



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:57 am GMT

PDB ID : 4V6C
Title : Crystal structure of the E. coli 70S ribosome in an intermediate state of ratcheting
Authors : Zhang, W.; Dunkle, J.A.; Cate, J.H.D.
Deposited on : 2009-06-27
Resolution : 3.19 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

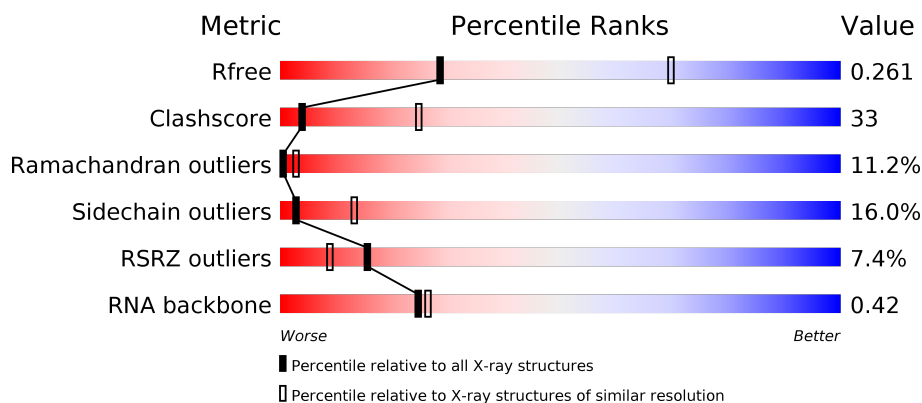
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)
RNA backbone	2435	1045 (3.60-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AB	241	<div> <div>7%</div> <div>18% 49% 21% 10%</div> </div>
1	CB	241	<div> <div>5%</div> <div>23% 53% 14% 10%</div> </div>
2	AC	233	<div> <div>0%</div> <div>33% 43% 10% 12%</div> </div>
2	CC	233	<div> <div>6%</div> <div>34% 41% 12% 12%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AD	206	
3	CD	206	
4	AE	167	
4	CE	167	
5	AF	135	
5	CF	135	
6	AG	179	
6	CG	179	
7	AH	130	
7	CH	130	
8	AI	130	
8	CI	130	
9	AJ	103	
9	CJ	103	
10	AK	129	
10	CK	129	
11	AL	124	
11	CL	124	
12	AM	118	
12	CM	118	
13	AN	101	
13	CN	101	
14	AO	89	
14	CO	89	
15	AP	82	

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Mol	Chain	Length	Quality of chain
15	CP	82	
16	AQ	84	
16	CQ	84	
17	AR	75	
17	CR	75	
18	AS	92	
18	CS	92	
19	AT	87	
19	CT	87	
20	AU	71	
20	CU	71	
21	AA	1533	
22	BA	2903	
22	DA	2903	
23	BB	118	
24	BC	273	
24	DC	273	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	179	
27	DF	179	
28	BG	177	
28	DG	177	

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Mol	Chain	Length	Quality of chain
29	BH	149	
29	DH	149	
30	BI	142	
30	DI	142	
31	BJ	142	
31	DJ	142	
32	BK	123	
32	DK	123	
33	BL	144	
33	DL	144	
34	BM	136	
34	DM	136	
35	BN	127	
35	DN	127	
36	BO	117	
36	DO	117	
37	BP	115	
37	DP	115	
38	BQ	118	
38	DQ	118	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	
41	BT	100	

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Mol	Chain	Length	Quality of chain
41	DT	100	
42	BU	104	
42	DU	104	
43	BV	94	
43	DV	94	
44	BW	85	
44	DW	85	
45	BX	78	
45	DX	78	
46	BY	63	
46	DY	63	
47	BZ	59	
47	DZ	59	
48	B0	57	
48	D0	57	
49	B1	55	
49	D1	55	
50	B2	46	
50	D2	46	
51	B3	65	
51	D3	65	
52	B4	38	
52	D4	38	
53	CA	1530	
54	DB	117	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3028	-	-	-	X
55	MG	BA	3037	-	-	-	X
55	MG	BA	3038	-	-	-	X
55	MG	BA	3058	-	-	-	X
55	MG	BA	3072	-	-	-	X
55	MG	BA	3084	-	-	-	X
55	MG	BA	3105	-	-	-	X
55	MG	BA	3110	-	-	-	X
55	MG	BA	3117	-	-	-	X
55	MG	BA	3125	-	-	-	X
55	MG	BA	3132	-	-	-	X
55	MG	BA	3137	-	-	-	X
55	MG	CA	1625	-	-	-	X
55	MG	CA	1628	-	-	-	X
55	MG	DA	3002	-	-	-	X
55	MG	DA	3070	-	-	-	X
55	MG	DA	3085	-	-	-	X
55	MG	DA	3098	-	-	-	X
55	MG	DA	3101	-	-	-	X
55	MG	DA	3109	-	-	-	X
55	MG	DA	3116	-	-	-	X
55	MG	DA	3131	-	-	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 284450 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S2.

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

- 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	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
6	CG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	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	95	Total	C	N	O	S	0	0	0
			769	480	159	127	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	80	Total	C	N	O	S	0	0	0
			648	411	121	113	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	79	Total	C	N	O	S	0	0	0
			637	408	120	107	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 S21.

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

- Molecule 21 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
22	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
27	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L11.

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

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

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

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

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

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

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

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a RNA chain called 16S rRNA.

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

- Molecule 54 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	DB	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BB	4	Total	Mg	0	0
			4	4		
55	BA	137	Total	Mg	0	0
			137	137		
55	CA	42	Total	Mg	0	0
			42	42		
55	DJ	1	Total	Mg	0	0
			1	1		
55	AA	43	Total	Mg	0	0
			43	43		
55	DA	135	Total	Mg	0	0
			135	135		
55	DB	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AE	1	Total	O	0	0
			1	1		
57	AL	3	Total	O	0	0
			3	3		
57	AN	6	Total	O	0	0
			6	6		
57	AT	2	Total	O	0	0
			2	2		
57	AU	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	195	Total 195	O 195	0	0
57	BA	610	Total 610	O 610	0	0
57	BB	20	Total 20	O 20	0	0
57	BC	10	Total 10	O 10	0	0
57	BD	2	Total 2	O 2	0	0
57	BL	4	Total 4	O 4	0	0
57	BN	3	Total 3	O 3	0	0
57	BQ	1	Total 1	O 1	0	0
57	BT	2	Total 2	O 2	0	0
57	B0	1	Total 1	O 1	0	0
57	B2	1	Total 1	O 1	0	0
57	B3	3	Total 3	O 3	0	0
57	B4	3	Total 3	O 3	0	0
57	CE	5	Total 5	O 5	0	0
57	CI	1	Total 1	O 1	0	0
57	CL	1	Total 1	O 1	0	0
57	CN	3	Total 3	O 3	0	0
57	CT	3	Total 3	O 3	0	0
57	CU	2	Total 2	O 2	0	0
57	CA	192	Total 192	O 192	0	0
57	DA	599	Total 599	O 599	0	0

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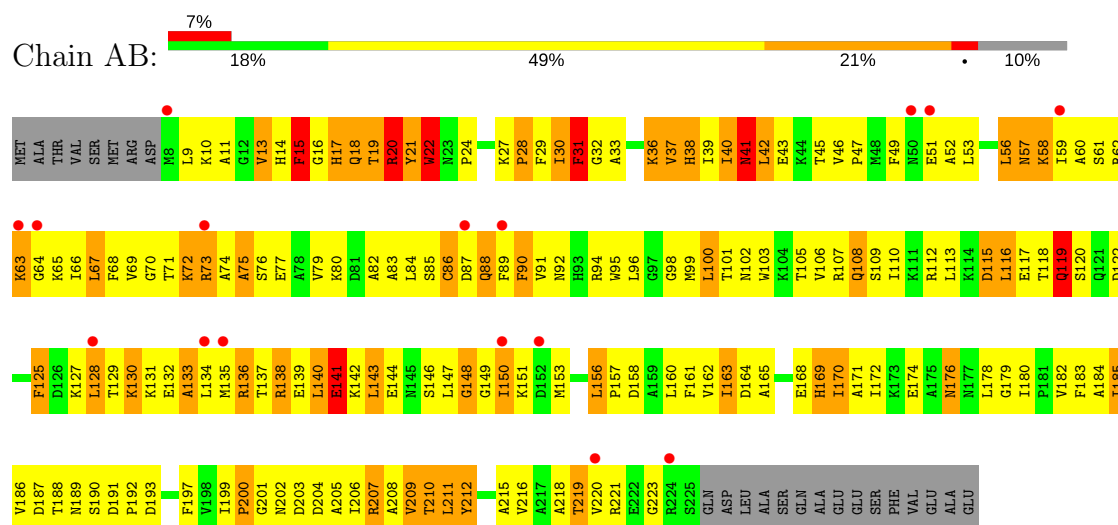
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DB	4	Total 4	O 4	0	0
57	DC	13	Total 13	O 13	0	0
57	DD	4	Total 4	O 4	0	0
57	DE	3	Total 3	O 3	0	0
57	DJ	3	Total 3	O 3	0	0
57	DL	5	Total 5	O 5	0	0
57	DN	2	Total 2	O 2	0	0
57	DT	2	Total 2	O 2	0	0
57	DU	1	Total 1	O 1	0	0
57	DV	1	Total 1	O 1	0	0
57	D2	1	Total 1	O 1	0	0
57	D3	1	Total 1	O 1	0	0
57	D4	4	Total 4	O 4	0	0

