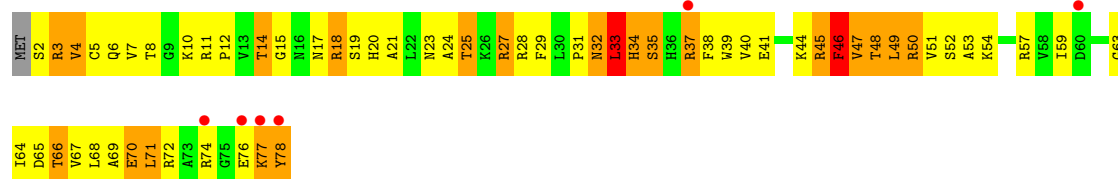


Chain DT: 



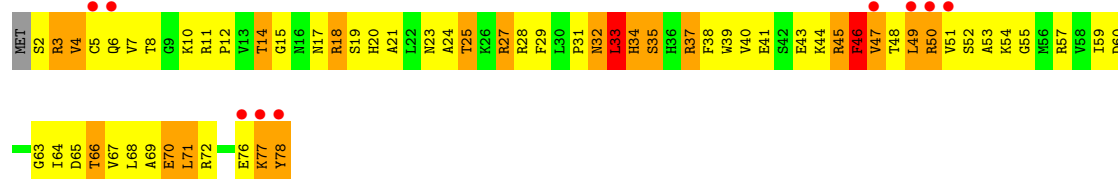
- Molecule 51: 50S ribosomal protein L28

Chain BZ: 



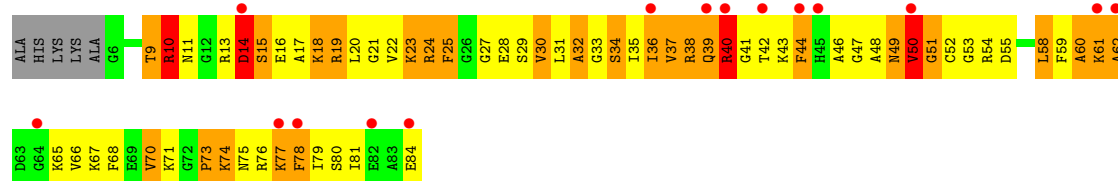
- Molecule 51: 50S ribosomal protein L28

Chain DZ: 



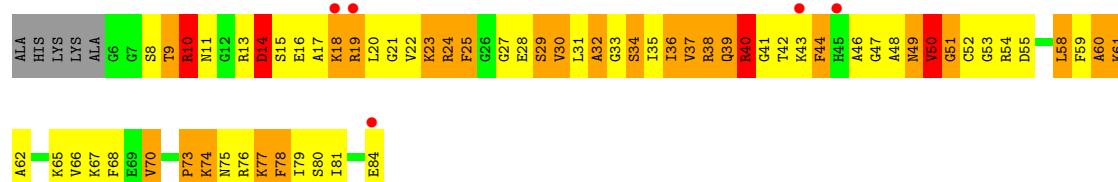
- Molecule 52: 50S ribosomal protein L27

Chain BW: 



- Molecule 52: 50S ribosomal protein L27

Chain DW: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.54 138.41 – 3.55	Depositor EDS
% Data completeness (in resolution range)	88.8 (70.00-3.54) 89.9 (138.41-3.55)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.58Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.281 , 0.320 0.259 , 0.285	Depositor DCC
$R_{free}$ test set	30217 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	125.1	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 20.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 627888 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	284252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% 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, LLL

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	0.26	2/36762 (0.0%)	0.76	22/57350 (0.0%)
1	CA	0.26	3/36762 (0.0%)	0.76	23/57350 (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	0.23	0/1118	0.45	0/1504
5	AF	0.24	0/835	0.44	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	0.46	0/1375
8	CI	0.24	0/1034	0.46	0/1375
9	AJ	0.22	0/796	0.48	0/1077
9	CJ	0.22	0/796	0.47	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	0.46	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AN	0.24	0/785	0.45	0/1043
13	CN	0.24	0/785	0.45	0/1043
14	AO	0.23	0/722	0.47	0/964
14	CO	0.22	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	0.24	0/657	0.46	0/881
16	CQ	0.24	0/666	0.46	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AR	0.23	0/462	0.46	0/621
17	CR	0.23	0/462	0.46	0/621
18	AS	0.25	0/652	0.46	0/877
18	CS	0.25	0/660	0.48	0/888
19	AT	0.24	0/671	0.39	0/888
19	CT	0.24	0/671	0.39	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	0.47	0/570
21	CU	0.26	0/430	0.47	0/570
22	BA	0.23	0/2803	0.74	0/4371
22	DA	0.23	0/2803	0.74	0/4371
23	BB	0.29	10/68314 (0.0%)	0.77	47/106569 (0.0%)
23	DB	0.28	9/68314 (0.0%)	0.78	58/106569 (0.1%)
24	BI	0.24	0/1046	0.46	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	0.53	0/1258
27	DK	0.24	0/939	0.53	0/1258
28	BP	0.24	0/929	0.50	0/1242
28	DP	0.24	0/929	0.50	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	0.48	0/605
30	DY	0.23	0/453	0.48	0/605
31	B0	0.22	0/450	0.53	0/599
31	D0	0.22	0/450	0.53	0/599
32	B4	0.23	0/303	0.46	0/397
32	D4	0.23	0/303	0.46	0/397
33	B1	0.27	0/416	0.48	0/554
33	D1	0.27	0/416	0.48	0/554
34	B3	0.24	0/513	0.47	0/676
34	D3	0.24	0/513	0.47	0/676
35	BV	0.25	0/766	0.42	0/1025
35	DV	0.25	0/766	0.42	0/1025
36	B2	0.25	0/380	0.45	0/498
36	D2	0.25	0/380	0.45	0/498
37	BL	0.23	0/1054	0.47	0/1403
37	DL	0.24	0/1054	0.47	0/1403
38	BM	0.25	0/1093	0.47	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DM	0.25	0/1093	0.47	0/1460
39	BX	0.24	0/510	0.52	0/677
39	DX	0.24	0/510	0.52	0/677
40	BH	0.25	0/1122	0.47	0/1515
40	DH	0.25	0/1122	0.47	0/1515
41	BJ	0.23	0/1152	0.48	0/1551
41	DJ	0.23	0/1152	0.48	0/1551
42	BN	0.24	0/973	0.51	0/1301
42	DN	0.24	0/973	0.51	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	0.47	0/1278
44	DQ	0.25	0/960	0.47	0/1278
45	BS	0.22	0/864	0.51	0/1156
45	DS	0.22	0/864	0.51	0/1156
46	BU	0.25	0/787	0.46	0/1051
46	DU	0.26	0/787	0.46	0/1051
47	BF	0.26	0/1444	0.50	0/1937
47	DF	0.26	0/1444	0.50	0/1937
48	BG	0.23	0/1343	0.47	0/1816
48	DG	0.23	0/1343	0.47	0/1816
49	BR	0.25	0/829	0.48	0/1107
49	DR	0.25	0/829	0.48	0/1107
50	BT	0.22	0/744	0.53	0/994
50	DT	0.22	0/744	0.54	0/994
51	BZ	0.25	0/635	0.50	0/848
51	DZ	0.25	0/635	0.50	0/848
52	BW	0.28	0/603	0.48	0/797
52	DW	0.28	0/603	0.48	0/797
All	All	0.26	24/306360 (0.0%)	0.70	150/457969 (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	15
1	CA	1	15
23	BB	0	41
23	DB	0	40
All	All	1	111

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-16.49	1.26	1.41
23	DB	1086	A	C5-C6	-16.38	1.26	1.41
23	BB	2322	A	O3'-P	14.51	1.78	1.61
23	BB	2318	G	O3'-P	-12.62	1.46	1.61
23	DB	1088	A	C6-N1	-10.61	1.28	1.35

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1213	A	O5'-P-OP1	-32.89	71.23	110.70
23	DB	2204	G	O5'-P-OP1	-29.68	75.08	110.70
1	AA	1213	A	O5'-P-OP2	-28.32	76.72	110.70
23	BB	2204	G	O5'-P-OP2	-28.25	76.80	110.70
23	BB	2791	G	O5'-P-OP1	-28.20	76.86	110.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	CA	366	A	C3'

5 of 111 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	437	U	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	1241	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CA	32831	0	16521	1247	0
2	AC	1624	0	1699	150	0
2	CC	1624	0	1699	150	0
3	AD	1643	0	1710	174	0
3	CD	1643	0	1710	174	0
4	AE	1105	0	1148	94	0
4	CE	1105	0	1148	93	0
5	AF	817	0	808	99	0
5	CF	817	0	808	93	0
6	AG	1174	0	1230	105	0
6	CG	1196	0	1246	98	0
7	AH	979	0	1034	82	0
7	CH	979	0	1034	79	0
8	AI	1022	0	1070	133	0
8	CI	1022	0	1070	132	0
9	AJ	786	0	828	81	0
9	CJ	786	0	828	87	0
10	AK	877	0	887	106	0
10	CK	877	0	887	104	0
11	AL	955	0	1019	95	0
11	CL	955	0	1019	95	0
12	AM	883	0	944	107	0
12	CM	876	0	937	111	0
13	AN	774	0	827	108	0
13	CN	774	0	827	110	0
14	AO	714	0	734	47	0
14	CO	714	0	734	41	0
15	AP	649	0	666	65	0
15	CP	638	0	656	66	0
16	AQ	648	0	691	76	0
16	CQ	657	0	702	67	0
17	AR	455	0	478	48	0
17	CR	455	0	478	44	0
18	AS	637	0	665	87	0
18	CS	644	0	675	93	0
19	AT	665	0	714	56	0
19	CT	665	0	714	55	0
20	AB	1704	0	1732	218	0
20	CB	1704	0	1732	205	0
21	AU	425	0	449	75	0
21	CU	425	0	449	69	0
22	BA	2507	0	1270	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	2507	0	1270	96	0
23	BB	60995	0	30678	2199	0
23	DB	60995	0	30677	2300	0
24	BI	1032	0	1088	106	0
24	DI	1032	0	1088	176	0
25	BC	2082	0	2157	243	0
25	DC	2082	0	2157	245	0
26	BD	1565	0	1616	196	0
26	DD	1565	0	1616	186	0
27	BK	930	0	1000	110	0
27	DK	930	0	1000	108	0
28	BP	917	0	965	111	0
28	DP	917	0	965	109	0
29	BE	1552	0	1619	165	0
29	DE	1552	0	1619	153	0
30	BY	449	0	491	54	0
30	DY	449	0	491	59	0
31	B0	444	0	461	41	0
31	D0	444	0	461	45	0
32	B4	302	0	340	40	0
32	D4	302	0	340	42	0
33	B1	409	0	440	52	0
33	D1	409	0	440	47	0
34	B3	504	0	574	53	0
34	D3	504	0	574	45	0
35	BV	753	0	780	89	0
35	DV	753	0	780	97	0
36	B2	377	0	418	31	0
36	D2	377	0	418	34	0
37	BL	1045	0	1117	132	0
37	DL	1045	0	1117	153	0
38	BM	1074	0	1157	117	0
38	DM	1074	0	1157	119	0
39	BX	509	0	543	71	0
39	DX	509	0	543	72	0
40	BH	1111	0	1148	197	0
40	DH	1111	0	1148	150	0
41	BJ	1129	0	1162	143	0
41	DJ	1129	0	1162	144	0
42	BN	960	0	1000	118	0
42	DN	960	0	1000	118	0
43	BO	892	0	923	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DO	892	0	923	103	0
44	BQ	947	0	1022	144	0
44	DQ	947	0	1022	141	0
45	BS	857	0	922	83	0
45	DS	857	0	922	87	0
46	BU	779	0	834	113	0
46	DU	779	0	834	114	0
47	BF	1420	0	1460	225	0
47	DF	1420	0	1460	228	0
48	BG	1323	0	1374	189	0
48	DG	1323	0	1374	191	0
49	BR	816	0	839	109	0
49	DR	816	0	839	112	0
50	BT	738	0	807	124	0
50	DT	738	0	807	128	0
51	BZ	625	0	652	80	0
51	DZ	625	0	652	77	0
52	BW	596	0	610	128	0
52	DW	596	0	610	131	0
53	AA	60	0	0	0	0
53	BB	110	0	0	0	0
53	CA	61	0	0	0	0
53	CN	1	0	0	0	0
53	DB	111	0	0	0	0
54	AA	93	0	117	6	0
54	BB	31	0	39	1	0
54	CA	93	0	117	5	0
54	DB	31	0	39	0	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	292	0	0	1	0
56	AE	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	2	0	0	0	0
56	AN	2	0	0	0	0
56	AT	2	0	0	0	0
56	B2	1	0	0	0	0
56	BB	492	0	0	7	0
56	BC	7	0	0	0	0
56	BE	3	0	0	0	0
56	BH	1	0	0	0	0
56	BL	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CA	297	0	0	2	0
56	CE	2	0	0	0	0
56	CK	1	0	0	0	0
56	CL	2	0	0	0	0
56	CN	4	0	0	0	0
56	CT	2	0	0	0	0
56	DB	502	0	0	8	0
56	DC	4	0	0	0	0
56	DE	2	0	0	0	0
56	DL	4	0	0	0	0
All	All	284252	0	190973	16353	0

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 35.

The worst 5 of 16353 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	1.42	1.17
23:DB:855:G:H21	52:DW:23:LYS:HG2	1.12	1.14
26:BD:106:LYS:HB3	26:BD:206:ALA:H	1.13	1.11
26:DD:106:LYS:HB3	26:DD:206:ALA:H	1.13	1.09
37:BL:143:GLU:HG2	37:BL:144:GLU:H	1.18	1.08

There are no symmetry-related clashes.

## 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%)	157 (77%)	34 (17%)	13 (6%)	2	30
2	CC	204/232 (88%)	156 (76%)	35 (17%)	13 (6%)	2	30
3	AD	203/205 (99%)	144 (71%)	45 (22%)	14 (7%)	2	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CD	203/205 (99%)	143 (70%)	45 (22%)	15 (7%)	2	25
4	AE	148/166 (89%)	114 (77%)	30 (20%)	4 (3%)	8	57
4	CE	148/166 (89%)	115 (78%)	29 (20%)	4 (3%)	8	57
5	AF	98/135 (73%)	71 (72%)	17 (17%)	10 (10%)	1	15
5	CF	98/135 (73%)	70 (71%)	19 (19%)	9 (9%)	1	18
6	AG	148/178 (83%)	117 (79%)	22 (15%)	9 (6%)	2	31
6	CG	150/178 (84%)	121 (81%)	18 (12%)	11 (7%)	2	26
7	AH	127/129 (98%)	99 (78%)	24 (19%)	4 (3%)	7	54
7	CH	127/129 (98%)	99 (78%)	23 (18%)	5 (4%)	5	47
8	AI	125/129 (97%)	88 (70%)	28 (22%)	9 (7%)	2	26
8	CI	125/129 (97%)	86 (69%)	29 (23%)	10 (8%)	1	22
9	AJ	96/103 (93%)	71 (74%)	15 (16%)	10 (10%)	1	15
9	CJ	96/103 (93%)	70 (73%)	15 (16%)	11 (12%)	1	13
10	AK	115/128 (90%)	83 (72%)	26 (23%)	6 (5%)	3	36
10	CK	115/128 (90%)	84 (73%)	25 (22%)	6 (5%)	3	36
11	AL	121/123 (98%)	79 (65%)	34 (28%)	8 (7%)	2	29
11	CL	121/123 (98%)	79 (65%)	34 (28%)	8 (7%)	2	29
12	AM	112/117 (96%)	76 (68%)	28 (25%)	8 (7%)	2	27
12	CM	111/117 (95%)	77 (69%)	26 (23%)	8 (7%)	2	26
13	AN	92/100 (92%)	61 (66%)	21 (23%)	10 (11%)	1	13
13	CN	92/100 (92%)	58 (63%)	24 (26%)	10 (11%)	1	13
14	AO	86/89 (97%)	63 (73%)	19 (22%)	4 (5%)	4	40
14	CO	86/89 (97%)	64 (74%)	19 (22%)	3 (4%)	6	51
15	AP	80/82 (98%)	57 (71%)	19 (24%)	4 (5%)	3	38
15	CP	78/82 (95%)	55 (70%)	18 (23%)	5 (6%)	2	30
16	AQ	78/83 (94%)	56 (72%)	16 (20%)	6 (8%)	1	24
16	CQ	79/83 (95%)	56 (71%)	17 (22%)	6 (8%)	2	24
17	AR	53/74 (72%)	39 (74%)	11 (21%)	3 (6%)	3	34
17	CR	53/74 (72%)	40 (76%)	10 (19%)	3 (6%)	3	34
18	AS	77/91 (85%)	60 (78%)	11 (14%)	6 (8%)	1	23
18	CS	78/91 (86%)	61 (78%)	11 (14%)	6 (8%)	1	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AT	83/86 (96%)	63 (76%)	15 (18%)	5 (6%)	2	32
19	CT	83/86 (96%)	64 (77%)	14 (17%)	5 (6%)	2	32
20	AB	216/240 (90%)	149 (69%)	52 (24%)	15 (7%)	2	28
20	CB	216/240 (90%)	149 (69%)	51 (24%)	16 (7%)	2	25
21	AU	49/70 (70%)	28 (57%)	14 (29%)	7 (14%)	0	7
21	CU	49/70 (70%)	27 (55%)	15 (31%)	7 (14%)	0	7
24	BI	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	5	50
24	DI	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	5	50
25	BC	269/272 (99%)	168 (62%)	58 (22%)	43 (16%)	0	5
25	DC	269/272 (99%)	167 (62%)	59 (22%)	43 (16%)	0	5
26	BD	207/209 (99%)	119 (58%)	59 (28%)	29 (14%)	0	8
26	DD	207/209 (99%)	119 (58%)	59 (28%)	29 (14%)	0	8
27	BK	119/123 (97%)	79 (66%)	22 (18%)	18 (15%)	0	6
27	DK	119/123 (97%)	78 (66%)	23 (19%)	18 (15%)	0	6
28	BP	112/114 (98%)	61 (54%)	36 (32%)	15 (13%)	0	9
28	DP	112/114 (98%)	60 (54%)	37 (33%)	15 (13%)	0	9
29	BE	199/201 (99%)	126 (63%)	48 (24%)	25 (13%)	0	11
29	DE	199/201 (99%)	127 (64%)	46 (23%)	26 (13%)	0	10
30	BY	56/58 (97%)	40 (71%)	13 (23%)	3 (5%)	3	36
30	DY	56/58 (97%)	40 (71%)	13 (23%)	3 (5%)	3	36
31	B0	54/56 (96%)	43 (80%)	6 (11%)	5 (9%)	1	18
31	D0	54/56 (96%)	42 (78%)	7 (13%)	5 (9%)	1	18
32	B4	36/38 (95%)	18 (50%)	7 (19%)	11 (31%)	0	0
32	D4	36/38 (95%)	18 (50%)	7 (19%)	11 (31%)	0	0
33	B1	48/54 (89%)	31 (65%)	12 (25%)	5 (10%)	1	15
33	D1	48/54 (89%)	33 (69%)	10 (21%)	5 (10%)	1	15
34	B3	62/64 (97%)	41 (66%)	16 (26%)	5 (8%)	1	22
34	D3	62/64 (97%)	41 (66%)	16 (26%)	5 (8%)	1	22
35	BV	92/94 (98%)	67 (73%)	20 (22%)	5 (5%)	3	36
35	DV	92/94 (98%)	67 (73%)	21 (23%)	4 (4%)	4	43
36	B2	44/46 (96%)	37 (84%)	4 (9%)	3 (7%)	2	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	D2	44/46 (96%)	37 (84%)	4 (9%)	3 (7%)	2	28
37	BL	141/144 (98%)	90 (64%)	29 (21%)	22 (16%)	0	5
37	DL	141/144 (98%)	90 (64%)	27 (19%)	24 (17%)	0	4
38	BM	134/136 (98%)	80 (60%)	40 (30%)	14 (10%)	1	15
38	DM	134/136 (98%)	81 (60%)	39 (29%)	14 (10%)	1	15
39	BX	61/63 (97%)	38 (62%)	16 (26%)	7 (12%)	1	13
39	DX	61/63 (97%)	37 (61%)	17 (28%)	7 (12%)	1	13
40	BH	147/149 (99%)	83 (56%)	27 (18%)	37 (25%)	0	1
40	DH	147/149 (99%)	89 (60%)	30 (20%)	28 (19%)	0	3
41	BJ	140/142 (99%)	86 (61%)	36 (26%)	18 (13%)	0	10
41	DJ	140/142 (99%)	85 (61%)	36 (26%)	19 (14%)	0	8
42	BN	118/127 (93%)	77 (65%)	30 (25%)	11 (9%)	1	18
42	DN	118/127 (93%)	76 (64%)	30 (25%)	12 (10%)	1	15
43	BO	114/117 (97%)	79 (69%)	24 (21%)	11 (10%)	1	17
43	DO	114/117 (97%)	80 (70%)	23 (20%)	11 (10%)	1	17
44	BQ	115/117 (98%)	75 (65%)	33 (29%)	7 (6%)	2	31
44	DQ	115/117 (98%)	77 (67%)	30 (26%)	8 (7%)	2	27
45	BS	108/110 (98%)	67 (62%)	29 (27%)	12 (11%)	1	13
45	DS	108/110 (98%)	66 (61%)	29 (27%)	13 (12%)	1	12
46	BU	100/103 (97%)	58 (58%)	25 (25%)	17 (17%)	0	4
46	DU	100/103 (97%)	59 (59%)	23 (23%)	18 (18%)	0	4
47	BF	176/178 (99%)	101 (57%)	49 (28%)	26 (15%)	0	6
47	DF	176/178 (99%)	102 (58%)	49 (28%)	25 (14%)	0	8
48	BG	174/176 (99%)	95 (55%)	48 (28%)	31 (18%)	0	4
48	DG	174/176 (99%)	94 (54%)	50 (29%)	30 (17%)	0	4
49	BR	101/103 (98%)	62 (61%)	26 (26%)	13 (13%)	0	10
49	DR	101/103 (98%)	62 (61%)	26 (26%)	13 (13%)	0	10
50	BT	91/100 (91%)	52 (57%)	23 (25%)	16 (18%)	0	4
50	DT	91/100 (91%)	51 (56%)	23 (25%)	17 (19%)	0	3
51	BZ	75/78 (96%)	51 (68%)	14 (19%)	10 (13%)	0	9
51	DZ	75/78 (96%)	50 (67%)	15 (20%)	10 (13%)	0	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	BW	77/84 (92%)	32 (42%)	22 (29%)	23 (30%)	0	0
52	DW	77/84 (92%)	30 (39%)	24 (31%)	23 (30%)	0	0
All	All	11241/11914 (94%)	7497 (67%)	2537 (23%)	1207 (11%)	1	14