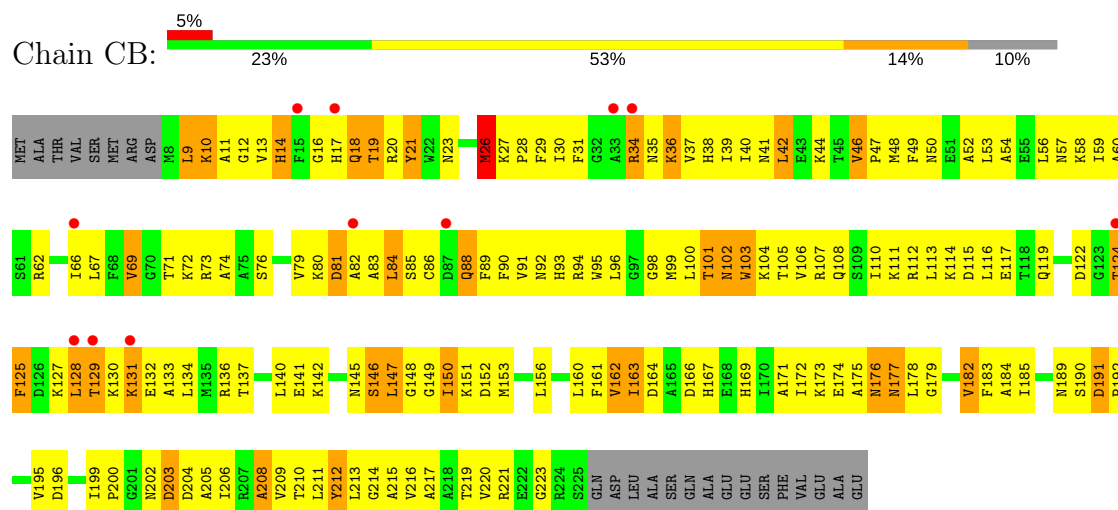
3 Residue-property plots

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

• Molecule 1: 30S ribosomal protein S2

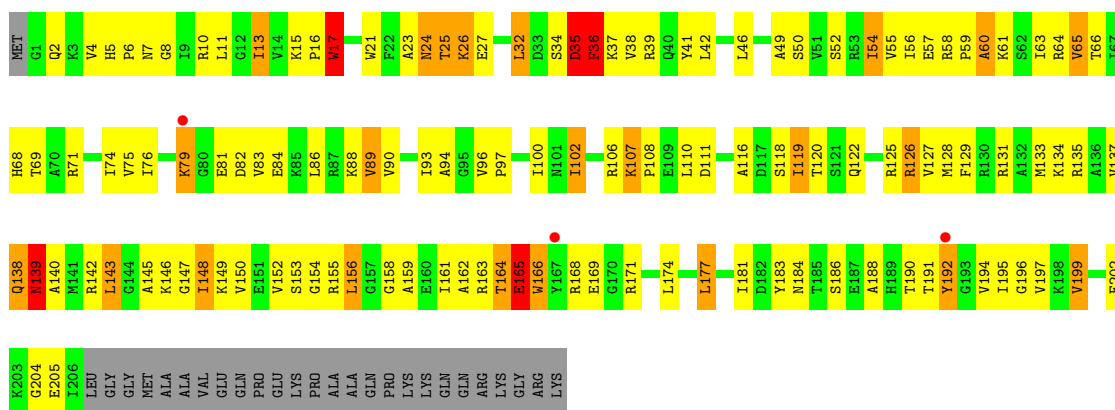


• Molecule 1: 30S ribosomal protein S2

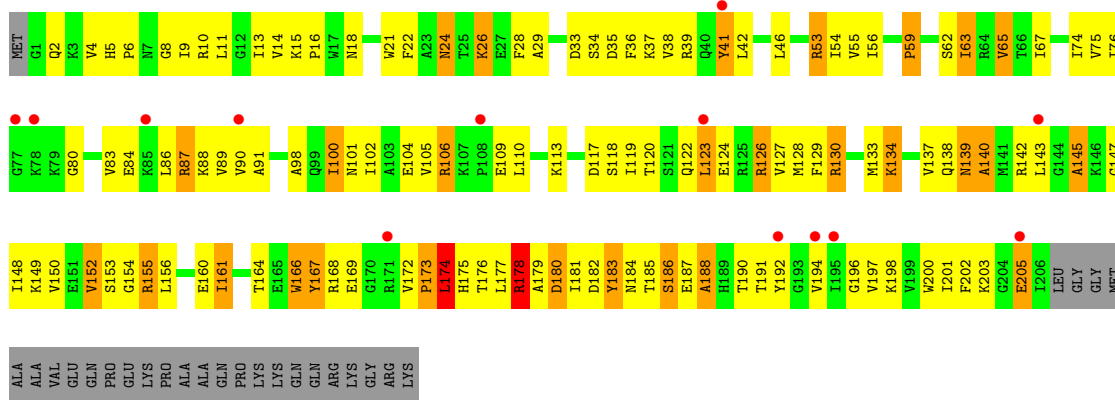


• Molecule 2: 30S ribosomal protein S3

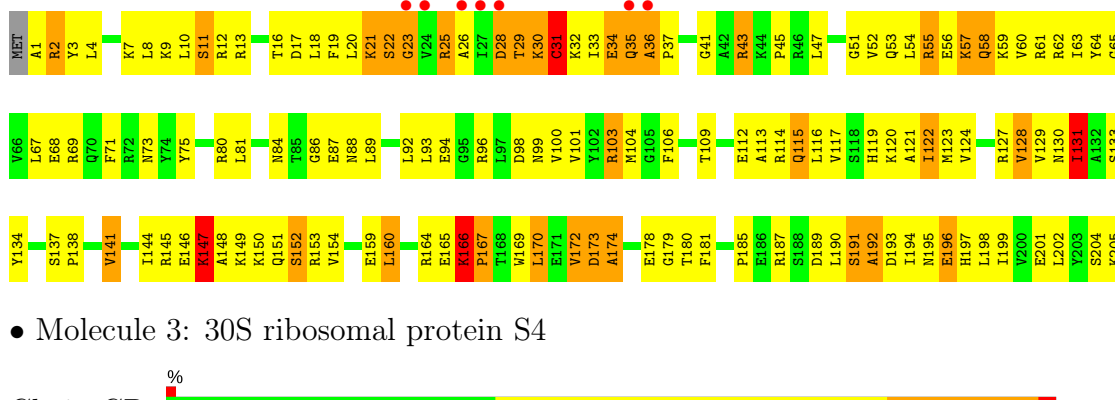




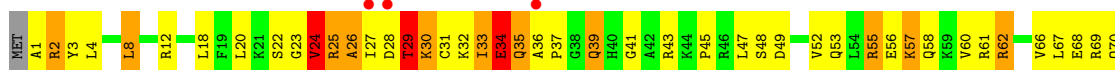
• Molecule 2: 30S ribosomal protein S3

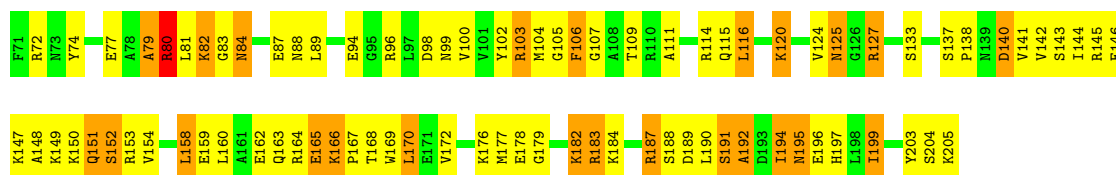


• Molecule 3: 30S ribosomal protein S4

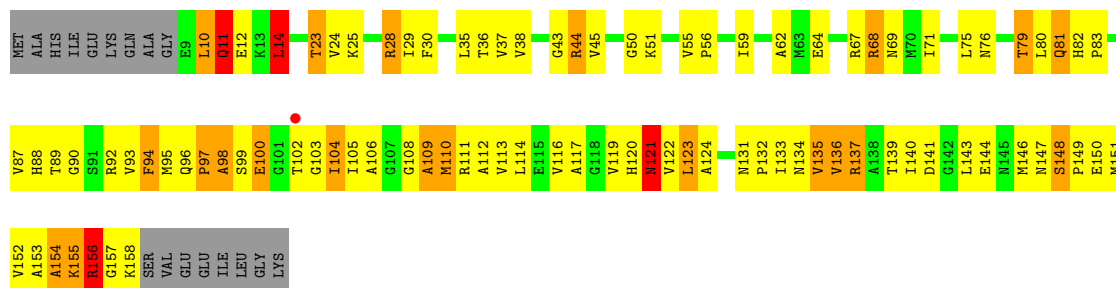


• Molecule 3: 30S ribosomal protein S4

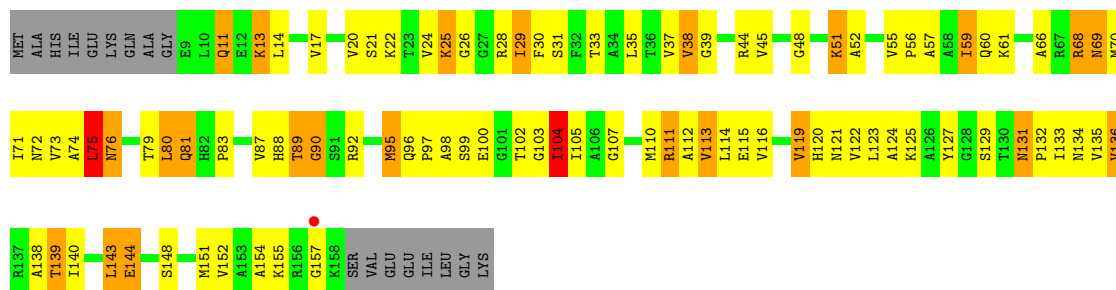




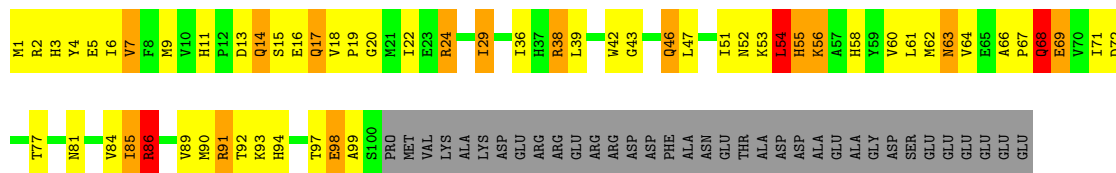
• Molecule 4: 30S ribosomal protein S5



• Molecule 4: 30S ribosomal protein S5

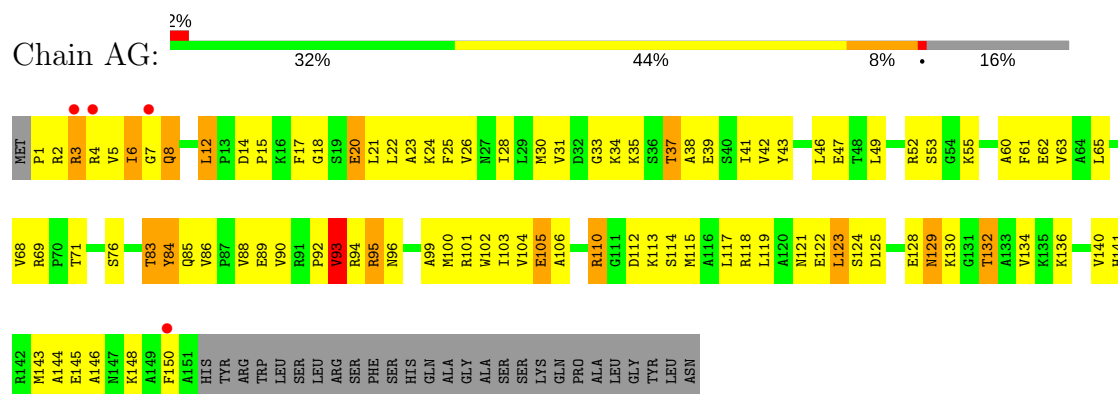


• Molecule 5: 30S ribosomal protein S6

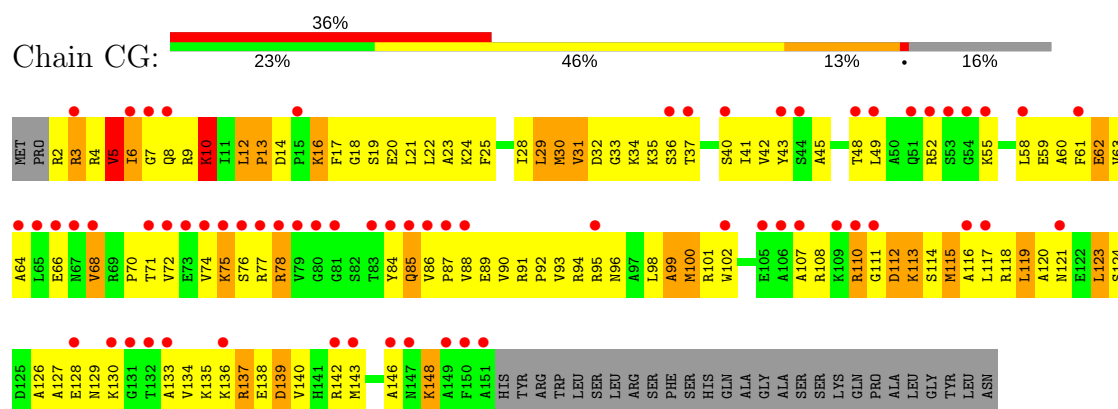


GLU
GLU
GLU

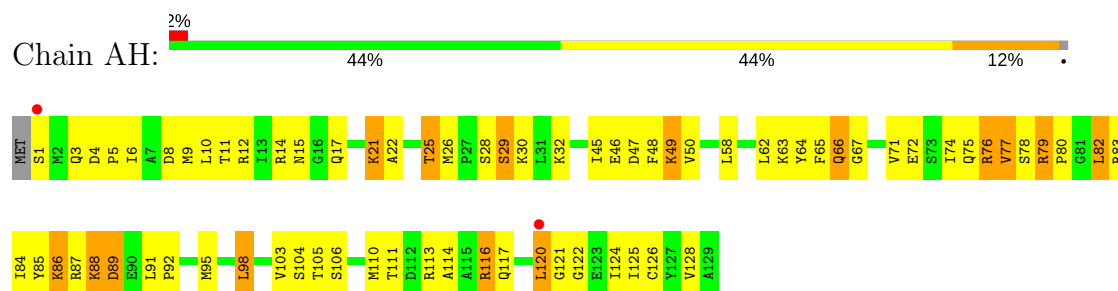
• Molecule 6: 30S ribosomal protein S7



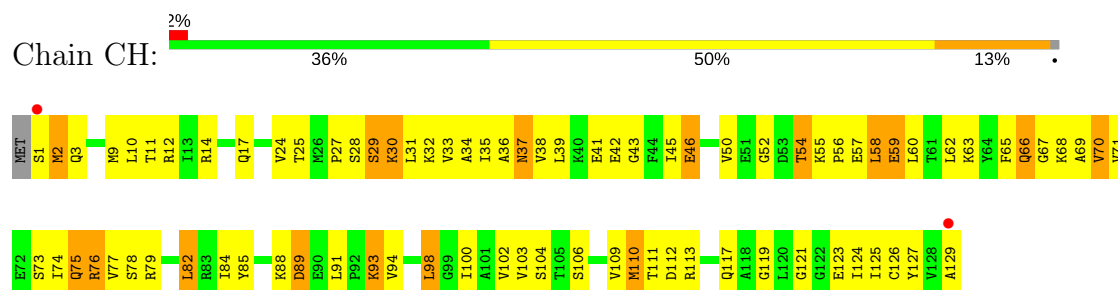
• Molecule 6: 30S ribosomal protein S7



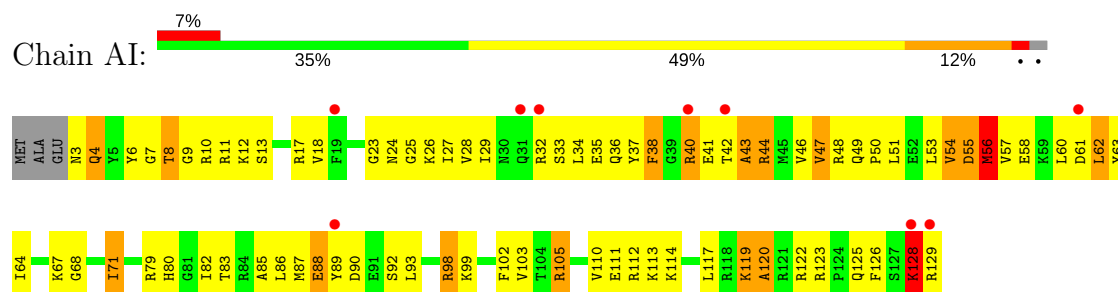
• Molecule 7: 30S ribosomal protein S8



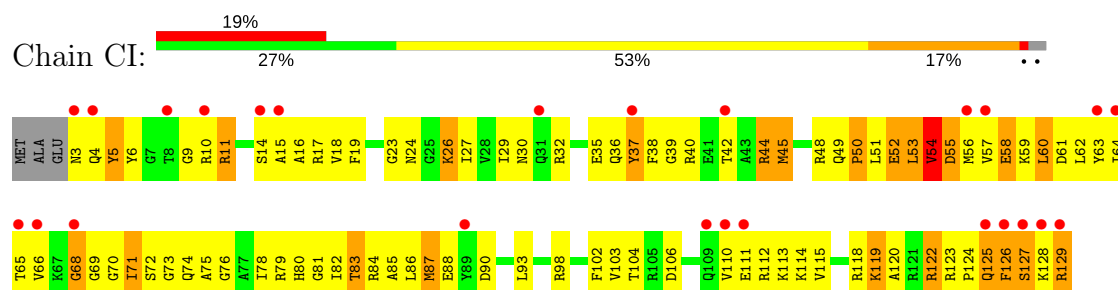
• Molecule 7: 30S ribosomal protein S8



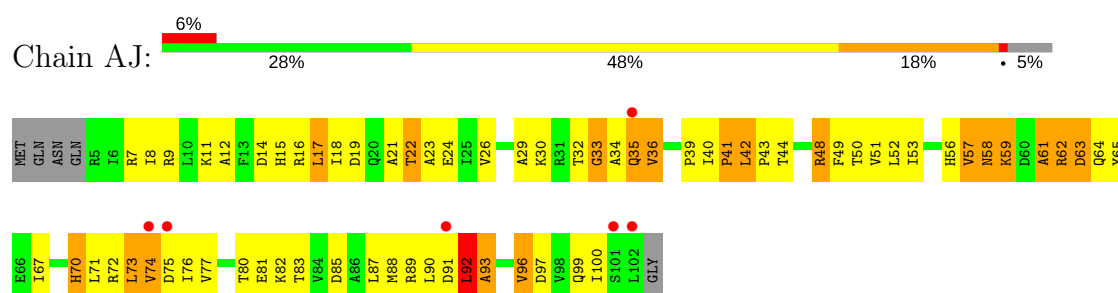
- Molecule 8: 30S ribosomal protein S9



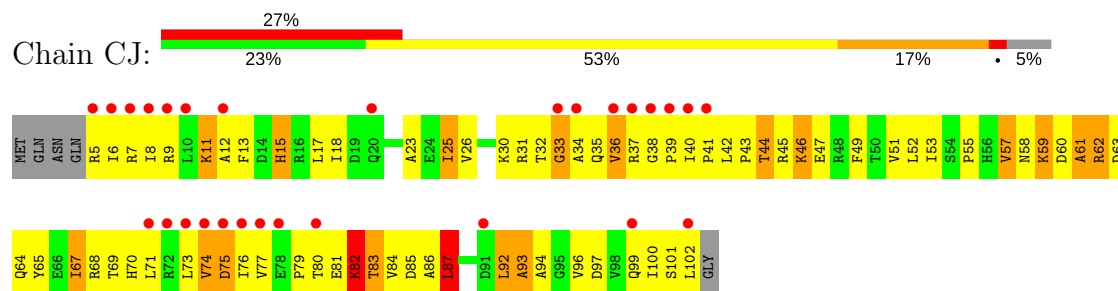
- Molecule 8: 30S ribosomal protein S9



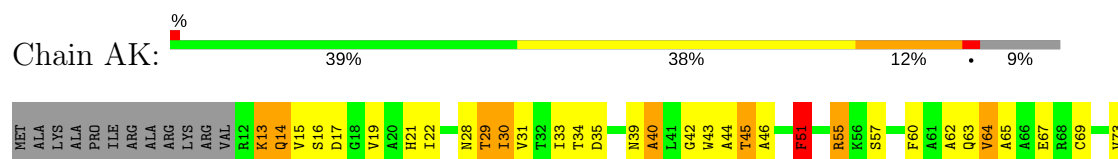
- Molecule 9: 30S ribosomal protein S10



- Molecule 9: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S11

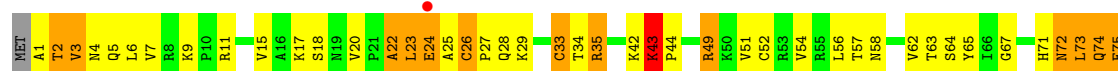
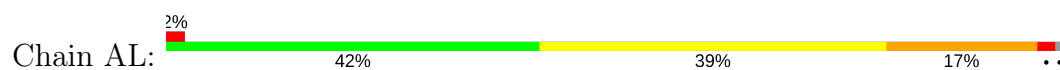




- Molecule 10: 30S ribosomal protein S11



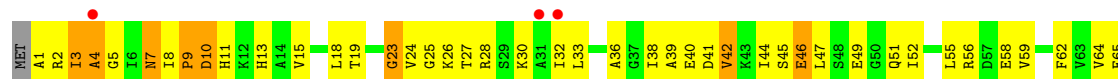
- Molecule 11: 30S ribosomal protein S12



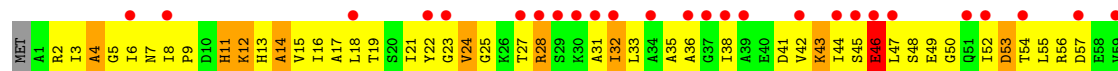
- Molecule 11: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S13