5 of 1207 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	54	ILE
2	AC	205	GLU
3	AD	24	VAL
3	AD	192	ALA

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AC	170/189 (90%)	145 (85%)	25 (15%)	4	27
2	CC	170/189 (90%)	145 (85%)	25 (15%)	4	27
3	AD	172/172 (100%)	148 (86%)	24 (14%)	5	29
3	CD	172/172 (100%)	148 (86%)	24 (14%)	5	29
4	AE	113/125 (90%)	102 (90%)	11 (10%)	12	51
4	CE	113/125 (90%)	102 (90%)	11 (10%)	12	51
5	AF	87/116 (75%)	70 (80%)	17 (20%)	2	12
5	CF	87/116 (75%)	70 (80%)	17 (20%)	2	12
6	AG	123/146 (84%)	109 (89%)	14 (11%)	8	40
6	CG	125/146 (86%)	114 (91%)	11 (9%)	14	57
7	AH	104/104 (100%)	97 (93%)	7 (7%)	23	71
7	CH	104/104 (100%)	97 (93%)	7 (7%)	23	71
8	AI	105/106 (99%)	89 (85%)	16 (15%)	4	25
8	CI	105/106 (99%)	89 (85%)	16 (15%)	4	25
9	AJ	86/90 (96%)	74 (86%)	12 (14%)	5	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	CJ	86/90 (96%)	75 (87%)	11 (13%)	6	33
10	AK	90/98 (92%)	76 (84%)	14 (16%)	4	23
10	CK	90/98 (92%)	77 (86%)	13 (14%)	5	27
11	AL	103/103 (100%)	92 (89%)	11 (11%)	10	45
11	CL	103/103 (100%)	92 (89%)	11 (11%)	10	45
12	AM	92/95 (97%)	79 (86%)	13 (14%)	5	29
12	CM	91/95 (96%)	79 (87%)	12 (13%)	6	32
13	AN	79/83 (95%)	64 (81%)	15 (19%)	2	13
13	CN	79/83 (95%)	64 (81%)	15 (19%)	2	13
14	AO	76/77 (99%)	69 (91%)	7 (9%)	13	54
14	CO	76/77 (99%)	69 (91%)	7 (9%)	13	54
15	AP	65/65 (100%)	59 (91%)	6 (9%)	13	54
15	CP	65/65 (100%)	58 (89%)	7 (11%)	9	44
16	AQ	74/77 (96%)	59 (80%)	15 (20%)	2	10
16	CQ	75/77 (97%)	62 (83%)	13 (17%)	3	17
17	AR	48/64 (75%)	41 (85%)	7 (15%)	5	27
17	CR	48/64 (75%)	41 (85%)	7 (15%)	5	27
18	AS	70/78 (90%)	56 (80%)	14 (20%)	2	11
18	CS	71/78 (91%)	56 (79%)	15 (21%)	1	9
19	AT	65/65 (100%)	58 (89%)	7 (11%)	9	44
19	CT	65/65 (100%)	58 (89%)	7 (11%)	9	44
20	AB	180/198 (91%)	149 (83%)	31 (17%)	3	18
20	CB	180/198 (91%)	147 (82%)	33 (18%)	2	14
21	AU	44/60 (73%)	33 (75%)	11 (25%)	1	6
21	CU	44/60 (73%)	33 (75%)	11 (25%)	1	6
24	BI	109/109 (100%)	107 (98%)	2 (2%)	71	94
24	DI	109/109 (100%)	103 (94%)	6 (6%)	30	78
25	BC	216/217 (100%)	182 (84%)	34 (16%)	4	23
25	DC	216/217 (100%)	183 (85%)	33 (15%)	4	25
26	BD	164/164 (100%)	139 (85%)	25 (15%)	4	25
26	DD	164/164 (100%)	138 (84%)	26 (16%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BK	102/104 (98%)	77 (76%)	25 (24%)	1	6
27	DK	102/104 (98%)	77 (76%)	25 (24%)	1	6
28	BP	99/99 (100%)	81 (82%)	18 (18%)	2	15
28	DP	99/99 (100%)	81 (82%)	18 (18%)	2	15
29	BE	165/165 (100%)	144 (87%)	21 (13%)	6	34
29	DE	165/165 (100%)	144 (87%)	21 (13%)	6	34
30	BY	48/48 (100%)	37 (77%)	11 (23%)	1	7
30	DY	48/48 (100%)	37 (77%)	11 (23%)	1	7
31	B0	47/47 (100%)	38 (81%)	9 (19%)	2	13
31	D0	47/47 (100%)	38 (81%)	9 (19%)	2	13
32	B4	34/34 (100%)	28 (82%)	6 (18%)	3	16
32	D4	34/34 (100%)	28 (82%)	6 (18%)	3	16
33	B1	45/48 (94%)	36 (80%)	9 (20%)	2	11
33	D1	45/48 (94%)	37 (82%)	8 (18%)	2	16
34	B3	51/51 (100%)	46 (90%)	5 (10%)	12	50
34	D3	51/51 (100%)	46 (90%)	5 (10%)	12	50
35	BV	78/78 (100%)	63 (81%)	15 (19%)	2	12
35	DV	78/78 (100%)	63 (81%)	15 (19%)	2	12
36	B2	38/38 (100%)	31 (82%)	7 (18%)	2	14
36	D2	38/38 (100%)	31 (82%)	7 (18%)	2	14
37	BL	102/103 (99%)	91 (89%)	11 (11%)	9	44
37	DL	102/103 (99%)	91 (89%)	11 (11%)	9	44
38	BM	109/109 (100%)	92 (84%)	17 (16%)	4	23
38	DM	109/109 (100%)	93 (85%)	16 (15%)	4	27
39	BX	55/55 (100%)	49 (89%)	6 (11%)	9	44
39	DX	55/55 (100%)	49 (89%)	6 (11%)	9	44
40	BH	114/114 (100%)	86 (75%)	28 (25%)	1	6
40	DH	114/114 (100%)	91 (80%)	23 (20%)	2	11
41	BJ	116/116 (100%)	98 (84%)	18 (16%)	4	24
41	DJ	116/116 (100%)	98 (84%)	18 (16%)	4	24
42	BN	100/103 (97%)	85 (85%)	15 (15%)	4	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	DN	100/103 (97%)	86 (86%)	14 (14%)	5	29
43	BO	86/87 (99%)	68 (79%)	18 (21%)	1	10
43	DO	86/87 (99%)	68 (79%)	18 (21%)	1	10
44	BQ	89/89 (100%)	81 (91%)	8 (9%)	14	55
44	DQ	89/89 (100%)	80 (90%)	9 (10%)	11	49
45	BS	93/93 (100%)	78 (84%)	15 (16%)	3	22
45	DS	93/93 (100%)	76 (82%)	17 (18%)	2	14
46	BU	83/84 (99%)	68 (82%)	15 (18%)	2	15
46	DU	83/84 (99%)	68 (82%)	15 (18%)	2	15
47	BF	149/149 (100%)	117 (78%)	32 (22%)	1	9
47	DF	149/149 (100%)	116 (78%)	33 (22%)	1	8
48	BG	137/137 (100%)	113 (82%)	24 (18%)	3	17
48	DG	137/137 (100%)	113 (82%)	24 (18%)	3	17
49	BR	84/84 (100%)	71 (84%)	13 (16%)	4	24
49	DR	84/84 (100%)	71 (84%)	13 (16%)	4	24
50	BT	80/84 (95%)	69 (86%)	11 (14%)	5	29
50	DT	80/84 (95%)	68 (85%)	12 (15%)	4	26
51	BZ	67/68 (98%)	53 (79%)	14 (21%)	1	10
51	DZ	67/68 (98%)	54 (81%)	13 (19%)	2	12
52	BW	59/62 (95%)	44 (75%)	15 (25%)	1	6
52	DW	59/62 (95%)	44 (75%)	15 (25%)	1	6
All	All	9333/9700 (96%)	7889 (84%)	1444 (16%)	4	24

5 of 1444 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BG	54	ARG
6	CG	109	LYS
47	DF	2	LYS
49	BR	4	VAL
2	CC	41	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 326 such sidechains are listed below:

Mol	Chain	Res	Type
47	BF	126	ASN
7	CH	3	GLN
45	DS	40	ASN
48	BG	63	GLN
2	CC	31	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	246 (16%)	21 (1%)
1	CA	1529/1542 (99%)	231 (15%)	19 (1%)
22	BA	116/120 (96%)	16 (13%)	0
22	DA	116/120 (96%)	14 (12%)	0
23	BB	2837/2904 (97%)	424 (14%)	20 (0%)
23	DB	2837/2904 (97%)	424 (14%)	21 (0%)
All	All	8964/9132 (98%)	1355 (15%)	81 (0%)

5 of 1355 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 81 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2756	U
1	CA	279	A
23	DB	2336	A
23	BB	2798	U
1	CA	51	A

## 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 353 ligands modelled in this entry, 345 are monoatomic - leaving 8 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$
54	LLL	AA	2061	-	33,33,33	2.35	12 (36%)	49,49,49	1.39	6 (12%)
54	LLL	AA	2062	-	33,33,33	2.39	13 (39%)	49,49,49	1.40	6 (12%)
54	LLL	AA	2063	-	33,33,33	2.35	13 (39%)	49,49,49	1.47	6 (12%)
54	LLL	BB	3111	-	33,33,33	2.39	12 (36%)	49,49,49	1.36	6 (12%)
54	LLL	CA	2062	-	33,33,33	2.35	11 (33%)	49,49,49	1.31	5 (10%)
54	LLL	CA	2063	-	33,33,33	2.41	13 (39%)	49,49,49	1.38	5 (10%)
54	LLL	CA	2064	-	33,33,33	2.29	12 (36%)	49,49,49	1.32	4 (8%)
54	LLL	DB	3112	-	33,33,33	2.39	12 (36%)	49,49,49	1.34	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	LLL	AA	2061	-	-	0/12/65/65	0/3/3/3
54	LLL	AA	2062	-	-	0/12/65/65	0/3/3/3
54	LLL	AA	2063	-	-	0/12/65/65	0/3/3/3
54	LLL	BB	3111	-	-	0/12/65/65	0/3/3/3
54	LLL	CA	2062	-	-	0/12/65/65	0/3/3/3
54	LLL	CA	2063	-	-	0/12/65/65	0/3/3/3
54	LLL	CA	2064	-	-	0/12/65/65	0/3/3/3
54	LLL	DB	3112	-	-	0/12/65/65	0/3/3/3

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	CA	2063	LLL	O53-C53	5.86	1.52	1.43
54	AA	2062	LLL	O53-C53	5.76	1.52	1.43
54	DB	3112	LLL	O53-C53	5.72	1.52	1.43
54	BB	3111	LLL	O53-C53	5.71	1.52	1.43
54	AA	2061	LLL	O53-C53	5.66	1.52	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	AA	2063	LLL	C53-O53-C13	5.12	118.52	111.22
54	CA	2063	LLL	C53-O53-C13	4.80	118.06	111.22
54	AA	2062	LLL	C53-O53-C13	4.69	117.90	111.22
54	CA	2062	LLL	C53-O53-C13	4.66	117.85	111.22
54	BB	3111	LLL	C53-O53-C13	4.59	117.76	111.22