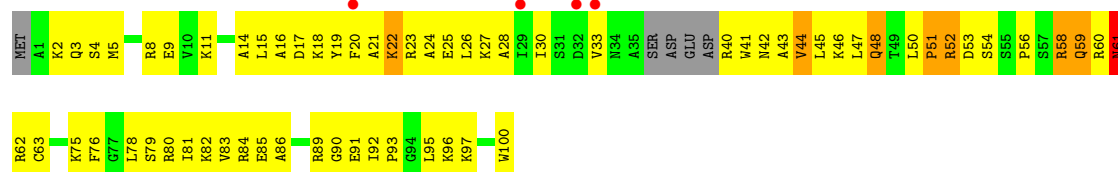


- Molecule 12: 30S ribosomal protein S13

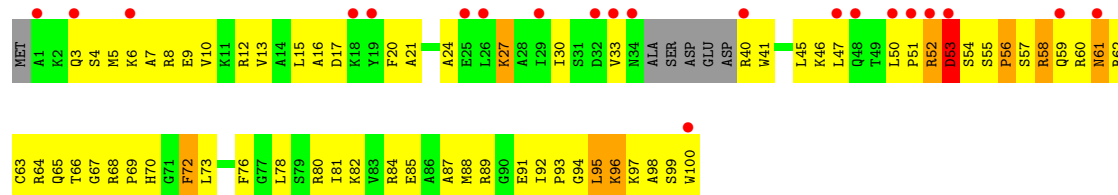




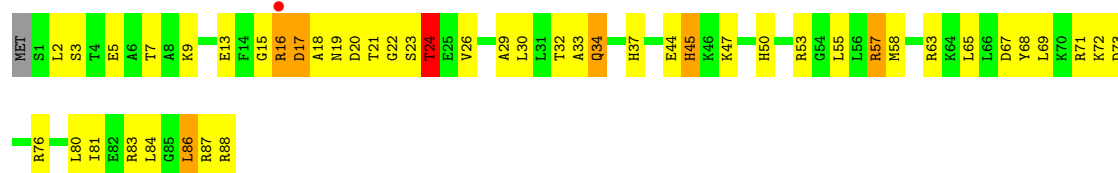
- Molecule 13: 30S ribosomal protein S14



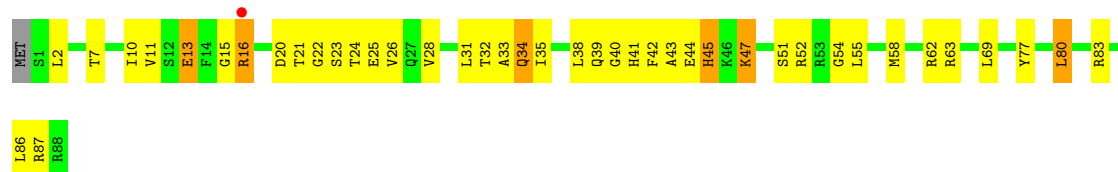
- Molecule 13: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S15

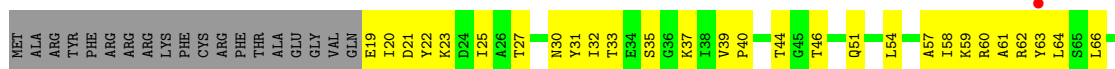


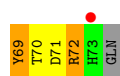
- Molecule 14: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S16



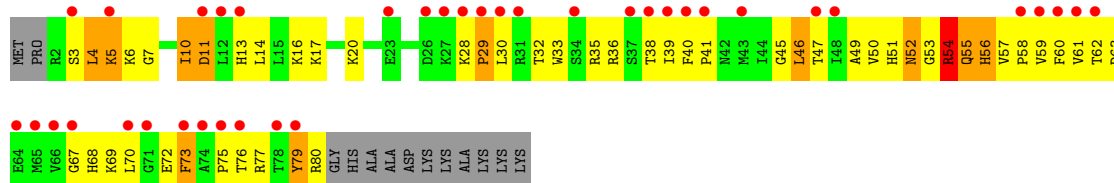




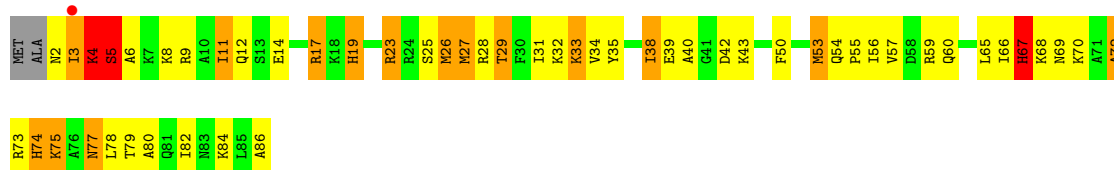
• Molecule 18: 30S ribosomal protein S19



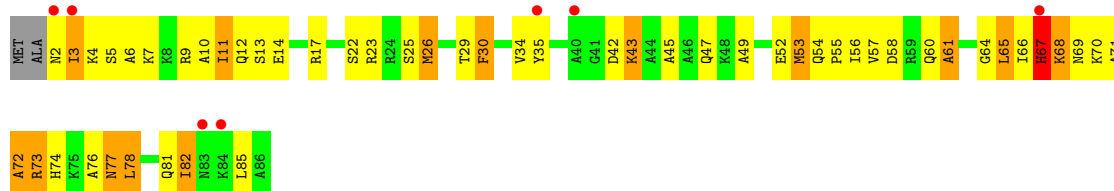
• Molecule 18: 30S ribosomal protein S19



• Molecule 19: 30S ribosomal protein S20



• Molecule 19: 30S ribosomal protein S20



• Molecule 20: 30S ribosomal protein S21



ALA
ARG
GLU
ASN
ALA
ARG
ARG
ARG
THR
LEU
TYR

• Molecule 20: 30S ribosomal protein S21

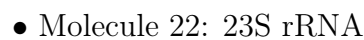


MET PRO VAL I3 K4 E7 E8 E9 P10 F11 B12 V13 A14 L15 R16 R17 R18 F18 K19 R20 R21 S21 C22 E23 K24 A25 A26 G26 V27 L28 L29 A29 E30 V31 R32 R33 R34 E35 F36 Y37 E38 K39 P40 T41 T42 E43 E44 K45 K53 ARG HIS ALA LYS LYS LEU ALA ARG GLU ASN ARG ARG ARG

• Molecule 21: 16S rRNA

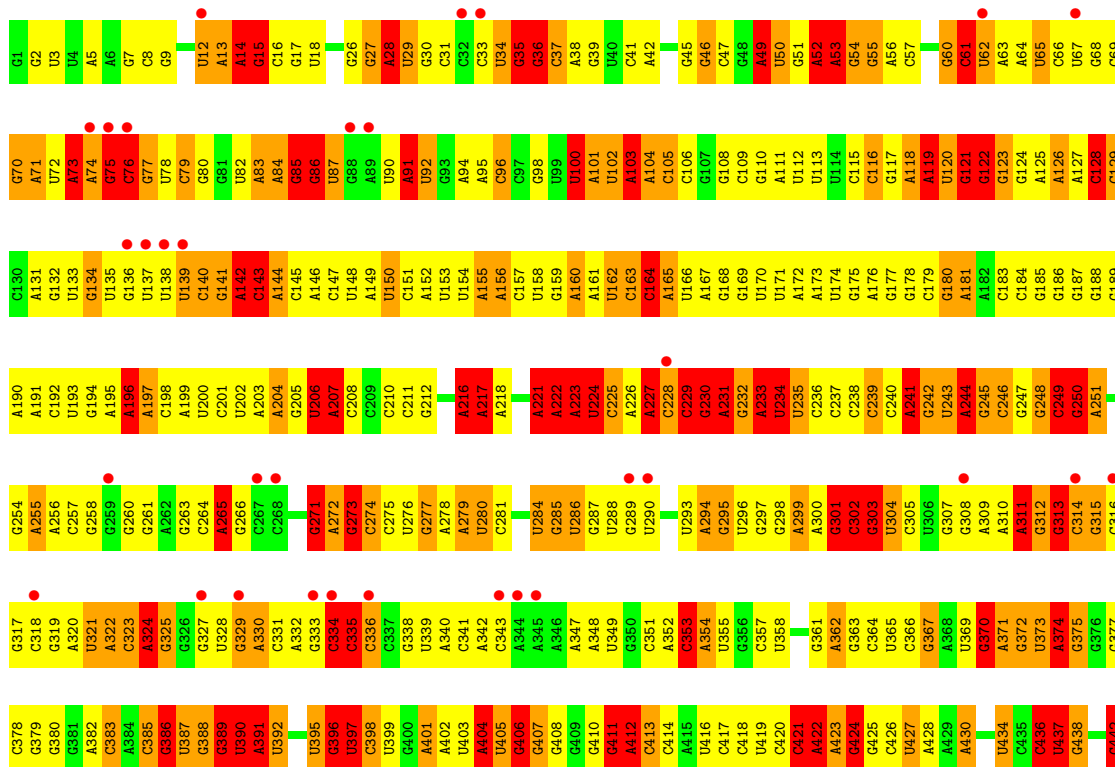


A2 A3 U4 U5 G6 A7 A8 A9 A10 G11 G12 U13 U14 G15 A16 U17 U18 U19 C18 A19 U20 U21 G21 G22 C23 U24 G31 A32 A33 C34 G35 G36 U37 G38 G39 G46 G47 C48 U49 A50 A51 C52 G113 U114 A53 U56 G57 G58 A59 A60 G61 G62 G63 G64 A65 A66 G67 G68 G69 U70 A71 A72 G73 A74 G75 G76 G77 A78 G79 A80 A81 G82 C83 C84 U84 U85 U86 G87 G88 U89 U90 U91 U92 U93 G94 C95 C96 G97 A98 C99 G100 A101 G102 U103 G104 G105 C106 G107 G108 G109 C110 G111 G112 G113 U114 G115 A116 G117 G118 U119 A120 G121 U122 G123 G126 A127 G128 G129 A130 A131 C132 U133 G134 C135 C136 U137 G138 A139 U140 G141 G142 A143 G144 G147 G148 A149 U150 U151 A152 A155 A156 U157 G158 G159 C163 C169 U170 A171 A172 U173 A174 C175 G176 G177 A181 A182 C183 G184 U185 C186 G187 C188 A189 A190 G191 A192 G193 C194 A195 A196 A197 G198 G199 G200 G201 C202 G203 G204 A205 C206 G207 U208 G209 C210 G211 G212 C213 A214 G215 U216 C217 U218 U219 G220 U224 C225 G226 G227 U230 G231 G232 C233 G240 U243 U244 U245 A246 U248 C250 G251 G252 U253 G254 G255 U256 G257 G258 G259 G260 U261 G262 A263 G264 G265 U266 G267 C268 G269 A270 C271 C272 U273 A274 G275 G276 A279 C280 G281 A282 U283 C284 C285 C286 U287 A288 G289 G292 G299 A300 A303 U304 G305 A306 C307 C308 A309 A315 C316 C317 U317 A320 A321 C322 U323 A324 A325 G326 A327 C328 A329 C330 G331 G332 U333 C334 A338 G339 U340 C341 G342 U343 A344 C345 G346 G347 G351 C352 C353 G354 C355 A356 G357 U358 C359 A363 A364 U365 A366 A367 U368 U369 G370 A371 C372 C373 A374 U375 G376 A382 A383 A384 C385 C386 U387 G388 A389 C391 C392 A393 G394 C395 A396 C397 U398 G399 C400 C403 C404 U405 U406 U407 U408 U409 G410 U411 U412 U413 U414 U415 U416 U417 U418 U419 U420 U421 U422 U423 U424 U425 U426 U427 U428 U429 U430 U431 U432 U433 U434 U435 U436 U437 U438 U439 U440 U441 U442 U443 U444 U445 U446 U447 U448 U449 U450 U451 U452 U453 U454 U455 U456 U457 U458 U459 U460 U461 U462 U463 U464 U465 U466 U467 U468 U469 U470 U471 U472 U473 U474 U475 U476 U477 U478 U479 U480 U481 U482 U483 U484 U485 U486 U487 U488 U489 U490 U491 U492 U493 U494 U495 U496 U497 U498 U499 U500 U501 U502 U503 U504 U505 U506 U507 U508 U509 U510 U511 U512 U513 U514 U515 U516 U517 U518 U519 U520 U521 U522 U523 U524 U525 U526 U527 U528 U529 U530 U531 U532 U533 U534 U535 U536 U537 U538 U539 U540 U541 U542 U543 U544 U545 U546 U547 U548 U549 U550 U551 U552 U553 U554 U555 C556 C557 A558 U559 U560 U561 U562 U563 U564 U565 U566 U567 U568 U569 U570 U571 U572 U573 U574 U575 U576 U577 U578 U579 U580 U581 U582 U583 U584 U585 U586 U587 U588 U589 U590 U591 U592 U593 U594 U595 U596 U597 U598 U599 U600 U601 U602 U603 U604 U605 U606 U607 U608 U609 U610 U611 U612 U613 U614 U615 U616 U617 U618 U619 U620 U621 U622 U623 U624 G625 G626 G627 G628 G629 G630 G631 G632 G633 G634 G635 U641 U642 U643 U644 U645 U652 U653 U654 U655 U656 U657 U658 U659 U660 U661 U662 U663 U664 U665 U666 U667 U672 U673 U674 U675 U676 U677 U678 U679 U680 U681 U682 U683 U684 U685 U686 U687 U688 U689 U692 U693 U694 U695 U696 U697 U698 U699 U700 U701 U702 U703 U704 U705 U706 U707 U708 U709 U710 U711 U712 U713 U714 U715 U716 U717 U718 U719 U720 U721 U722 U723 U724 U725 U726 U727 U728 U729 U730 U731 U732 U733 U734 U735 U736 U737 U738 U739 U740 U741 U742 U743 U744 U745 U746 U747 U748 U749 U750 U751 U752 U753 U754 U755 U756 U757 U758 U759 U760 U761 U762 U763 U764 U765 U766 U767 U768 U769 U770 U771 U772 U773 U774









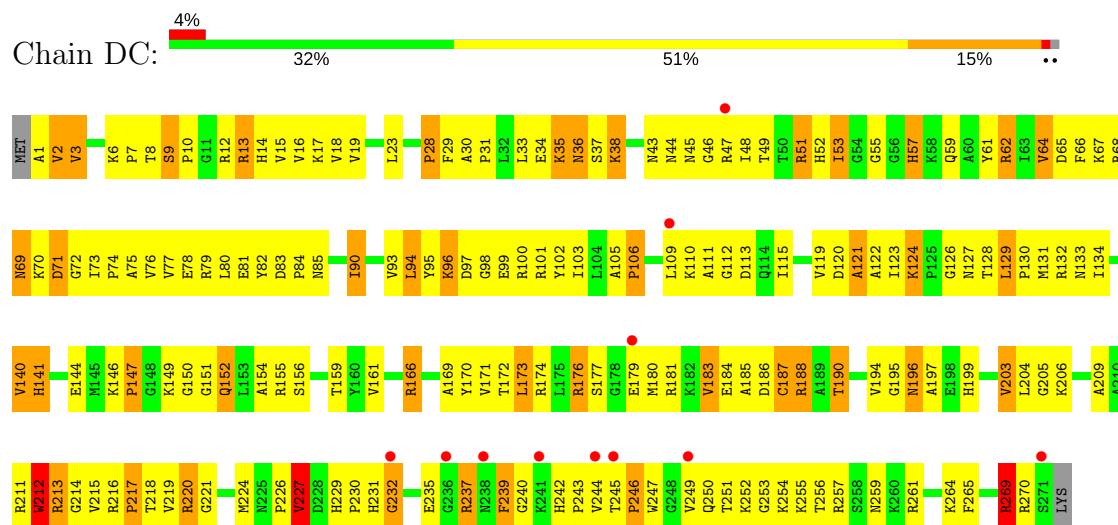
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G1345	G1280	A1214	A1146	A1084	G1022	U958	G	G830	A764	G701	A633	A572	A506	C445
G1346	G1281	A1085	A1147	A1085	U1023	A959	A	G831	C765	G701	C634	U573	A507	C446
A1347	G1282	U1148	G1148	A1086	G1024	A960	C	U832	U766	U703	C635	A574	A508	A447
G1348	G1283	G1067	U1149	G1067	G1025	G961	U	A833	G704	G704	G636	A575	C509	U448
C1349	A1284	A1088	C1153	A1088	G1026	G962	U	G834	U769	A705	A637	U576	C510	A449
C1350	A1285	A1089	G1154	A1089	A1027	U963	A	C835	G770	A706	U638	G577	U511	A450
C1351	A1286	A1090	G1154	A1090	A1028	G964	C	G836	G771	A707	U639	G578	U512	A451
U1352	A1287	G1091	A1155	C1091	A1029	U965		C837	U773	A708	U640	G579	A513	A452
A1353	G1288	C1092	A1156	C1092	G1030	G966		C838	G774	G708	U641	U580	A514	A453
A1354	C1289	G1093	G1157	U1094	G1031	U967			G775	U709	U642	C581	A515	A454
A1355	C1290	U1094	C1158	U1094	A1032	C968	C902	G841	G776	U710	A643	C584	C455	A455
C1356	C1291	A1095	U1159	A1095	U1033	G969	G903	U842	G777	G711	A644	C585	C456	A456
C1357	G1292	A1096	C1160	A1096	G1034	U970	G904	U843	G778	G712	C645	G586	C457	A457
C1358		U1097	C1161	U1097	U1035	G971	A905	G844	U779	G713	U646	A586	G458	U459
A1359		A1098	U1173	A1098	G1036	A972		A845	G780	U714	G647	C587	U459	A460
G1360		G1099	G1166	C1099	A1040	A973	A910	U846	A781	A715	G648	U588	U525	A461
G1361	G1299	C1100	C1167	U1101	G1041	G974	C912	U847	G782	A716	G649	U589	U526	
C1362	A1300	U1101	G1168	U1101	G1042	A975	U913	C848	A783	C717	C650	A590	A526	
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G1364	G1302	A1103	G1170	A1103	C1044	U977		U850	G785	C719	U652	A592	A528	
G1365	G1303	C1104	G1171	C1104	C1045	C978	G915	C851	C786	U720	U653	A593	A465	
A1366	A1304	U1105	U1172	U1105	C1046	A980	A917	U852	G787	A721	A654	U594	A467	
C1368	C1305	U1106	C1173	U1106	A1047	A981	A918	C853	A788		A655	C595	C531	
	C1306	G1107	U1174	G1107	G1047	C982	U919	C854	A789	U724	G656	U596	A532	
G1371	A1307	U1108	A1175	U1108	A1048	A983	A920	G855	U790	G725	U657	G597	A532	
U1372	G1308	C1109	C1176	C1109	C1049	A984	C921	C856	C791	G726	U658	U598	G583	
A1373	G1309	A1110	U1177	A1110	A1050	C985	C922	C857	A792	A727	G659	A599	A472	
G1374	G1310	C1111	C1178	A1111	G1051		G923	C858	A793	G728	C660	G600	A473	
U1375	G1311	U1112	C1179	U1112	C1052	A988	G924	C859	A794	G729	A661	C601	G537	
C1376	U1312	U1113	U1180	U1113	A1053	G989	A925	U860	C795	A730	G662	A602	A538	
C1377	U1313	C1114	U1181	C1114	G1054	A990	G926	A861	C796	C731	G663	G539	G539	
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U1379	C1315	U1183	U1183	U1183	G1056	C992	A928	A863	G798	G733	U665	G605	A541	
G1380	U1316	U1184	U1184	U1184	A1057	C993	U929	C864	G799	A734	A666	U606	A478	
G1381	G1317	U1185	U1185	U1185	G1058	C995	G930	C865	A800	A735	U667	U607	A479	
G1382		G1186	G1186	G1186	G1059	A996	U931	A866	G801	C736	A668	A608	C544	
A1383	C1320	C1212	U1187	C1212	U1060	G997	U932	C867	A802	G737	G669	A609	U545	
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A1404	A1277	C1211	C1211	A1443	U1081		U955	C	U827			G630	U569	