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%)	-0.49	11 (0%) 84 56	22, 85, 131, 156	0
1	CA	1530/1542 (99%)	-0.51	7 (0%) 88 65	5, 60, 120, 167	0
2	AC	206/232 (88%)	0.65	12 (5%) 22 10	14, 72, 111, 136	0
2	CC	206/232 (88%)	0.48	7 (3%) 43 20	5, 74, 103, 160	0
3	AD	205/205 (100%)	1.03	33 (16%) 2 3	21, 87, 115, 135	0
3	CD	205/205 (100%)	0.68	14 (6%) 17 8	8, 65, 107, 121	0
4	AE	150/166 (90%)	0.70	12 (8%) 12 7	6, 74, 105, 134	0
4	CE	150/166 (90%)	0.85	16 (10%) 6 5	5, 59, 96, 125	0
5	AF	100/135 (74%)	1.18	24 (24%) 1 2	22, 72, 115, 148	0
5	CF	100/135 (74%)	0.90	6 (6%) 21 10	12, 72, 109, 123	0
6	AG	150/178 (84%)	0.52	15 (10%) 8 5	47, 89, 116, 152	0
6	CG	152/178 (85%)	0.21	7 (4%) 31 14	29, 80, 115, 134	0
7	AH	129/129 (100%)	0.87	19 (14%) 3 3	31, 80, 112, 136	0
7	CH	129/129 (100%)	0.45	6 (4%) 30 13	5, 56, 91, 112	0
8	AI	127/129 (98%)	0.51	12 (9%) 9 6	31, 83, 118, 143	0
8	CI	127/129 (98%)	0.37	3 (2%) 56 27	35, 84, 118, 157	0
9	AJ	98/103 (95%)	0.78	11 (11%) 6 4	22, 87, 121, 135	0
9	CJ	98/103 (95%)	0.68	9 (9%) 9 6	33, 84, 110, 125	0
10	AK	117/128 (91%)	0.41	2 (1%) 67 35	5, 67, 102, 117	0
10	CK	117/128 (91%)	0.20	3 (2%) 53 25	5, 56, 101, 119	0
11	AL	123/123 (100%)	0.63	9 (7%) 15 7	22, 75, 110, 146	0
11	CL	123/123 (100%)	0.49	4 (3%) 44 21	5, 47, 103, 123	0
12	AM	114/117 (97%)	0.36	4 (3%) 42 20	58, 96, 124, 147	0
12	CM	113/117 (96%)	0.45	5 (4%) 33 15	48, 89, 116, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AN	96/100 (96%)	0.39	1 (1%) 79 48	27, 85, 121, 154	0
13	CN	96/100 (96%)	0.50	7 (7%) 15 7	40, 87, 114, 142	0
14	AO	88/89 (98%)	0.82	7 (7%) 12 7	38, 80, 109, 133	0
14	CO	88/89 (98%)	0.38	3 (3%) 43 20	5, 56, 107, 128	0
15	AP	82/82 (100%)	1.11	12 (14%) 3 3	48, 88, 121, 135	0
15	CP	80/82 (97%)	0.62	6 (7%) 14 7	11, 59, 109, 147	0
16	AQ	80/83 (96%)	1.04	12 (15%) 3 3	31, 87, 117, 124	0
16	CQ	81/83 (97%)	0.44	0 100 100	9, 58, 99, 121	0
17	AR	55/74 (74%)	0.61	4 (7%) 15 7	19, 76, 118, 138	0
17	CR	55/74 (74%)	0.67	6 (10%) 6 5	19, 68, 119, 131	0
18	AS	79/91 (86%)	0.59	4 (5%) 27 12	68, 100, 124, 136	0
18	CS	80/91 (87%)	0.78	13 (16%) 2 2	48, 94, 127, 153	0
19	AT	85/86 (98%)	0.48	1 (1%) 75 43	39, 92, 123, 144	0
19	CT	85/86 (98%)	0.25	3 (3%) 42 20	19, 61, 106, 125	0
20	AB	218/240 (90%)	0.48	12 (5%) 24 11	20, 87, 113, 132	0
20	CB	218/240 (90%)	0.65	20 (9%) 9 6	29, 89, 118, 144	0
21	AU	51/70 (72%)	0.88	5 (9%) 8 5	36, 89, 126, 134	0
21	CU	51/70 (72%)	0.82	8 (15%) 3 3	46, 78, 116, 132	0
22	BA	117/120 (97%)	-0.55	2 (1%) 67 35	47, 78, 117, 140	0
22	DA	117/120 (97%)	-0.41	2 (1%) 67 35	30, 80, 115, 155	0
23	BB	2841/2904 (97%)	-0.24	25 (0%) 81 51	9, 58, 127, 165	0
23	DB	2841/2904 (97%)	-0.25	15 (0%) 88 65	5, 45, 124, 163	0
24	BI	141/141 (100%)	2.01	63 (44%) 1 1	59, 117, 149, 158	0
24	DI	141/141 (100%)	0.93	16 (11%) 6 4	70, 117, 148, 160	0
25	BC	271/272 (99%)	0.85	29 (10%) 6 5	5, 47, 88, 105	0
25	DC	271/272 (99%)	0.78	21 (7%) 13 7	5, 32, 80, 112	0
26	BD	209/209 (100%)	0.68	24 (11%) 5 4	12, 71, 107, 141	0
26	DD	209/209 (100%)	0.81	26 (12%) 5 4	5, 49, 98, 135	0
27	BK	121/123 (98%)	1.43	32 (26%) 1 2	16, 67, 106, 134	0
27	DK	121/123 (98%)	0.84	7 (5%) 22 10	5, 37, 90, 130	0
28	BP	114/114 (100%)	1.64	44 (38%) 1 1	25, 81, 113, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DP	114/114 (100%)	0.75	8 (7%) 16 8	7, 49, 94, 112	0
29	BE	201/201 (100%)	0.99	29 (14%) 3 3	5, 65, 104, 147	0
29	DE	201/201 (100%)	0.55	14 (6%) 16 8	5, 62, 107, 138	0
30	BY	58/58 (100%)	0.68	5 (8%) 11 6	26, 69, 107, 137	0
30	DY	58/58 (100%)	0.46	2 (3%) 43 20	6, 64, 110, 117	0
31	B0	56/56 (100%)	0.82	6 (10%) 6 5	5, 71, 113, 136	0
31	D0	56/56 (100%)	0.23	0 100 100	10, 43, 99, 104	0
32	B4	38/38 (100%)	0.81	4 (10%) 7 5	33, 76, 108, 125	0
32	D4	38/38 (100%)	0.36	0 100 100	15, 65, 94, 105	0
33	B1	50/54 (92%)	1.75	12 (24%) 1 2	50, 75, 102, 115	0
33	D1	50/54 (92%)	0.96	5 (10%) 8 5	27, 74, 105, 118	0
34	B3	64/64 (100%)	0.81	8 (12%) 5 3	9, 55, 82, 106	0
34	D3	64/64 (100%)	0.61	3 (4%) 30 13	5, 39, 84, 101	0
35	BV	94/94 (100%)	0.69	7 (7%) 14 7	31, 86, 115, 129	0
35	DV	94/94 (100%)	0.65	13 (13%) 4 3	8, 79, 108, 125	0
36	B2	46/46 (100%)	0.61	2 (4%) 34 15	8, 40, 81, 113	0
36	D2	46/46 (100%)	0.69	2 (4%) 34 15	5, 28, 69, 113	0
37	BL	143/144 (99%)	0.63	7 (4%) 28 13	9, 63, 99, 134	0
37	DL	143/144 (99%)	0.85	23 (16%) 2 3	5, 55, 95, 123	0
38	BM	136/136 (100%)	0.89	13 (9%) 8 6	5, 65, 100, 131	0
38	DM	136/136 (100%)	0.51	4 (2%) 49 24	5, 55, 94, 134	0
39	BX	63/63 (100%)	0.77	4 (6%) 19 9	18, 76, 110, 123	0
39	DX	63/63 (100%)	0.20	1 (1%) 68 36	36, 82, 107, 142	0
40	BH	149/149 (100%)	2.29	69 (46%) 1 1	25, 98, 122, 146	0
40	DH	149/149 (100%)	1.21	26 (17%) 2 2	18, 88, 112, 141	0
41	BJ	142/142 (100%)	0.76	13 (9%) 9 6	16, 70, 106, 118	0
41	DJ	142/142 (100%)	0.63	6 (4%) 35 15	5, 60, 101, 131	0
42	BN	120/127 (94%)	0.73	12 (10%) 8 5	14, 65, 101, 145	0
42	DN	120/127 (94%)	0.40	3 (2%) 54 26	5, 42, 75, 118	0
43	BO	116/117 (99%)	0.95	18 (15%) 3 3	40, 78, 104, 128	0
43	DO	116/117 (99%)	0.45	4 (3%) 43 20	5, 73, 106, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BQ	117/117 (100%)	0.21	2 (1%) 67 35	5, 60, 95, 109	0
44	DQ	117/117 (100%)	0.52	6 (5%) 27 12	5, 50, 92, 120	0
45	BS	110/110 (100%)	1.29	25 (22%) 1 2	6, 56, 98, 118	0
45	DS	110/110 (100%)	1.22	20 (18%) 2 2	5, 48, 95, 128	0
46	BU	102/103 (99%)	1.08	15 (14%) 3 3	9, 71, 105, 123	0
46	DU	102/103 (99%)	0.36	3 (2%) 49 24	34, 80, 112, 130	0
47	BF	178/178 (100%)	0.69	16 (8%) 10 6	40, 95, 125, 140	0
47	DF	178/178 (100%)	1.16	31 (17%) 2 2	38, 85, 125, 138	0
48	BG	176/176 (100%)	0.92	26 (14%) 3 3	37, 88, 114, 146	0
48	DG	176/176 (100%)	0.73	21 (11%) 5 4	17, 82, 110, 133	0
49	BR	103/103 (100%)	0.51	6 (5%) 22 10	13, 78, 112, 120	0
49	DR	103/103 (100%)	0.79	10 (9%) 8 6	15, 72, 111, 128	0
50	BT	93/100 (93%)	0.86	14 (15%) 3 3	14, 70, 112, 124	0
50	DT	93/100 (93%)	0.78	10 (10%) 6 5	8, 66, 108, 120	0
51	BZ	77/78 (98%)	0.92	6 (7%) 13 7	5, 54, 93, 115	0
51	DZ	77/78 (98%)	0.73	9 (11%) 5 4	5, 43, 87, 114	0
52	BW	79/84 (94%)	1.12	15 (18%) 2 2	8, 75, 111, 136	0
52	DW	79/84 (94%)	0.63	5 (6%) 19 9	12, 65, 103, 122	0
All	All	20417/21046 (97%)	0.27	1244 (6%) 21 9	5, 68, 120, 167	0

The worst 5 of 1244 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	CI	129	ARG	10.7
23	BB	139	U	9.2
33	B1	52	LYS	9.0
22	DA	88	C	9.0
23	BB	140	C	8.4