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A2369	G2239	G	G2239	U	G2044	U1980	U1911	U1834	C1774	G1707	C1638	C1574	G1511	U1442
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A2322	U2259	U2190	U2259	U	C2063	U1998	U1932		G1792	C1728	U1662	U1595	A1529	C1462
G2323	C2260	A2191	C2260	U	C2064	A1999	G1935	G1862	U1793	U1729	G1663	A1596	C1530	
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A2330	A2266	G2138	A2266	G	A2071	G2010	U1940		A1735	U1736		A1603	G1537	
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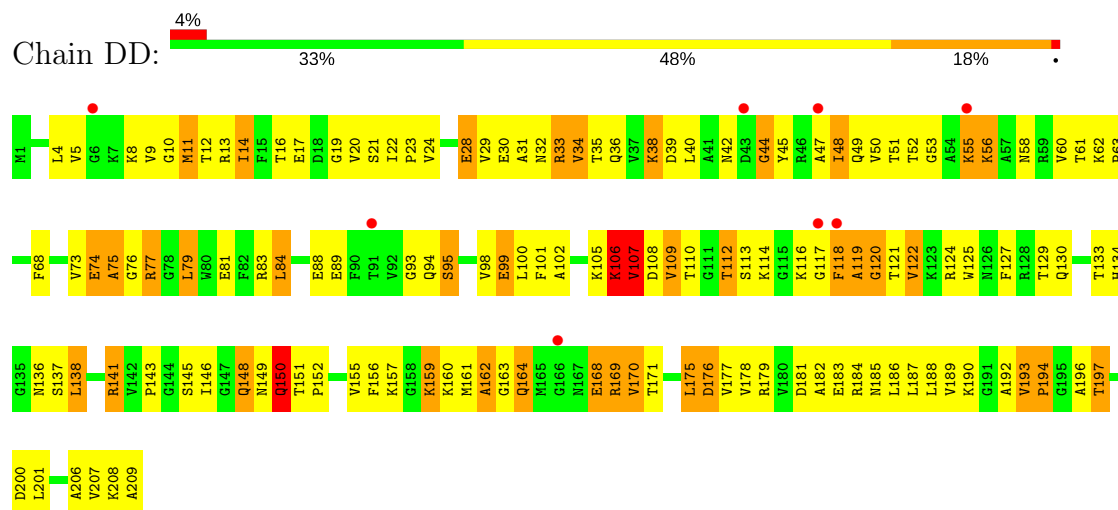
• Molecule 24: 50S ribosomal protein L2



• Molecule 25: 50S ribosomal protein L3

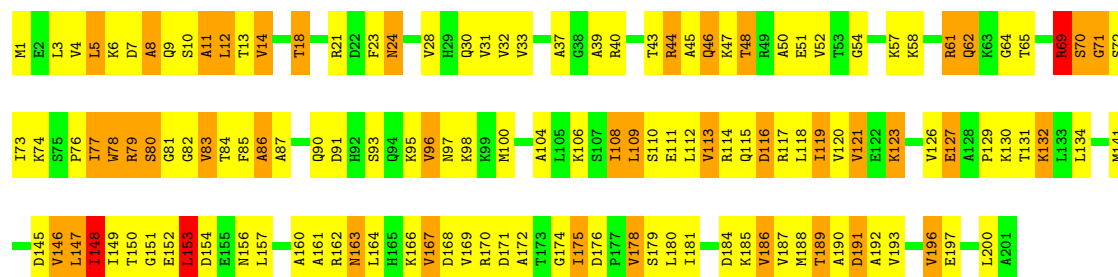


• Molecule 25: 50S ribosomal protein L3



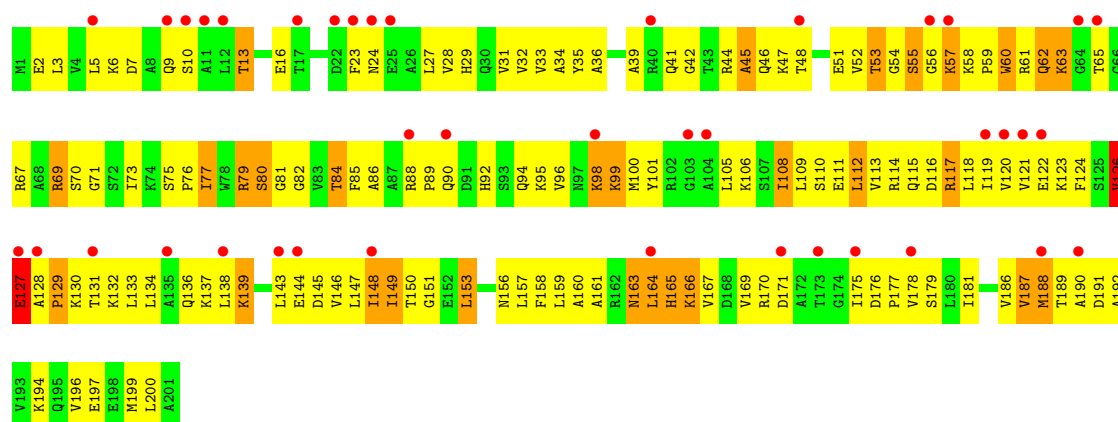
• Molecule 26: 50S ribosomal protein L4

Chain BE:  32% 46% 20% .



• Molecule 26: 50S ribosomal protein L4

Chain DE:  29% 55% 14% .



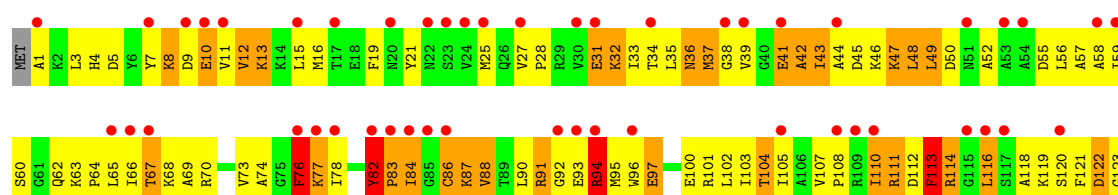
• Molecule 27: 50S ribosomal protein L5

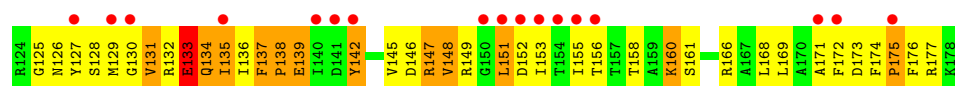
Chain BF:  44% 40% 13% ..



• Molecule 27: 50S ribosomal protein L5

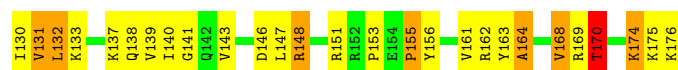
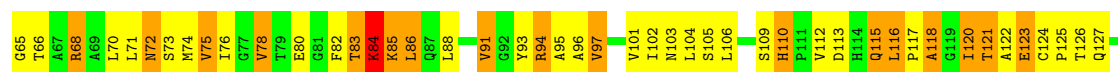
Chain DF:  26% 47% 23% ..





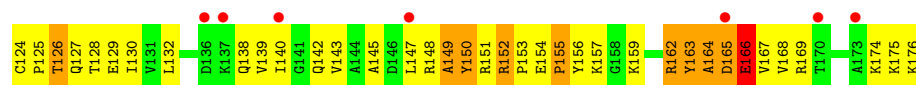
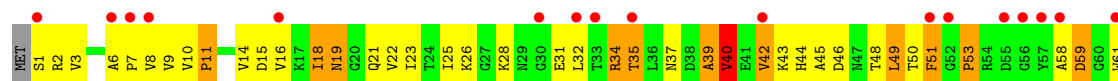
• Molecule 28: 50S ribosomal protein L6

Chain BG: 31% 45% 22%



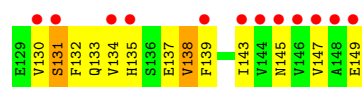
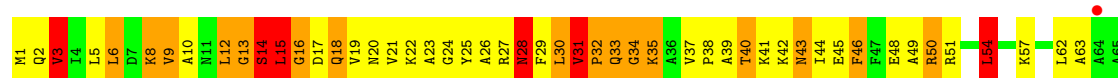
• Molecule 28: 50S ribosomal protein L6

Chain DG: 23% 32% 49% 16%



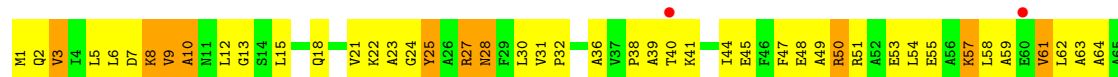
• Molecule 29: 50S ribosomal protein L9

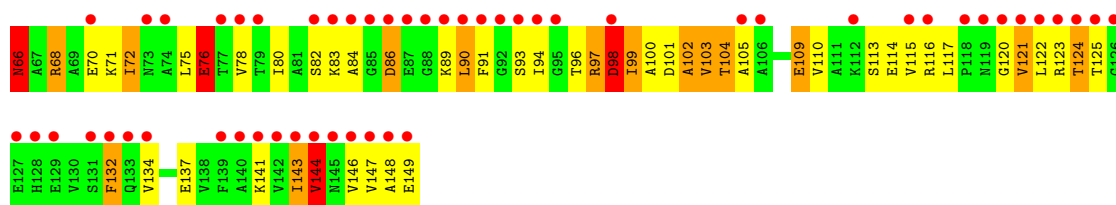
Chain BH: 40% 32% 42% 20% 5%



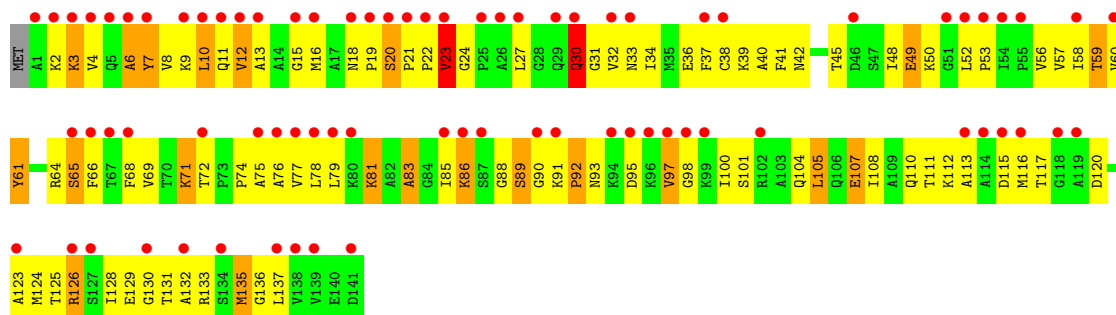
• Molecule 29: 50S ribosomal protein L9

Chain DH: 37% 36% 46% 16%

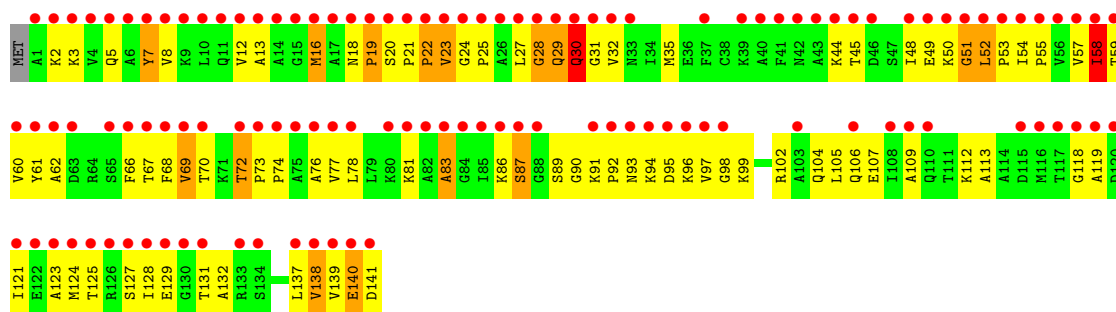
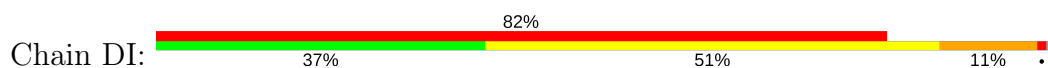




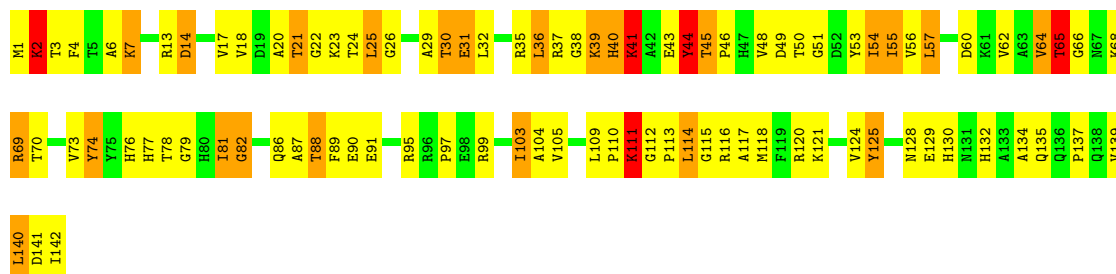
• Molecule 30: 50S ribosomal protein L11



• Molecule 30: 50S ribosomal protein L11

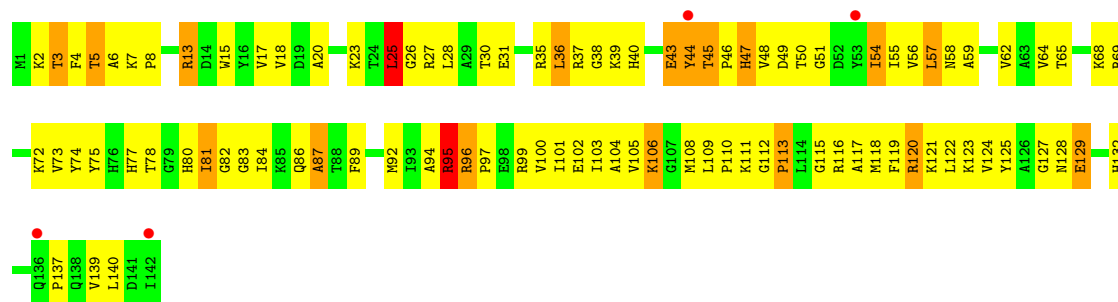


• Molecule 31: 50S ribosomal protein L13



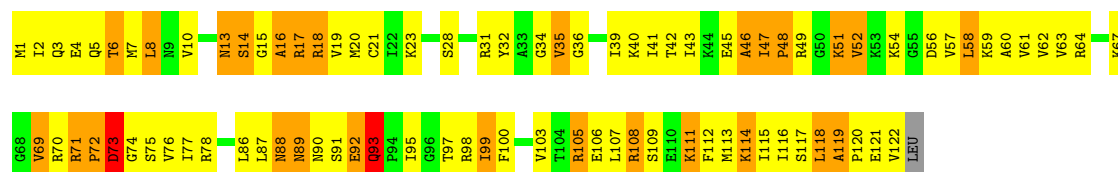
• Molecule 31: 50S ribosomal protein L13





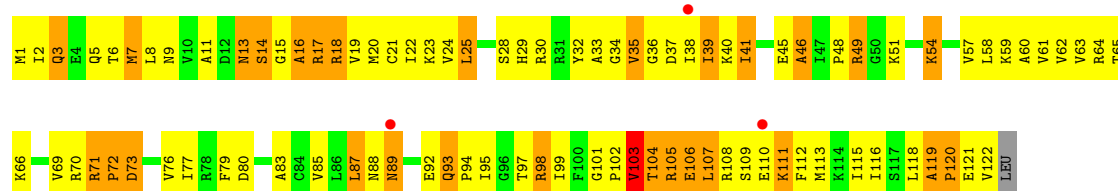
• Molecule 32: 50S ribosomal protein L14

Chain BK: 27% 49% 22% ..



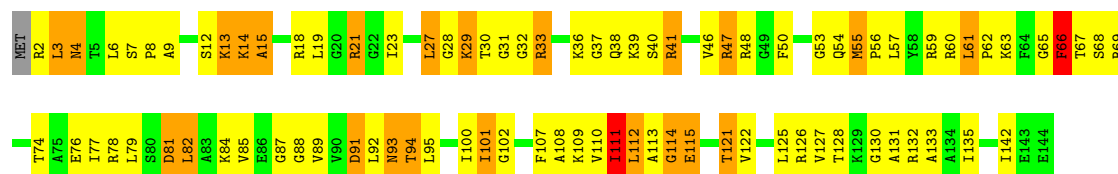
• Molecule 32: 50S ribosomal protein L14

Chain DK: 29% 24% 51% 23% ..



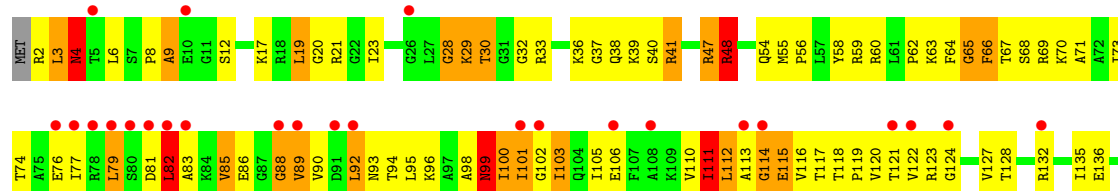
• Molecule 33: 50S ribosomal protein L15

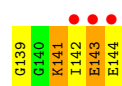
Chain BL: 38% 44% 16% ..



• Molecule 33: 50S ribosomal protein L15

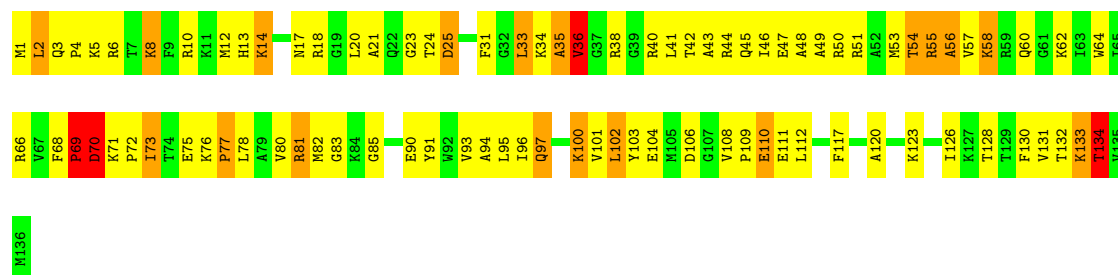
Chain DL: 19% 35% 44% 16% ..





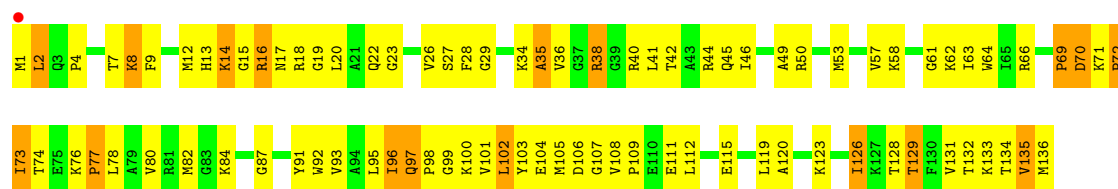
• Molecule 34: 50S ribosomal protein L16

Chain BM: 35% 49% 13%



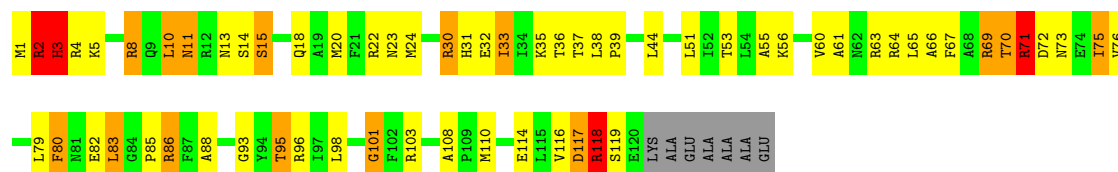
• Molecule 34: 50S ribosomal protein L16

Chain DM: 36% 51% 13%



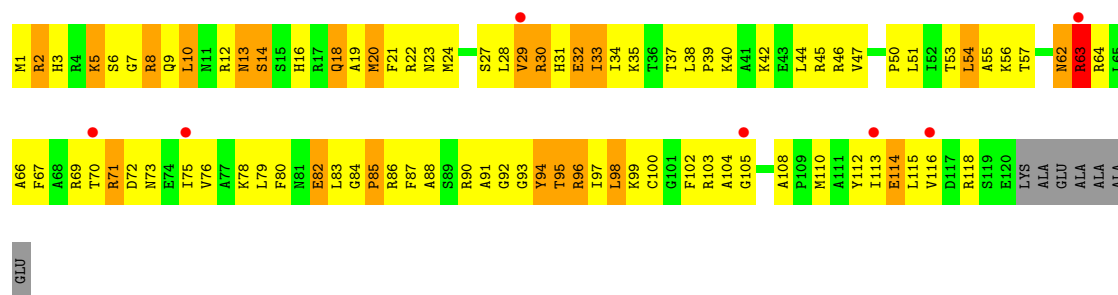
• Molecule 35: 50S ribosomal protein L17

Chain BN: 44% 35% 12% 6%

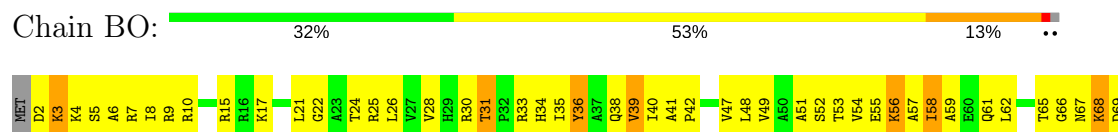


• Molecule 35: 50S ribosomal protein L17

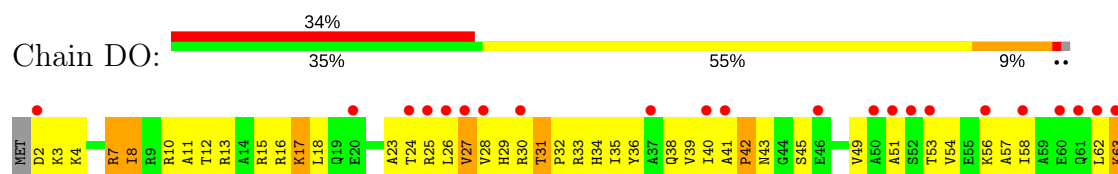
Chain DN: 24% 53% 17% 6%



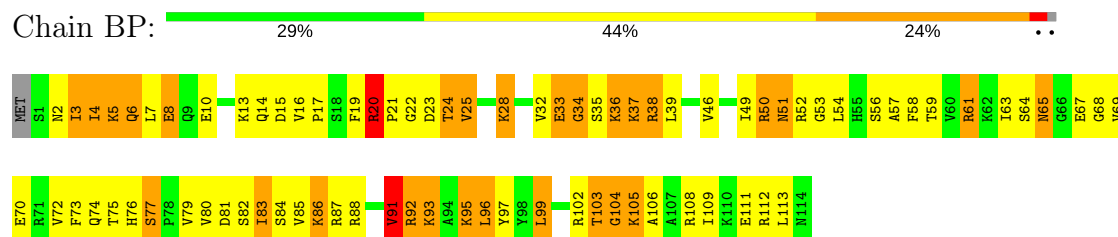
• Molecule 36: 50S ribosomal protein L18



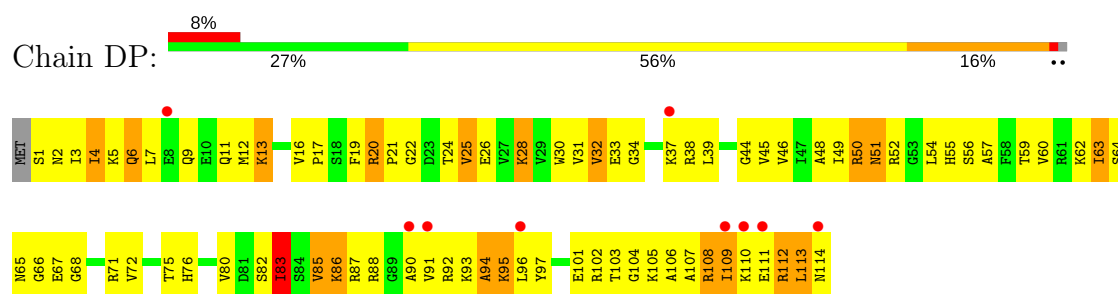
- Molecule 36: 50S ribosomal protein L18



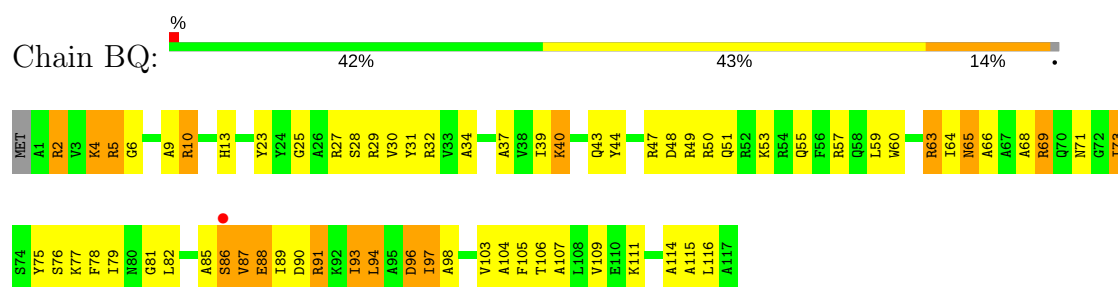
- Molecule 37: 50S ribosomal protein L19



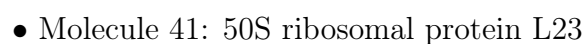
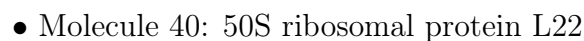
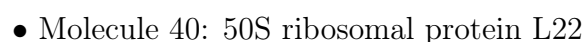
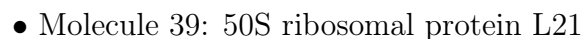
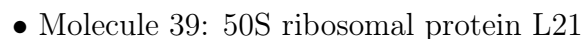
- Molecule 37: 50S ribosomal protein L19

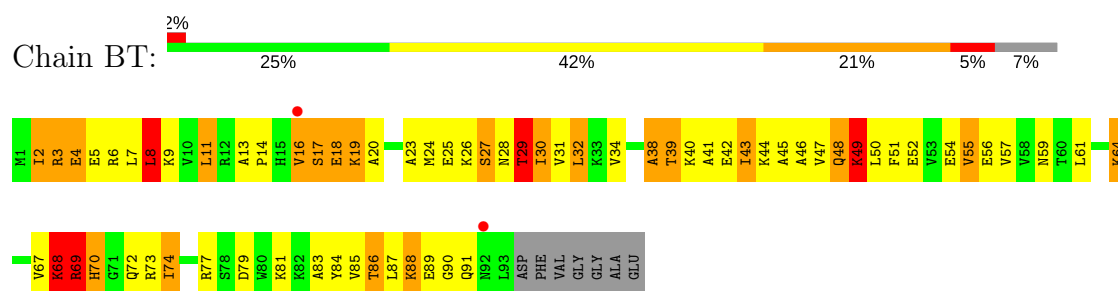


- Molecule 38: 50S ribosomal protein L20

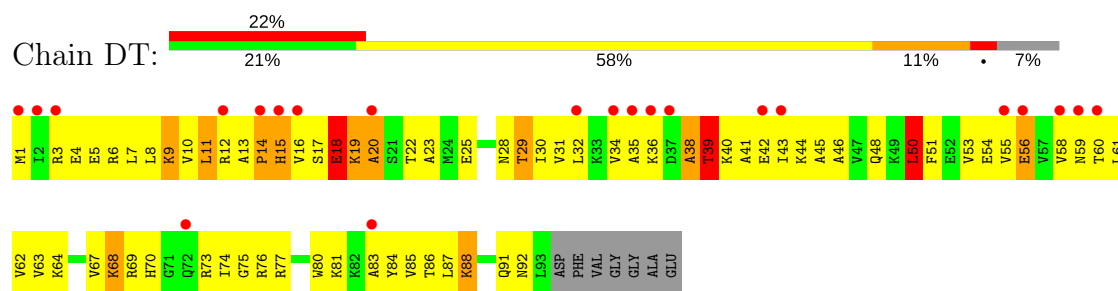


- Molecule 38: 50S ribosomal protein L20

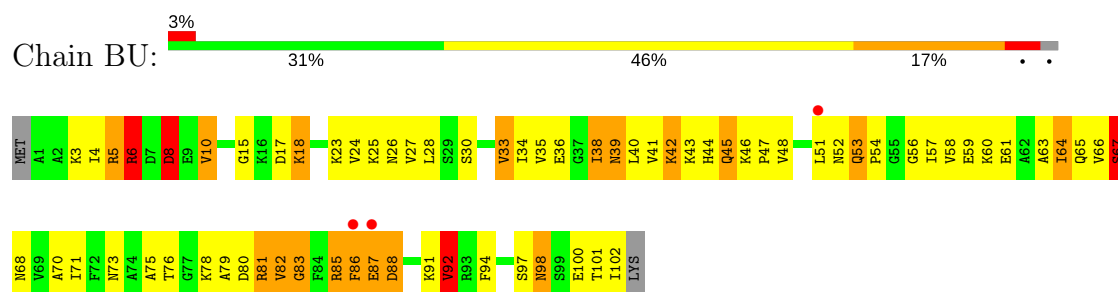




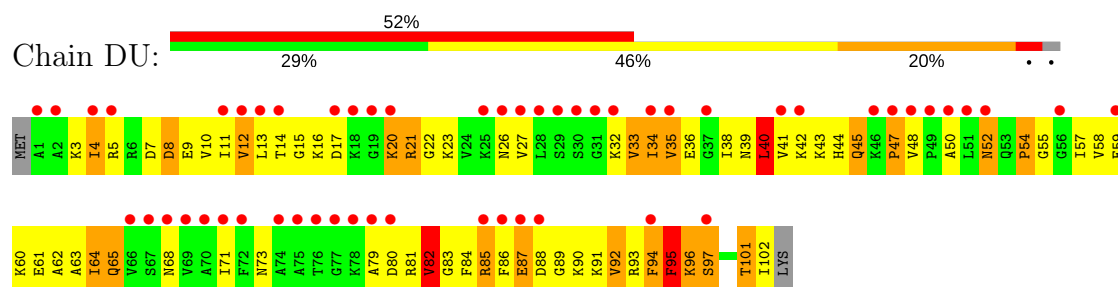
- Molecule 41: 50S ribosomal protein L23