## 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
53	MG	DB	3058	1/1	0.77	41.86	96,96,96,96	0
53	MG	CA	2020	1/1	0.51	41.01	85,85,85,85	0
53	MG	BB	3033	1/1	0.46	26.82	90,90,90,90	0
53	MG	AA	2023	1/1	0.49	22.47	44,44,44,44	1
53	MG	AA	2059	1/1	0.35	18.10	102,102,102,102	0
53	MG	AA	2047	1/1	0.47	16.67	73,73,73,73	0
53	MG	AA	2037	1/1	0.53	16.60	87,87,87,87	0
54	LLL	AA	2063	31/31	0.46	15.48	62,62,62,62	31
54	LLL	AA	2062	31/31	0.46	14.77	73,73,73,73	31
53	MG	AA	2057	1/1	0.39	14.61	80,80,80,80	0
53	MG	DB	3089	1/1	0.29	14.15	52,52,52,52	0
53	MG	AA	2051	1/1	0.20	10.11	66,66,66,66	0
53	MG	CA	2026	1/1	0.41	9.25	40,40,40,40	1
54	LLL	BB	3111	31/31	0.43	8.43	67,67,67,67	31
53	MG	AA	2025	1/1	0.21	7.62	50,50,50,50	1
54	LLL	CA	2063	31/31	0.33	7.43	70,70,70,70	0
53	MG	CA	2029	1/1	0.19	7.30	57,57,57,57	1
54	LLL	DB	3112	31/31	0.30	6.58	54,54,54,54	0
53	MG	BB	3043	1/1	0.24	5.59	86,86,86,86	0
53	MG	CA	2022	1/1	0.12	5.25	105,105,105,105	0
53	MG	BB	3084	1/1	0.27	5.15	67,67,67,67	0
53	MG	AA	2056	1/1	0.22	4.49	103,103,103,103	0
53	MG	CA	2058	1/1	0.29	4.23	63,63,63,63	0
53	MG	AA	2024	1/1	0.15	3.71	73,73,73,73	0
53	MG	CA	2038	1/1	0.17	3.26	77,77,77,77	0
53	MG	DB	3091	1/1	0.27	2.91	45,45,45,45	0
53	MG	AA	2032	1/1	0.16	2.83	67,67,67,67	0
53	MG	CA	2045	1/1	0.19	2.68	77,77,77,77	0
53	MG	AA	2002	1/1	0.31	2.61	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	BB	3087	1/1	0.23	2.55	73,73,73,73	0
53	MG	CA	2019	1/1	0.18	2.46	63,63,63,63	0
53	MG	BB	3093	1/1	0.38	2.41	80,80,80,80	0
53	MG	DB	3101	1/1	0.24	2.41	26,26,26,26	0
53	MG	AA	2022	1/1	0.48	2.36	100,100,100,100	0
53	MG	AA	2019	1/1	0.15	2.35	87,87,87,87	0
53	MG	CA	2027	1/1	0.14	2.30	55,55,55,55	1
53	MG	DB	3052	1/1	0.25	2.21	62,62,62,62	0
53	MG	DB	3083	1/1	0.24	2.16	56,56,56,56	0
53	MG	BB	3063	1/1	0.21	2.12	51,51,51,51	0
53	MG	BB	3078	1/1	0.25	1.99	67,67,67,67	0
53	MG	DB	3011	1/1	0.24	1.98	35,35,35,35	0
53	MG	DB	3037	1/1	0.19	1.82	5,5,5,5	0
53	MG	DB	3030	1/1	0.26	1.74	26,26,26,26	0
53	MG	DB	3097	1/1	0.19	1.66	42,42,42,42	0
53	MG	AA	2039	1/1	0.46	1.55	92,92,92,92	0
53	MG	DB	3111	1/1	0.23	1.27	43,43,43,43	0
53	MG	DB	3088	1/1	0.24	1.14	18,18,18,18	0
53	MG	BB	3036	1/1	0.16	1.09	57,57,57,57	0
53	MG	BB	3011	1/1	0.26	1.09	21,21,21,21	0
54	LLL	CA	2064	31/31	0.31	0.90	41,41,41,41	31
53	MG	DB	3098	1/1	0.25	0.83	23,23,23,23	0
53	MG	BB	3018	1/1	0.19	0.67	54,54,54,54	0
54	LLL	AA	2061	31/31	0.30	0.61	20,20,20,20	0
53	MG	BB	3022	1/1	0.26	0.56	44,44,44,44	0
53	MG	AA	2040	1/1	0.15	0.54	65,65,65,65	0
53	MG	BB	3038	1/1	0.15	0.50	77,77,77,77	0
53	MG	CA	2006	1/1	0.19	0.42	73,73,73,73	0
53	MG	CA	2048	1/1	0.19	0.20	65,65,65,65	0
53	MG	BB	3095	1/1	0.15	0.14	59,59,59,59	0
53	MG	BB	3075	1/1	0.21	0.14	33,33,33,33	0
53	MG	BB	3097	1/1	0.12	0.14	56,56,56,56	0
53	MG	DB	3007	1/1	0.21	0.07	18,18,18,18	0
53	MG	BB	3060	1/1	0.20	0.03	59,59,59,59	0
53	MG	DB	3110	1/1	0.21	0.00	29,29,29,29	0
54	LLL	CA	2062	31/31	0.19	-0.05	9,9,9,9	0
53	MG	DB	3004	1/1	0.19	-0.07	21,21,21,21	0
53	MG	DB	3104	1/1	0.20	-0.10	55,55,55,55	0
53	MG	DB	3099	1/1	0.20	-0.15	5,5,5,5	0
53	MG	CA	2053	1/1	0.11	-0.16	51,51,51,51	0
53	MG	BB	3081	1/1	0.22	-0.16	40,40,40,40	0
53	MG	DB	3065	1/1	0.19	-0.18	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	CA	2033	1/1	0.15	-0.21	57,57,57,57	0
53	MG	AA	2015	1/1	0.16	-0.22	78,78,78,78	0
53	MG	BB	3057	1/1	0.24	-0.26	72,72,72,72	0
53	MG	BB	3110	1/1	0.13	-0.28	74,74,74,74	0
53	MG	DB	3013	1/1	0.17	-0.28	37,37,37,37	0
53	MG	BB	3034	1/1	0.19	-0.29	52,52,52,52	0
53	MG	DB	3059	1/1	0.17	-0.37	100,100,100,100	0
53	MG	CA	2050	1/1	0.15	-0.39	5,5,5,5	0
53	MG	DB	3087	1/1	0.19	-0.40	63,63,63,63	0
53	MG	DB	3005	1/1	0.22	-0.43	6,6,6,6	0
53	MG	AA	2045	1/1	0.11	-0.43	48,48,48,48	0
53	MG	CA	2035	1/1	0.11	-0.47	85,85,85,85	0
53	MG	BB	3040	1/1	0.17	-0.52	40,40,40,40	0
53	MG	BB	3039	1/1	0.15	-0.53	35,35,35,35	0
53	MG	BB	3098	1/1	0.18	-0.56	43,43,43,43	0
53	MG	DB	3096	1/1	0.18	-0.57	5,5,5,5	0
53	MG	BB	3044	1/1	0.14	-0.64	55,55,55,55	0
53	MG	CA	2015	1/1	0.09	-0.67	108,108,108,108	0
53	MG	CA	2036	1/1	0.10	-0.70	74,74,74,74	0
53	MG	AA	2035	1/1	0.09	-0.71	71,71,71,71	0
53	MG	DB	3034	1/1	0.21	-0.75	74,74,74,74	0
53	MG	BB	3092	1/1	0.10	-0.82	40,40,40,40	0
53	MG	AA	2052	1/1	0.11	-0.82	69,69,69,69	0
53	MG	CA	2007	1/1	0.11	-0.89	47,47,47,47	0
53	MG	CA	2014	1/1	0.07	-0.92	72,72,72,72	0
53	MG	DB	3057	1/1	0.08	-0.93	53,53,53,53	0
53	MG	AA	2049	1/1	0.07	-0.98	93,93,93,93	0
53	MG	BB	3107	1/1	0.12	-1.00	41,41,41,41	0
53	MG	DB	3031	1/1	0.16	-1.02	8,8,8,8	0
53	MG	CA	2039	1/1	0.12	-1.02	19,19,19,19	0
53	MG	DB	3024	1/1	0.15	-1.03	53,53,53,53	0
53	MG	DB	3051	1/1	0.18	-1.05	57,57,57,57	0
53	MG	BB	3073	1/1	0.18	-1.05	33,33,33,33	0
53	MG	AA	2053	1/1	0.12	-1.07	58,58,58,58	0
53	MG	AA	2011	1/1	0.08	-1.07	41,41,41,41	0
53	MG	BB	3083	1/1	0.20	-1.08	33,33,33,33	0
53	MG	CA	2025	1/1	0.16	-1.09	72,72,72,72	0
53	MG	DB	3060	1/1	0.11	-1.10	79,79,79,79	0
53	MG	BB	3021	1/1	0.11	-1.11	22,22,22,22	0
53	MG	AA	2060	1/1	0.15	-1.13	46,46,46,46	0
53	MG	BB	3023	1/1	0.21	-1.14	11,11,11,11	0
53	MG	BB	3085	1/1	0.17	-1.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
53	MG	CA	2059	1/1	0.09	-1.16	51,51,51,51	0
53	MG	CN	201	1/1	0.06	-1.19	50,50,50,50	0
53	MG	CA	2013	1/1	0.11	-1.19	48,48,48,48	0
53	MG	DB	3102	1/1	0.12	-1.21	16,16,16,16	0
53	MG	AA	2018	1/1	0.11	-1.24	76,76,76,76	0
53	MG	CA	2049	1/1	0.11	-1.29	63,63,63,63	0
55	ZN	D4	101	1/1	0.07	-1.31	45,45,45,45	0
53	MG	AA	2036	1/1	0.07	-1.32	62,62,62,62	0
53	MG	AA	2007	1/1	0.09	-1.37	70,70,70,70	0
53	MG	AA	2004	1/1	0.14	-1.37	35,35,35,35	0
53	MG	CA	2051	1/1	0.08	-1.39	38,38,38,38	0
53	MG	DB	3014	1/1	0.07	-1.39	13,13,13,13	0
53	MG	DB	3077	1/1	0.16	-1.40	50,50,50,50	0
53	MG	BB	3086	1/1	0.19	-1.42	5,5,5,5	0
53	MG	BB	3037	1/1	0.10	-1.42	29,29,29,29	0
53	MG	BB	3010	1/1	0.11	-1.43	73,73,73,73	0
53	MG	AA	2031	1/1	0.13	-1.43	49,49,49,49	0
53	MG	DB	3029	1/1	0.09	-1.46	66,66,66,66	0
53	MG	DB	3082	1/1	0.09	-1.50	42,42,42,42	0
53	MG	BB	3005	1/1	0.18	-1.50	5,5,5,5	0
53	MG	DB	3095	1/1	0.15	-1.51	96,96,96,96	0
53	MG	BB	3053	1/1	0.07	-1.52	59,59,59,59	0
53	MG	BB	3089	1/1	0.19	-1.53	63,63,63,63	0
53	MG	AA	2009	1/1	0.15	-1.54	27,27,27,27	0
53	MG	BB	3080	1/1	0.15	-1.56	56,56,56,56	0
53	MG	BB	3072	1/1	0.15	-1.57	57,57,57,57	0
53	MG	AA	2041	1/1	0.07	-1.60	57,57,57,57	0
53	MG	DB	3023	1/1	0.06	-1.60	13,13,13,13	0
53	MG	AA	2013	1/1	0.04	-1.62	70,70,70,70	0
53	MG	DB	3084	1/1	0.17	-1.64	25,25,25,25	0
53	MG	CA	2042	1/1	0.09	-1.66	66,66,66,66	0
53	MG	AA	2010	1/1	0.04	-1.67	45,45,45,45	0
53	MG	BB	3006	1/1	0.14	-1.69	19,19,19,19	0
53	MG	DB	3074	1/1	0.12	-1.75	5,5,5,5	0
53	MG	BB	3028	1/1	0.16	-1.80	16,16,16,16	0
53	MG	BB	3099	1/1	0.16	-1.83	56,56,56,56	0
53	MG	DB	3012	1/1	0.15	-1.85	14,14,14,14	0
53	MG	BB	3104	1/1	0.15	-1.90	18,18,18,18	0
53	MG	DB	3042	1/1	0.11	-1.91	22,22,22,22	0
53	MG	DB	3041	1/1	0.13	-1.91	41,41,41,41	0
53	MG	CA	2060	1/1	0.05	-1.95	55,55,55,55	0
53	MG	BB	3105	1/1	0.14	-1.97	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	CA	2023	1/1	0.05	-2.02	54,54,54,54	0
53	MG	BB	3082	1/1	0.17	-2.03	5,5,5,5	0
53	MG	CA	2012	1/1	0.07	-2.05	49,49,49,49	0
53	MG	AA	2020	1/1	0.06	-2.05	91,91,91,91	0
53	MG	DB	3036	1/1	0.12	-2.06	26,26,26,26	0
53	MG	BB	3046	1/1	0.12	-2.06	50,50,50,50	0
53	MG	DB	3100	1/1	0.10	-2.09	5,5,5,5	0
55	ZN	B4	101	1/1	0.07	-2.11	82,82,82,82	0
53	MG	CA	2041	1/1	0.09	-2.14	69,69,69,69	0
53	MG	AA	2003	1/1	0.17	-2.16	29,29,29,29	0
53	MG	AA	2008	1/1	0.09	-2.18	81,81,81,81	0
53	MG	CA	2054	1/1	0.08	-2.19	91,91,91,91	0
53	MG	CA	2037	1/1	0.07	-2.20	69,69,69,69	0
53	MG	CA	2016	1/1	0.09	-2.21	10,10,10,10	0
53	MG	AA	2017	1/1	0.13	-2.22	76,76,76,76	0
53	MG	DB	3018	1/1	0.14	-2.23	48,48,48,48	0
53	MG	DB	3073	1/1	0.12	-2.24	33,33,33,33	0
53	MG	AA	2016	1/1	0.08	-2.27	36,36,36,36	0
53	MG	DB	3078	1/1	0.08	-2.31	48,48,48,48	0
53	MG	AA	2033	1/1	0.05	-2.31	69,69,69,69	0
53	MG	AA	2029	1/1	0.11	-2.33	50,50,50,50	0
53	MG	DB	3106	1/1	0.12	-2.35	37,37,37,37	0
53	MG	BB	3003	1/1	0.09	-2.38	17,17,17,17	0
53	MG	DB	3050	1/1	0.10	-2.38	73,73,73,73	0
53	MG	BB	3109	1/1	0.11	-2.41	37,37,37,37	0
53	MG	DB	3094	1/1	0.03	-2.42	14,14,14,14	0
53	MG	DB	3109	1/1	0.11	-2.52	28,28,28,28	0
53	MG	DB	3038	1/1	0.15	-2.54	17,17,17,17	0
53	MG	DB	3105	1/1	0.12	-2.55	30,30,30,30	0
53	MG	BB	3103	1/1	0.12	-2.58	5,5,5,5	0
53	MG	DB	3003	1/1	0.11	-2.59	17,17,17,17	0
53	MG	BB	3077	1/1	0.12	-2.59	44,44,44,44	0
53	MG	AA	2012	1/1	0.07	-2.62	70,70,70,70	0
53	MG	DB	3047	1/1	0.19	-2.65	5,5,5,5	0
53	MG	BB	3045	1/1	0.07	-2.68	19,19,19,19	0
53	MG	DB	3063	1/1	0.10	-2.69	21,21,21,21	0
53	MG	DB	3076	1/1	0.15	-2.70	43,43,43,43	0
53	MG	AA	2043	1/1	0.10	-2.73	44,44,44,44	0
53	MG	BB	3088	1/1	0.09	-2.73	26,26,26,26	0
53	MG	DB	3079	1/1	0.14	-2.76	43,43,43,43	0
53	MG	BB	3065	1/1	0.09	-2.76	44,44,44,44	0
53	MG	AA	2038	1/1	0.08	-2.77	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	AA	2006	1/1	0.06	-2.82	57,57,57,57	0
53	MG	AA	2034	1/1	0.07	-2.82	42,42,42,42	0
53	MG	AA	2001	1/1	0.09	-2.83	27,27,27,27	0
53	MG	AA	2028	1/1	0.08	-2.86	53,53,53,53	0
53	MG	DB	3020	1/1	0.17	-2.88	5,5,5,5	0
53	MG	DB	3062	1/1	0.06	-2.89	43,43,43,43	0
53	MG	AA	2027	1/1	0.17	-2.91	56,56,56,56	0
53	MG	DB	3068	1/1	0.13	-2.91	5,5,5,5	0
53	MG	BB	3079	1/1	0.14	-2.94	52,52,52,52	0
53	MG	DB	3107	1/1	0.10	-2.96	15,15,15,15	0
53	MG	BB	3108	1/1	0.12	-2.96	12,12,12,12	0
53	MG	DB	3055	1/1	0.11	-2.97	11,11,11,11	0
53	MG	CA	2011	1/1	0.10	-3.02	82,82,82,82	0
53	MG	CA	2005	1/1	0.10	-3.03	10,10,10,10	0
53	MG	DB	3017	1/1	0.13	-3.05	5,5,5,5	0
53	MG	DB	3033	1/1	0.13	-3.07	18,18,18,18	0
53	MG	BB	3070	1/1	0.15	-3.08	24,24,24,24	0
53	MG	DB	3027	1/1	0.14	-3.11	12,12,12,12	0
53	MG	BB	3059	1/1	0.09	-3.11	39,39,39,39	0
53	MG	CA	2046	1/1	0.07	-3.12	70,70,70,70	0
53	MG	BB	3054	1/1	0.06	-3.14	39,39,39,39	0
53	MG	BB	3027	1/1	0.14	-3.18	24,24,24,24	0
53	MG	BB	3062	1/1	0.16	-3.18	29,29,29,29	0
53	MG	BB	3012	1/1	0.09	-3.19	31,31,31,31	0
53	MG	DB	3032	1/1	0.09	-3.20	45,45,45,45	0
53	MG	BB	3009	1/1	0.08	-3.21	70,70,70,70	0
53	MG	DB	3048	1/1	0.09	-3.24	36,36,36,36	0
53	MG	CA	2032	1/1	0.12	-3.28	22,22,22,22	0
53	MG	DB	3015	1/1	0.10	-3.32	50,50,50,50	0
53	MG	AA	2030	1/1	0.07	-3.33	88,88,88,88	0
53	MG	CA	2021	1/1	0.09	-3.35	70,70,70,70	0
53	MG	BB	3055	1/1	0.16	-3.37	40,40,40,40	0
53	MG	AA	2042	1/1	0.06	-3.40	28,28,28,28	0
53	MG	BB	3013	1/1	0.10	-3.40	41,41,41,41	0
53	MG	DB	3045	1/1	0.09	-3.43	66,66,66,66	0
53	MG	BB	3047	1/1	0.09	-3.44	77,77,77,77	0
53	MG	BB	3024	1/1	0.06	-3.47	21,21,21,21	0
53	MG	DB	3085	1/1	0.11	-3.51	5,5,5,5	0