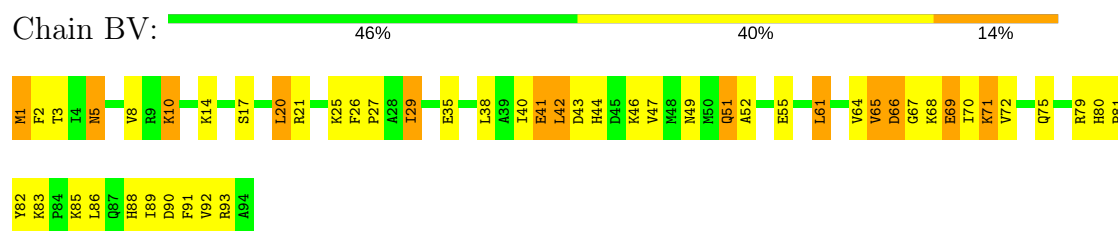
- Molecule 42: 50S ribosomal protein L24



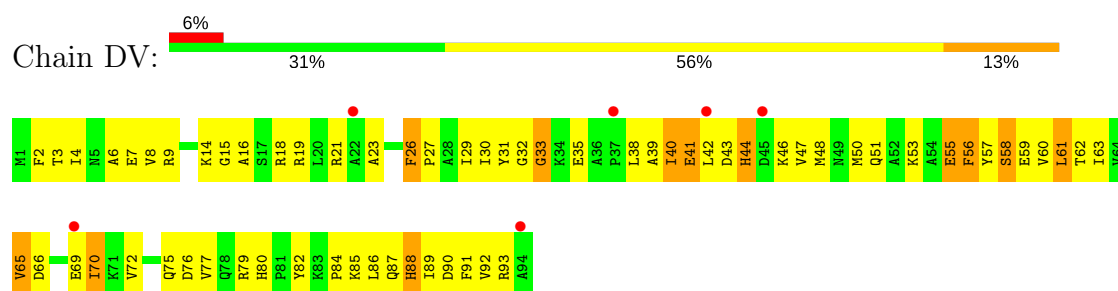
- Molecule 42: 50S ribosomal protein L24



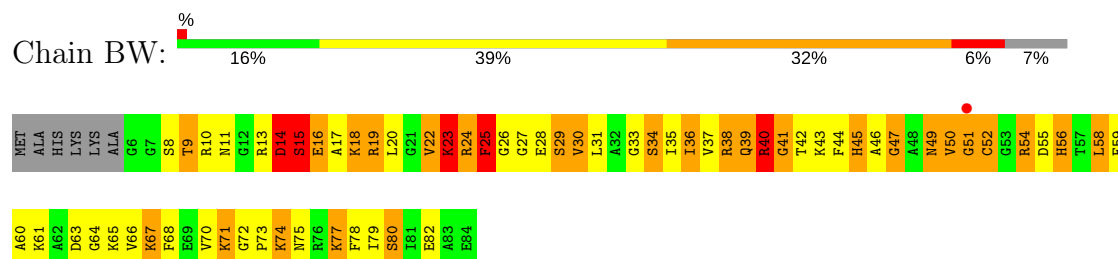
- Molecule 43: 50S ribosomal protein L25



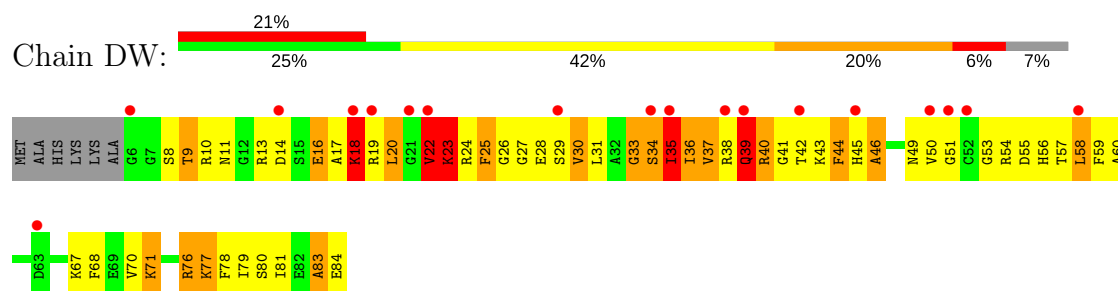
- Molecule 43: 50S ribosomal protein L25



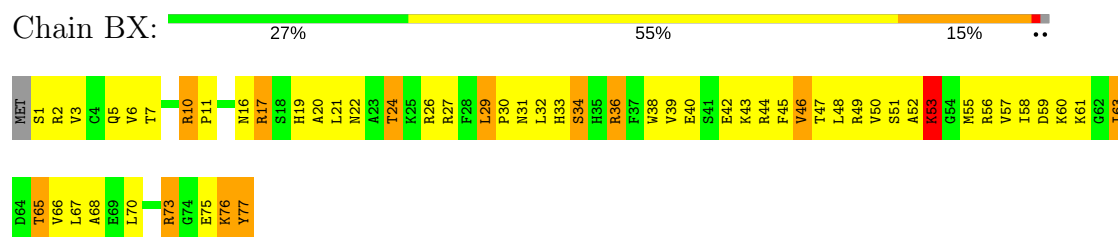
- Molecule 44: 50S ribosomal protein L27



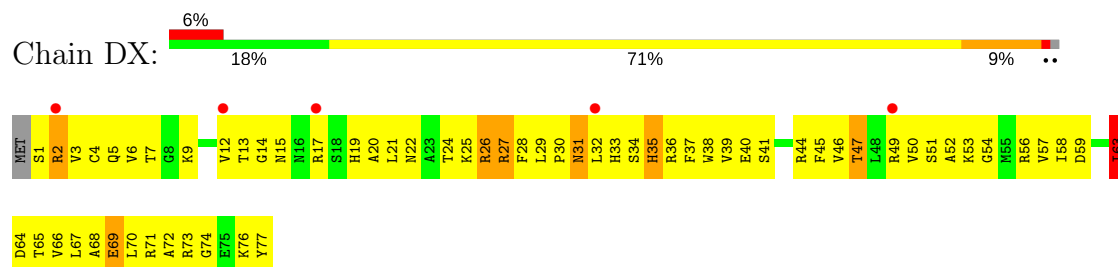
- Molecule 44: 50S ribosomal protein L27



- Molecule 45: 50S ribosomal protein L28



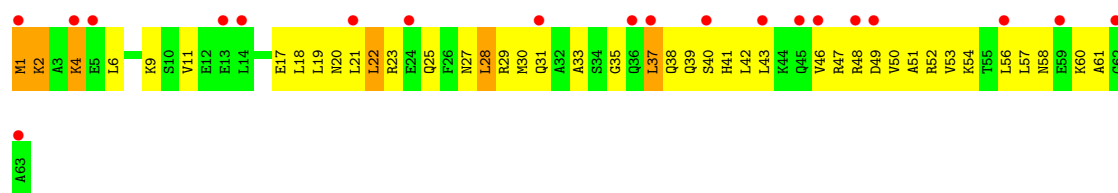
- Molecule 45: 50S ribosomal protein L28



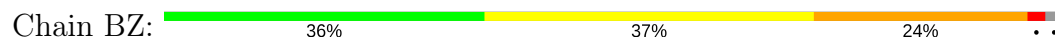
- Molecule 46: 50S ribosomal protein L29



- Molecule 46: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L30



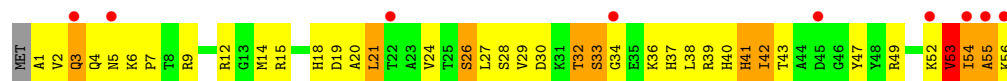
- Molecule 47: 50S ribosomal protein L30



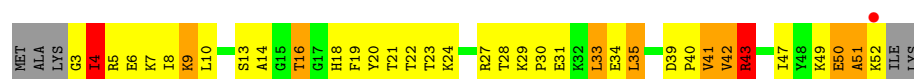
- Molecule 48: 50S ribosomal protein L32



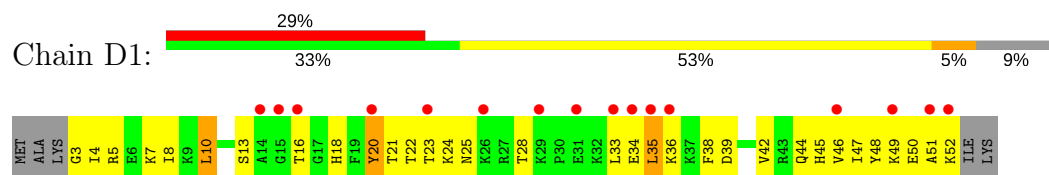
- Molecule 48: 50S ribosomal protein L32



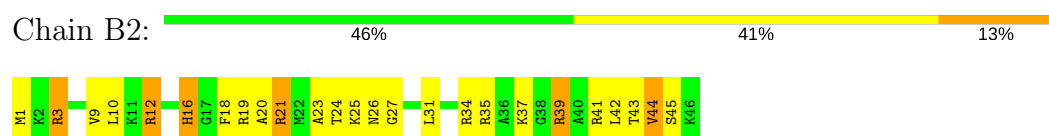
- Molecule 49: 50S ribosomal protein L33



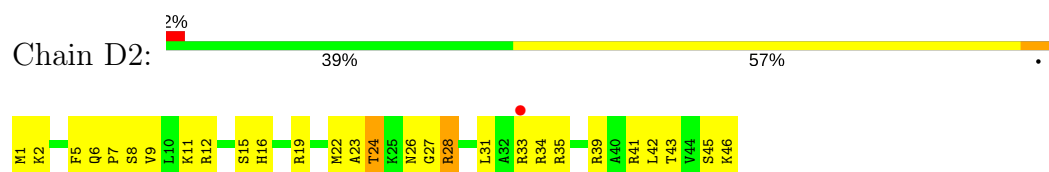
- Molecule 49: 50S ribosomal protein L33



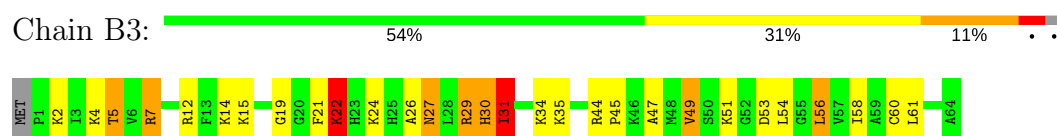
- Molecule 50: 50S ribosomal protein L34



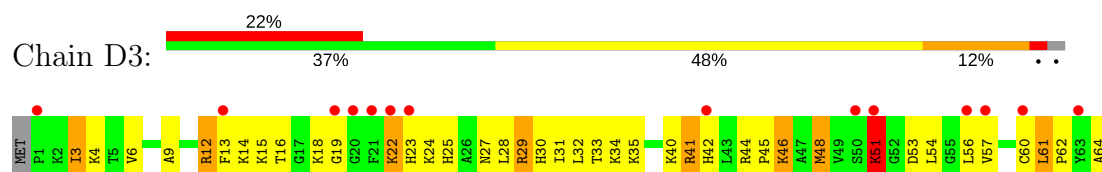
- Molecule 50: 50S ribosomal protein L34



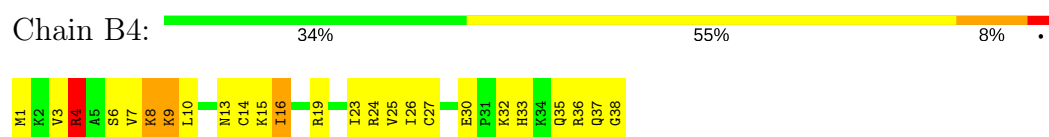
- Molecule 51: 50S ribosomal protein L35



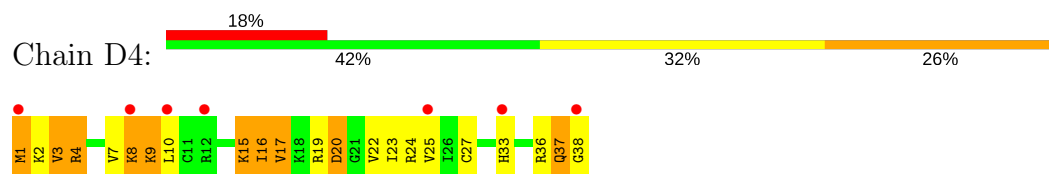
- Molecule 51: 50S ribosomal protein L35