53	MG	AA	2048	1/1	0.10	-3.52	48,48,48,48	0
53	MG	DB	3021	1/1	0.14	-3.55	5,5,5,5	0
53	MG	CA	2043	1/1	0.07	-3.61	31,31,31,31	0
53	MG	BB	3102	1/1	0.07	-3.62	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	BB	3020	1/1	0.11	-3.62	13,13,13,13	0
53	MG	AA	2046	1/1	0.09	-3.64	95,95,95,95	0
53	MG	DB	3086	1/1	0.15	-3.64	24,24,24,24	0
53	MG	DB	3067	1/1	0.09	-3.68	5,5,5,5	0
53	MG	DB	3108	1/1	0.08	-3.70	5,5,5,5	0
53	MG	BB	3025	1/1	0.08	-3.71	51,51,51,51	0
53	MG	BB	3042	1/1	0.08	-3.73	96,96,96,96	0
53	MG	DB	3090	1/1	0.11	-3.75	57,57,57,57	0
53	MG	DB	3035	1/1	0.07	-3.78	54,54,54,54	0
53	MG	BB	3032	1/1	0.20	-3.81	36,36,36,36	0
53	MG	DB	3049	1/1	0.07	-3.81	5,5,5,5	0
53	MG	DB	3081	1/1	0.11	-3.82	5,5,5,5	0
53	MG	BB	3100	1/1	0.11	-3.86	105,105,105,105	0
53	MG	BB	3091	1/1	0.10	-3.87	34,34,34,34	0
53	MG	CA	2047	1/1	0.06	-3.92	74,74,74,74	0
53	MG	DB	3025	1/1	0.11	-3.94	5,5,5,5	0
53	MG	BB	3076	1/1	0.08	-3.98	23,23,23,23	0
53	MG	DB	3056	1/1	0.10	-4.04	5,5,5,5	0
53	MG	CA	2008	1/1	0.07	-4.04	86,86,86,86	0
53	MG	BB	3002	1/1	0.09	-4.07	5,5,5,5	0
53	MG	BB	3048	1/1	0.05	-4.09	22,22,22,22	0
53	MG	DB	3080	1/1	0.09	-4.09	5,5,5,5	0
53	MG	CA	2024	1/1	0.06	-4.11	23,23,23,23	0
53	MG	CA	2009	1/1	0.05	-4.13	84,84,84,84	0
53	MG	DB	3064	1/1	0.04	-4.14	11,11,11,11	0
53	MG	BB	3051	1/1	0.10	-4.15	43,43,43,43	0
53	MG	BB	3094	1/1	0.12	-4.16	69,69,69,69	0
53	MG	BB	3101	1/1	0.07	-4.19	11,11,11,11	0
53	MG	CA	2044	1/1	0.07	-4.21	67,67,67,67	0
53	MG	BB	3066	1/1	0.10	-4.22	37,37,37,37	0
53	MG	DB	3010	1/1	0.08	-4.31	14,14,14,14	0
53	MG	AA	2050	1/1	0.06	-4.44	103,103,103,103	0
53	MG	BB	3096	1/1	0.14	-4.44	44,44,44,44	0
53	MG	DB	3093	1/1	0.15	-4.48	7,7,7,7	0
53	MG	DB	3053	1/1	0.07	-4.50	66,66,66,66	0
53	MG	CA	2018	1/1	0.13	-4.53	60,60,60,60	0
53	MG	CA	2061	1/1	0.07	-4.55	25,25,25,25	0
53	MG	BB	3090	1/1	0.09	-4.55	60,60,60,60	0
53	MG	CA	2030	1/1	0.08	-4.56	31,31,31,31	0
53	MG	CA	2034	1/1	0.12	-4.57	15,15,15,15	0
53	MG	DB	3022	1/1	0.07	-4.59	23,23,23,23	0
53	MG	CA	2055	1/1	0.08	-4.61	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	BB	3064	1/1	0.09	-4.62	37,37,37,37	0
53	MG	BB	3014	1/1	0.06	-4.66	39,39,39,39	0
53	MG	CA	2017	1/1	0.05	-4.68	5,5,5,5	0
53	MG	DB	3008	1/1	0.11	-4.68	8,8,8,8	0
53	MG	AA	2021	1/1	0.08	-4.70	23,23,23,23	0
53	MG	BB	3029	1/1	0.07	-4.73	5,5,5,5	0
53	MG	BB	3030	1/1	0.06	-4.73	53,53,53,53	0
53	MG	BB	3026	1/1	0.12	-4.75	24,24,24,24	0
53	MG	DB	3006	1/1	0.10	-4.86	5,5,5,5	0
53	MG	CA	2040	1/1	0.08	-5.04	12,12,12,12	0
53	MG	BB	3106	1/1	0.08	-5.05	31,31,31,31	0
53	MG	DB	3002	1/1	0.13	-5.08	12,12,12,12	0
53	MG	DB	3039	1/1	0.05	-5.10	36,36,36,36	0
53	MG	AA	2055	1/1	0.05	-5.16	57,57,57,57	0
53	MG	BB	3016	1/1	0.14	-5.27	43,43,43,43	0
53	MG	BB	3041	1/1	0.14	-5.28	18,18,18,18	0
53	MG	BB	3069	1/1	0.09	-5.29	5,5,5,5	0
53	MG	DB	3069	1/1	0.17	-5.33	21,21,21,21	0
53	MG	DB	3070	1/1	0.10	-5.33	43,43,43,43	0
53	MG	DB	3092	1/1	0.09	-5.39	76,76,76,76	0
53	MG	CA	2057	1/1	0.05	-5.62	61,61,61,61	0
53	MG	BB	3052	1/1	0.08	-5.63	26,26,26,26	0
53	MG	DB	3044	1/1	0.07	-5.66	18,18,18,18	0
53	MG	BB	3049	1/1	0.12	-5.67	20,20,20,20	0
53	MG	BB	3001	1/1	0.10	-5.69	8,8,8,8	0
53	MG	DB	3046	1/1	0.08	-5.72	5,5,5,5	0
53	MG	DB	3028	1/1	0.09	-5.74	37,37,37,37	0
53	MG	DB	3040	1/1	0.16	-5.85	5,5,5,5	0
53	MG	AA	2005	1/1	0.10	-5.88	72,72,72,72	0
53	MG	DB	3026	1/1	0.09	-5.92	33,33,33,33	0
53	MG	AA	2054	1/1	0.06	-6.07	66,66,66,66	0
53	MG	BB	3056	1/1	0.05	-6.08	22,22,22,22	0
53	MG	CA	2056	1/1	0.09	-6.38	32,32,32,32	0
53	MG	BB	3071	1/1	0.09	-6.39	63,63,63,63	0
53	MG	CA	2002	1/1	0.10	-6.41	27,27,27,27	0
53	MG	DB	3103	1/1	0.07	-6.61	7,7,7,7	0
53	MG	DB	3016	1/1	0.07	-6.64	17,17,17,17	0
53	MG	BB	3050	1/1	0.09	-6.71	18,18,18,18	0
53	MG	BB	3067	1/1	0.08	-6.74	40,40,40,40	0
53	MG	BB	3061	1/1	0.06	-6.75	45,45,45,45	0
53	MG	CA	2003	1/1	0.07	-6.77	44,44,44,44	0
53	MG	DB	3071	1/1	0.09	-6.92	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
53	MG	BB	3019	1/1	0.09	-6.96	49,49,49,49	0
53	MG	DB	3075	1/1	0.08	-7.24	41,41,41,41	0
53	MG	BB	3058	1/1	0.08	-7.33	32,32,32,32	0
53	MG	CA	2001	1/1	0.05	-7.37	5,5,5,5	0
53	MG	BB	3008	1/1	0.07	-7.38	80,80,80,80	0
53	MG	AA	2044	1/1	0.07	-7.48	48,48,48,48	0
53	MG	CA	2010	1/1	0.05	-7.71	59,59,59,59	0
53	MG	BB	3015	1/1	0.06	-7.78	5,5,5,5	0
53	MG	DB	3054	1/1	0.10	-7.81	13,13,13,13	0
53	MG	BB	3068	1/1	0.11	-7.82	37,37,37,37	0
53	MG	DB	3009	1/1	0.08	-8.11	5,5,5,5	0
53	MG	BB	3007	1/1	0.04	-8.21	60,60,60,60	0
53	MG	DB	3061	1/1	0.09	-8.26	58,58,58,58	0
53	MG	CA	2004	1/1	0.07	-8.30	13,13,13,13	0
53	MG	BB	3004	1/1	0.06	-8.76	43,43,43,43	0
53	MG	DB	3019	1/1	0.05	-9.28	6,6,6,6	0
53	MG	BB	3074	1/1	0.10	-9.30	9,9,9,9	0
53	MG	AA	2026	1/1	0.13	-9.40	51,51,51,51	1
53	MG	DB	3043	1/1	0.08	-9.42	5,5,5,5	0
53	MG	CA	2031	1/1	0.07	-9.56	37,37,37,37	0
53	MG	DB	3072	1/1	0.07	-9.92	25,25,25,25	0
53	MG	BB	3031	1/1	0.07	-10.28	32,32,32,32	0
53	MG	DB	3001	1/1	0.13	-11.32	5,5,5,5	0
53	MG	AA	2014	1/1	0.06	-12.67	72,72,72,72	0
53	MG	CA	2028	1/1	0.04	-15.83	77,77,77,77	0
53	MG	AA	2058	1/1	0.04	-17.00	94,94,94,94	0
53	MG	BB	3035	1/1	0.09	-19.45	35,35,35,35	0
53	MG	BB	3017	1/1	0.07	-24.50	16,16,16,16	0
53	MG	CA	2052	1/1	0.08	-29.00	66,66,66,66	0
53	MG	DB	3066	1/1	0.38	-	100,100,100,100	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.