- Molecule 52: 50S ribosomal protein L36

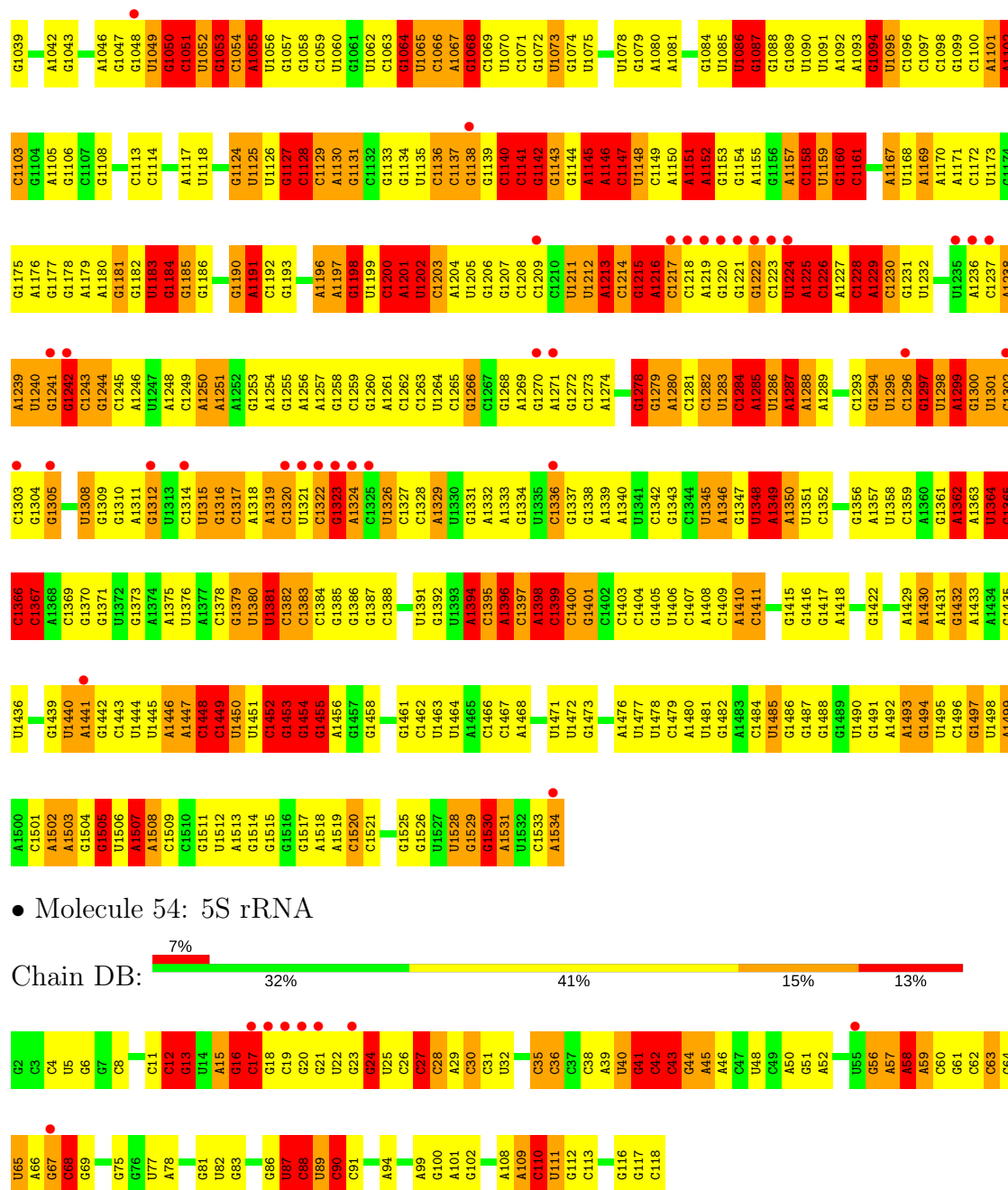


- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 16S rRNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.89Å 434.93Å 622.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.88 – 3.19 39.88 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.8 (39.88-3.19) 95.8 (39.88-3.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.195 , 0.252 0.206 , 0.261	Depositor DCC
R_{free} test set	18171 reflections (2.01%)	DCC
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 74.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	284450	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	AB	0.30	0/1735	0.52	0/2338
1	CB	0.27	0/1735	0.49	0/2338
2	AC	0.30	0/1651	0.53	1/2225 (0.0%)
2	CC	0.25	0/1651	0.45	0/2225
3	AD	0.31	0/1665	0.52	0/2227
3	CD	0.39	0/1665	0.60	0/2227
4	AE	0.36	0/1118	0.63	1/1504 (0.1%)
4	CE	0.34	0/1118	0.54	0/1504
5	AF	0.32	0/835	0.49	0/1128
5	CF	0.28	0/835	0.50	0/1128
6	AG	0.27	0/1195	0.48	0/1602
6	CG	0.25	0/1187	0.46	0/1591
7	AH	0.33	0/989	0.55	0/1326
7	CH	0.28	0/989	0.50	0/1326
8	AI	0.27	0/1034	0.49	0/1375
8	CI	0.24	0/1034	0.43	0/1375
9	AJ	0.29	0/796	0.53	0/1077
9	CJ	0.24	0/796	0.48	0/1077
10	AK	0.31	0/893	0.56	0/1205
10	CK	0.29	0/893	0.50	0/1205
11	AL	0.39	0/969	0.69	0/1300
11	CL	0.32	0/969	0.57	0/1300
12	AM	0.26	0/892	0.49	0/1193
12	CM	0.20	0/884	0.41	0/1181
13	AN	0.30	0/785	0.54	0/1043
13	CN	0.22	0/780	0.39	0/1036
14	AO	0.30	0/722	0.49	0/964
14	CO	0.26	0/722	0.45	0/964
15	AP	0.30	0/659	0.50	0/884
15	CP	0.30	0/648	0.51	0/870
16	AQ	0.39	0/657	0.59	0/881
16	CQ	0.31	0/657	0.51	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.30	0/462	0.50	0/621
17	CR	0.30	0/462	0.47	0/621
18	AS	0.28	0/652	0.49	0/877
18	CS	0.21	0/652	0.43	0/877
19	AT	0.35	0/671	0.56	0/888
19	CT	0.27	0/671	0.50	0/888
20	AU	0.39	0/430	0.54	0/570
20	CU	0.39	0/430	0.63	0/570
21	AA	0.55	1/36834 (0.0%)	1.38	581/57462 (1.0%)
22	BA	0.78	12/68626 (0.0%)	1.59	1420/107056 (1.3%)
22	DA	0.50	0/68314	1.35	1136/106569 (1.1%)
23	BB	0.71	0/2828	1.50	45/4410 (1.0%)
24	BC	0.44	0/2121	0.70	1/2852 (0.0%)
24	DC	0.31	0/2121	0.53	0/2852
25	BD	0.53	0/1586	0.76	1/2134 (0.0%)
25	DD	0.30	0/1586	0.56	0/2134
26	BE	0.43	0/1571	0.64	0/2113
26	DE	0.26	0/1571	0.47	0/2113
27	BF	0.33	0/1434	0.54	0/1926
27	DF	0.23	0/1444	0.47	0/1937
28	BG	0.40	0/1343	0.64	0/1816
28	DG	0.24	0/1343	0.48	0/1816
29	BH	0.31	0/1122	0.50	0/1515
29	DH	0.28	0/1122	0.50	0/1515
30	BI	0.23	0/1046	0.47	0/1410
30	DI	0.21	0/1046	0.43	0/1410
31	BJ	0.57	0/1152	0.80	1/1551 (0.1%)
31	DJ	0.28	0/1152	0.55	1/1551 (0.1%)
32	BK	0.51	0/947	0.77	0/1268
32	DK	0.33	0/947	0.56	0/1268
33	BL	0.43	0/1054	0.75	0/1403
33	DL	0.27	0/1054	0.52	0/1403
34	BM	0.50	0/1093	0.70	0/1460
34	DM	0.27	0/1093	0.46	0/1460
35	BN	0.47	0/973	0.70	0/1301
35	DN	0.28	0/973	0.50	0/1301
36	BO	0.42	0/902	0.63	0/1209
36	DO	0.22	0/902	0.42	0/1209
37	BP	0.50	0/929	0.73	0/1242
37	DP	0.30	0/929	0.50	0/1242
38	BQ	0.57	0/960	0.73	0/1278
38	DQ	0.29	0/960	0.46	0/1278
39	BR	0.60	1/829 (0.1%)	0.75	0/1107

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DR	0.28	0/829	0.49	0/1107
40	BS	0.53	0/864	0.72	0/1156
40	DS	0.29	0/864	0.52	0/1156
41	BT	0.46	0/744	0.74	0/994
41	DT	0.24	0/744	0.48	0/994
42	BU	0.44	0/787	0.70	0/1051
42	DU	0.25	0/787	0.47	0/1051
43	BV	0.42	0/766	0.58	0/1025
43	DV	0.25	0/766	0.43	0/1025
44	BW	0.56	0/603	0.87	0/797
44	DW	0.26	0/603	0.48	0/797
45	BX	0.42	0/635	0.70	1/848 (0.1%)
45	DX	0.27	0/635	0.55	0/848
46	BY	0.35	0/510	0.65	0/677
46	DY	0.22	0/510	0.45	0/677
47	BZ	0.51	0/453	0.77	0/605
47	DZ	0.26	0/453	0.49	0/605
48	B0	0.45	0/450	0.71	0/599
48	D0	0.28	0/450	0.51	0/599
49	B1	0.40	0/416	0.63	0/554
49	D1	0.27	0/416	0.46	0/554
50	B2	0.46	0/380	0.73	0/498
50	D2	0.28	0/380	0.50	0/498
51	B3	0.45	0/513	0.69	0/676
51	D3	0.27	0/513	0.51	0/676
52	B4	0.55	0/303	0.78	0/397
52	D4	0.27	0/303	0.49	0/397
53	CA	0.50	0/36762	1.32	542/57350 (0.9%)
54	DB	0.44	0/2803	1.26	34/4371 (0.8%)
All	All	0.55	14/306737 (0.0%)	1.26	3765/458565 (0.8%)

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
25	BD	0	1
32	BK	0	1
35	BN	0	1
51	B3	0	1
All	All	0	4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1142	A	N9-C4	-10.15	1.31	1.37
22	BA	2451	A	C8-N7	8.00	1.37	1.31
22	BA	2447	G	N9-C4	7.71	1.44	1.38
22	BA	984	A	N9-C4	-6.87	1.33	1.37
22	BA	1142	A	C8-N7	6.70	1.36	1.31

The worst 5 of 3765 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2447	G	C6-N1-C2	-18.49	114.00	125.10
22	BA	919	U	N1-C2-O2	18.00	135.40	122.80
22	BA	919	U	C2-N1-C1'	16.54	137.55	117.70
22	BA	302	C	N1-C1'-C2'	-16.46	92.60	114.00
22	BA	805	G	P-O3'-C3'	15.12	137.85	119.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	B3	29	ARG	Peptide
25	BD	9	VAL	Peptide
32	BK	15	GLY	Peptide
35	BN	101	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1704	0	1732	221	0
1	CB	1704	0	1732	174	0
2	AC	1624	0	1699	112	0
2	CC	1624	0	1699	143	0
3	AD	1643	0	1710	151	0
3	CD	1643	0	1710	152	0
4	AE	1105	0	1148	132	0
4	CE	1105	0	1148	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AF	817	0	808	73	0
5	CF	817	0	808	66	0
6	AG	1181	0	1240	87	0
6	CG	1174	0	1230	136	0
7	AH	979	0	1034	74	0
7	CH	979	0	1034	88	0
8	AI	1022	0	1070	83	0
8	CI	1022	0	1070	98	0
9	AJ	786	0	828	74	0
9	CJ	786	0	828	97	0
10	AK	877	0	887	89	0
10	CK	877	0	887	78	0
11	AL	955	0	1019	89	0
11	CL	955	0	1019	89	0
12	AM	883	0	944	74	0
12	CM	876	0	937	107	0
13	AN	774	0	827	76	0
13	CN	769	0	822	82	0
14	AO	714	0	737	54	0
14	CO	714	0	737	36	0
15	AP	649	0	666	52	0
15	CP	638	0	656	67	0
16	AQ	648	0	691	75	0
16	CQ	648	0	691	61	0
17	AR	455	0	478	25	0
17	CR	455	0	478	35	0
18	AS	637	0	665	52	0
18	CS	637	0	665	75	0
19	AT	665	0	714	72	0
19	CT	665	0	714	52	0
20	AU	425	0	449	88	0
20	CU	425	0	449	80	0
21	AA	32895	0	16553	1203	0
22	BA	61274	0	30819	1932	0
22	DA	60995	0	30679	3174	0
23	BB	2529	0	1281	63	0
24	BC	2082	0	2157	213	0
24	DC	2082	0	2157	210	0
25	BD	1565	0	1616	186	0
25	DD	1565	0	1616	179	0
26	BE	1552	0	1619	127	0
26	DE	1552	0	1619	172	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	BF	1410	0	1447	124	0
27	DF	1420	0	1460	170	0
28	BG	1323	0	1374	169	0
28	DG	1323	0	1374	137	0
29	BH	1111	0	1148	107	0
29	DH	1111	0	1148	102	0
30	BI	1032	0	1088	108	0
30	DI	1032	0	1088	77	0
31	BJ	1129	0	1162	154	0
31	DJ	1129	0	1162	141	0
32	BK	938	0	1012	99	0
32	DK	938	0	1012	111	0
33	BL	1045	0	1117	117	0
33	DL	1045	0	1117	115	0
34	BM	1074	0	1157	102	0
34	DM	1074	0	1157	96	0
35	BN	960	0	1000	82	0
35	DN	960	0	1000	122	0
36	BO	892	0	923	74	0
36	DO	892	0	923	75	0
37	BP	917	0	965	131	0
37	DP	917	0	965	112	0
38	BQ	947	0	1022	124	0
38	DQ	947	0	1022	131	0
39	BR	816	0	839	91	0
39	DR	816	0	839	91	0
40	BS	857	0	922	67	0
40	DS	857	0	922	76	0
41	BT	738	0	807	117	0
41	DT	738	0	807	98	0
42	BU	779	0	834	57	0
42	DU	779	0	834	89	0
43	BV	753	0	780	45	0
43	DV	753	0	780	64	0
44	BW	596	0	610	187	0
44	DW	596	0	610	111	0
45	BX	625	0	655	61	0
45	DX	625	0	655	63	0
46	BY	509	0	543	55	0
46	DY	509	0	543	58	0
47	BZ	449	0	491	39	0
47	DZ	449	0	491	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	B0	444	0	461	22	0
48	D0	444	0	461	53	0
49	B1	409	0	440	44	0
49	D1	409	0	440	31	0
50	B2	377	0	418	29	0
50	D2	377	0	418	41	0
51	B3	504	0	574	41	0
51	D3	504	0	574	58	0
52	B4	302	0	340	32	0
52	D4	302	0	340	29	0
53	CA	32831	0	16521	1452	0
54	DB	2507	0	1270	121	0
55	AA	43	0	0	0	0
55	BA	137	0	0	0	0
55	BB	4	0	0	0	0
55	CA	42	0	0	0	0
55	DA	135	0	0	0	0
55	DB	1	0	0	0	0
55	DJ	1	0	0	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	195	0	0	2	0
57	AE	1	0	0	0	0
57	AL	3	0	0	0	0
57	AN	6	0	0	0	0
57	AT	2	0	0	0	0
57	AU	1	0	0	0	0
57	B0	1	0	0	0	0
57	B2	1	0	0	0	0
57	B3	3	0	0	0	0
57	B4	3	0	0	0	0
57	BA	610	0	0	24	0
57	BB	20	0	0	1	0
57	BC	10	0	0	0	0
57	BD	2	0	0	1	0
57	BL	4	0	0	1	0
57	BN	3	0	0	0	0
57	BQ	1	0	0	0	0
57	BT	2	0	0	1	0
57	CA	192	0	0	8	0
57	CE	5	0	0	0	0
57	CI	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	CL	1	0	0	0	0
57	CN	3	0	0	0	0
57	CT	3	0	0	0	0
57	CU	2	0	0	0	0
57	D2	1	0	0	1	0
57	D3	1	0	0	0	0
57	D4	4	0	0	0	0
57	DA	599	0	0	9	0
57	DB	4	0	0	0	0
57	DC	13	0	0	1	0
57	DD	4	0	0	0	0
57	DE	3	0	0	0	0
57	DJ	3	0	0	0	0
57	DL	5	0	0	0	0
57	DN	2	0	0	2	0
57	DT	2	0	0	1	0
57	DU	1	0	0	0	0
57	DV	1	0	0	0	0
All	All	284450	0	190838	15808	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

The worst 5 of 15808 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BQ:63:ARG:NH1	38:BQ:96:ASP:HA	1.49	1.26
22:DA:1439:A:C2	22:DA:1552:A:C6	2.32	1.17
22:DA:1439:A:N1	22:DA:1552:A:C5	2.12	1.17
27:BF:35:LEU:HB3	27:BF:153:ILE:HG22	1.19	1.16
33:BL:93:ASN:HD22	33:BL:94:THR:N	1.44	1.16

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	
1	AB	216/241 (90%)	131 (61%)	49 (23%)	36 (17%)	0	1
1	CB	216/241 (90%)	149 (69%)	47 (22%)	20 (9%)	1	4
2	AC	204/233 (88%)	151 (74%)	35 (17%)	18 (9%)	1	5
2	CC	204/233 (88%)	144 (71%)	41 (20%)	19 (9%)	1	4
3	AD	203/206 (98%)	140 (69%)	36 (18%)	27 (13%)	0	1
3	CD	203/206 (98%)	142 (70%)	39 (19%)	22 (11%)	0	3
4	AE	148/167 (89%)	107 (72%)	25 (17%)	16 (11%)	0	3
4	CE	148/167 (89%)	111 (75%)	21 (14%)	16 (11%)	0	3
5	AF	98/135 (73%)	74 (76%)	15 (15%)	9 (9%)	1	4
5	CF	98/135 (73%)	68 (69%)	18 (18%)	12 (12%)	0	2
6	AG	149/179 (83%)	108 (72%)	34 (23%)	7 (5%)	3	20
6	CG	148/179 (83%)	99 (67%)	35 (24%)	14 (10%)	1	4
7	AH	127/130 (98%)	93 (73%)	30 (24%)	4 (3%)	5	31
7	CH	127/130 (98%)	96 (76%)	20 (16%)	11 (9%)	1	5
8	AI	125/130 (96%)	84 (67%)	31 (25%)	10 (8%)	1	7
8	CI	125/130 (96%)	90 (72%)	21 (17%)	14 (11%)	0	3
9	AJ	96/103 (93%)	67 (70%)	18 (19%)	11 (12%)	0	2
9	CJ	96/103 (93%)	55 (57%)	24 (25%)	17 (18%)	0	0
10	AK	115/129 (89%)	85 (74%)	21 (18%)	9 (8%)	1	7
10	CK	115/129 (89%)	85 (74%)	22 (19%)	8 (7%)	1	9
11	AL	121/124 (98%)	87 (72%)	20 (16%)	14 (12%)	0	2
11	CL	121/124 (98%)	85 (70%)	29 (24%)	7 (6%)	2	15
12	AM	112/118 (95%)	89 (80%)	16 (14%)	7 (6%)	1	12
12	CM	111/118 (94%)	60 (54%)	38 (34%)	13 (12%)	0	2
13	AN	92/101 (91%)	56 (61%)	24 (26%)	12 (13%)	0	2
13	CN	91/101 (90%)	60 (66%)	26 (29%)	5 (6%)	2	16
14	AO	86/89 (97%)	63 (73%)	20 (23%)	3 (4%)	4	28
14	CO	86/89 (97%)	62 (72%)	20 (23%)	4 (5%)	3	20
15	AP	80/82 (98%)	58 (72%)	14 (18%)	8 (10%)	1	4
15	CP	78/82 (95%)	50 (64%)	17 (22%)	11 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	AQ	78/84 (93%)	51 (65%)	15 (19%)	12 (15%)	0	1
16	CQ	78/84 (93%)	59 (76%)	10 (13%)	9 (12%)	0	2
17	AR	53/75 (71%)	40 (76%)	11 (21%)	2 (4%)	4	25
17	CR	53/75 (71%)	39 (74%)	12 (23%)	2 (4%)	4	25
18	AS	77/92 (84%)	59 (77%)	9 (12%)	9 (12%)	0	2
18	CS	77/92 (84%)	46 (60%)	24 (31%)	7 (9%)	1	4
19	AT	83/87 (95%)	56 (68%)	20 (24%)	7 (8%)	1	6
19	CT	83/87 (95%)	59 (71%)	16 (19%)	8 (10%)	1	4
20	AU	49/71 (69%)	25 (51%)	13 (26%)	11 (22%)	0	0
20	CU	49/71 (69%)	21 (43%)	11 (22%)	17 (35%)	0	0
24	BC	269/273 (98%)	194 (72%)	50 (19%)	25 (9%)	1	4
24	DC	269/273 (98%)	174 (65%)	63 (23%)	32 (12%)	0	2
25	BD	207/209 (99%)	146 (70%)	27 (13%)	34 (16%)	0	1
25	DD	207/209 (99%)	132 (64%)	43 (21%)	32 (16%)	0	1
26	BE	199/201 (99%)	155 (78%)	24 (12%)	20 (10%)	1	4
26	DE	199/201 (99%)	130 (65%)	46 (23%)	23 (12%)	0	2
27	BF	175/179 (98%)	134 (77%)	25 (14%)	16 (9%)	1	4
27	DF	176/179 (98%)	98 (56%)	43 (24%)	35 (20%)	0	0
28	BG	174/177 (98%)	111 (64%)	38 (22%)	25 (14%)	0	1
28	DG	174/177 (98%)	106 (61%)	38 (22%)	30 (17%)	0	0
29	BH	147/149 (99%)	68 (46%)	47 (32%)	32 (22%)	0	0
29	DH	147/149 (99%)	75 (51%)	54 (37%)	18 (12%)	0	2
30	BI	139/142 (98%)	84 (60%)	41 (30%)	14 (10%)	1	4
30	DI	139/142 (98%)	81 (58%)	39 (28%)	19 (14%)	0	1
31	BJ	140/142 (99%)	107 (76%)	21 (15%)	12 (9%)	1	5
31	DJ	140/142 (99%)	91 (65%)	38 (27%)	11 (8%)	1	7
32	BK	120/123 (98%)	86 (72%)	15 (12%)	19 (16%)	0	1
32	DK	120/123 (98%)	80 (67%)	20 (17%)	20 (17%)	0	1
33	BL	141/144 (98%)	101 (72%)	32 (23%)	8 (6%)	2	16
33	DL	141/144 (98%)	81 (57%)	40 (28%)	20 (14%)	0	1
34	BM	134/136 (98%)	97 (72%)	22 (16%)	15 (11%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	DM	134/136 (98%)	92 (69%)	29 (22%)	13 (10%)	1	4
35	BN	118/127 (93%)	92 (78%)	17 (14%)	9 (8%)	1	8
35	DN	118/127 (93%)	72 (61%)	30 (25%)	16 (14%)	0	1
36	BO	114/117 (97%)	91 (80%)	12 (10%)	11 (10%)	1	4
36	DO	114/117 (97%)	77 (68%)	30 (26%)	7 (6%)	2	13
37	BP	112/115 (97%)	77 (69%)	18 (16%)	17 (15%)	0	1
37	DP	112/115 (97%)	68 (61%)	27 (24%)	17 (15%)	0	1
38	BQ	115/118 (98%)	100 (87%)	9 (8%)	6 (5%)	2	17
38	DQ	115/118 (98%)	80 (70%)	25 (22%)	10 (9%)	1	5
39	BR	101/103 (98%)	80 (79%)	13 (13%)	8 (8%)	1	7
39	DR	101/103 (98%)	70 (69%)	21 (21%)	10 (10%)	1	4
40	BS	108/110 (98%)	86 (80%)	16 (15%)	6 (6%)	2	16
40	DS	108/110 (98%)	76 (70%)	23 (21%)	9 (8%)	1	6
41	BT	91/100 (91%)	52 (57%)	24 (26%)	15 (16%)	0	1
41	DT	91/100 (91%)	46 (50%)	31 (34%)	14 (15%)	0	1
42	BU	100/104 (96%)	69 (69%)	15 (15%)	16 (16%)	0	1
42	DU	100/104 (96%)	51 (51%)	26 (26%)	23 (23%)	0	0
43	BV	92/94 (98%)	77 (84%)	13 (14%)	2 (2%)	8	41
43	DV	92/94 (98%)	61 (66%)	23 (25%)	8 (9%)	1	5
44	BW	77/85 (91%)	30 (39%)	24 (31%)	23 (30%)	0	0
44	DW	77/85 (91%)	33 (43%)	27 (35%)	17 (22%)	0	0
45	BX	75/78 (96%)	56 (75%)	14 (19%)	5 (7%)	1	10
45	DX	75/78 (96%)	47 (63%)	20 (27%)	8 (11%)	0	3
46	BY	61/63 (97%)	38 (62%)	16 (26%)	7 (12%)	0	2
46	DY	61/63 (97%)	42 (69%)	14 (23%)	5 (8%)	1	6
47	BZ	56/59 (95%)	45 (80%)	9 (16%)	2 (4%)	4	27
47	DZ	56/59 (95%)	34 (61%)	16 (29%)	6 (11%)	0	3
48	B0	54/57 (95%)	41 (76%)	9 (17%)	4 (7%)	1	8
48	D0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	2
49	B1	48/55 (87%)	36 (75%)	7 (15%)	5 (10%)	0	3
49	D1	48/55 (87%)	37 (77%)	7 (15%)	4 (8%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	B2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	7	40
50	D2	44/46 (96%)	31 (70%)	10 (23%)	3 (7%)	1	10
51	B3	62/65 (95%)	53 (86%)	5 (8%)	4 (6%)	1	11
51	D3	62/65 (95%)	39 (63%)	18 (29%)	5 (8%)	1	6
52	B4	36/38 (95%)	31 (86%)	2 (6%)	3 (8%)	1	6
52	D4	36/38 (95%)	23 (64%)	7 (19%)	6 (17%)	0	1
All	All	11238/11970 (94%)	7646 (68%)	2332 (21%)	1260 (11%)	0	3

5 of 1260 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	18	GLN
1	AB	20	ARG
1	AB	40	ILE
1	AB	75	ALA
1	AB	119	GLN

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	
1	AB	180/199 (90%)	138 (77%)	42 (23%)	1	4
1	CB	180/199 (90%)	155 (86%)	25 (14%)	4	19
2	AC	170/190 (90%)	139 (82%)	31 (18%)	2	10
2	CC	170/190 (90%)	152 (89%)	18 (11%)	8	32
3	AD	172/173 (99%)	144 (84%)	28 (16%)	3	13
3	CD	172/173 (99%)	138 (80%)	34 (20%)	1	8
4	AE	113/126 (90%)	94 (83%)	19 (17%)	2	12
4	CE	113/126 (90%)	93 (82%)	20 (18%)	2	10
5	AF	87/116 (75%)	74 (85%)	13 (15%)	3	16
5	CF	87/116 (75%)	74 (85%)	13 (15%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AG	124/147 (84%)	109 (88%)	15 (12%)	6	26
6	CG	123/147 (84%)	99 (80%)	24 (20%)	1	8
7	AH	104/105 (99%)	88 (85%)	16 (15%)	3	15
7	CH	104/105 (99%)	90 (86%)	14 (14%)	4	20
8	AI	105/107 (98%)	88 (84%)	17 (16%)	3	13
8	CI	105/107 (98%)	91 (87%)	14 (13%)	4	21
9	AJ	86/90 (96%)	72 (84%)	14 (16%)	3	13
9	CJ	86/90 (96%)	77 (90%)	9 (10%)	8	32
10	AK	90/99 (91%)	71 (79%)	19 (21%)	1	6
10	CK	90/99 (91%)	78 (87%)	12 (13%)	4	21
11	AL	103/104 (99%)	81 (79%)	22 (21%)	1	6
11	CL	103/104 (99%)	84 (82%)	19 (18%)	2	9
12	AM	92/96 (96%)	88 (96%)	4 (4%)	33	71
12	CM	91/96 (95%)	80 (88%)	11 (12%)	6	26
13	AN	79/84 (94%)	73 (92%)	6 (8%)	15	51
13	CN	79/84 (94%)	67 (85%)	12 (15%)	3	15
14	AO	76/77 (99%)	69 (91%)	7 (9%)	11	38
14	CO	76/77 (99%)	70 (92%)	6 (8%)	14	49
15	AP	65/65 (100%)	54 (83%)	11 (17%)	2	11
15	CP	65/65 (100%)	53 (82%)	12 (18%)	2	9
16	AQ	74/78 (95%)	61 (82%)	13 (18%)	2	10
16	CQ	74/78 (95%)	63 (85%)	11 (15%)	3	16
17	AR	48/65 (74%)	45 (94%)	3 (6%)	21	59
17	CR	48/65 (74%)	46 (96%)	2 (4%)	34	72
18	AS	70/79 (89%)	62 (89%)	8 (11%)	7	28
18	CS	70/79 (89%)	62 (89%)	8 (11%)	7	28
19	AT	65/66 (98%)	48 (74%)	17 (26%)	0	2
19	CT	65/66 (98%)	54 (83%)	11 (17%)	2	11
20	AU	44/61 (72%)	32 (73%)	12 (27%)	0	1
20	CU	44/61 (72%)	34 (77%)	10 (23%)	1	4
24	BC	216/218 (99%)	173 (80%)	43 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	DC	216/218 (99%)	188 (87%)	28 (13%)	5	22
25	BD	164/164 (100%)	136 (83%)	28 (17%)	2	11
25	DD	164/164 (100%)	140 (85%)	24 (15%)	3	17
26	BE	165/165 (100%)	125 (76%)	40 (24%)	1	3
26	DE	165/165 (100%)	150 (91%)	15 (9%)	11	39
27	BF	148/150 (99%)	128 (86%)	20 (14%)	4	20
27	DF	149/150 (99%)	122 (82%)	27 (18%)	2	10
28	BG	137/138 (99%)	107 (78%)	30 (22%)	1	5
28	DG	137/138 (99%)	119 (87%)	18 (13%)	5	22
29	BH	114/114 (100%)	96 (84%)	18 (16%)	3	14
29	DH	114/114 (100%)	96 (84%)	18 (16%)	3	14
30	BI	109/110 (99%)	91 (84%)	18 (16%)	2	12
30	DI	109/110 (99%)	102 (94%)	7 (6%)	20	59
31	BJ	116/116 (100%)	89 (77%)	27 (23%)	1	4
31	DJ	116/116 (100%)	104 (90%)	12 (10%)	8	33
32	BK	103/104 (99%)	84 (82%)	19 (18%)	2	9
32	DK	103/104 (99%)	87 (84%)	16 (16%)	3	14
33	BL	102/103 (99%)	79 (78%)	23 (22%)	1	5
33	DL	102/103 (99%)	88 (86%)	14 (14%)	4	19
34	BM	109/109 (100%)	87 (80%)	22 (20%)	1	7
34	DM	109/109 (100%)	99 (91%)	10 (9%)	11	38
35	BN	100/103 (97%)	83 (83%)	17 (17%)	2	11
35	DN	100/103 (97%)	85 (85%)	15 (15%)	3	16
36	BO	86/87 (99%)	69 (80%)	17 (20%)	1	8
36	DO	86/87 (99%)	78 (91%)	8 (9%)	10	38
37	BP	99/100 (99%)	78 (79%)	21 (21%)	1	6
37	DP	99/100 (99%)	90 (91%)	9 (9%)	11	39
38	BQ	89/90 (99%)	74 (83%)	15 (17%)	2	11
38	DQ	89/90 (99%)	78 (88%)	11 (12%)	5	24
39	BR	84/84 (100%)	65 (77%)	19 (23%)	1	5
39	DR	84/84 (100%)	71 (84%)	13 (16%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BS	93/93 (100%)	73 (78%)	20 (22%)	1	6
40	DS	93/93 (100%)	76 (82%)	17 (18%)	2	9
41	BT	80/84 (95%)	61 (76%)	19 (24%)	1	3
41	DT	80/84 (95%)	74 (92%)	6 (8%)	16	52
42	BU	83/85 (98%)	66 (80%)	17 (20%)	1	6
42	DU	83/85 (98%)	74 (89%)	9 (11%)	7	31
43	BV	78/78 (100%)	61 (78%)	17 (22%)	1	6
43	DV	78/78 (100%)	66 (85%)	12 (15%)	3	15
44	BW	59/63 (94%)	42 (71%)	17 (29%)	0	1
44	DW	59/63 (94%)	44 (75%)	15 (25%)	0	2
45	BX	67/68 (98%)	53 (79%)	14 (21%)	1	6
45	DX	67/68 (98%)	58 (87%)	9 (13%)	4	21
46	BY	55/55 (100%)	43 (78%)	12 (22%)	1	6
46	DY	55/55 (100%)	52 (94%)	3 (6%)	25	64
47	BZ	48/49 (98%)	32 (67%)	16 (33%)	0	0
47	DZ	48/49 (98%)	41 (85%)	7 (15%)	3	17
48	B0	47/48 (98%)	43 (92%)	4 (8%)	12	44
48	D0	47/48 (98%)	40 (85%)	7 (15%)	3	16
49	B1	45/49 (92%)	36 (80%)	9 (20%)	1	7
49	D1	45/49 (92%)	41 (91%)	4 (9%)	11	41
50	B2	38/38 (100%)	31 (82%)	7 (18%)	2	9
50	D2	38/38 (100%)	34 (90%)	4 (10%)	8	32
51	B3	51/52 (98%)	44 (86%)	7 (14%)	4	19
51	D3	51/52 (98%)	42 (82%)	9 (18%)	2	10
52	B4	34/34 (100%)	30 (88%)	4 (12%)	6	27
52	D4	34/34 (100%)	29 (85%)	5 (15%)	3	16
All	All	9331/9756 (96%)	7837 (84%)	1494 (16%)	3	13

5 of 1494 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	BR	10	LYS
49	B1	41	VAL

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Mol	Chain	Res	Type
39	DR	75	VAL
40	BS	4	ILE
43	BV	41	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 333 such sidechains are listed below:

Mol	Chain	Res	Type
42	BU	52	ASN
2	CC	184	ASN
42	DU	45	GLN
43	BV	51	GLN
48	B0	4	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1532/1533 (99%)	471 (30%)	0
22	BA	2850/2903 (98%)	800 (28%)	0
22	DA	2837/2903 (97%)	1022 (36%)	0
23	BB	117/118 (99%)	29 (24%)	0
53	CA	1529/1530 (99%)	512 (33%)	0
54	DB	116/117 (99%)	36 (31%)	0
All	All	8981/9104 (98%)	2870 (31%)	0

5 of 2870 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	7	A
21	AA	8	A
21	AA	9	G

There are no RNA pucker outliers to report.

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 365 ligands modelled in this entry, 365 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	218/241 (90%)	0.17	16 (7%) 16 9	85, 115, 146, 164	0
1	CB	218/241 (90%)	0.32	11 (5%) 30 17	90, 125, 152, 170	0
2	AC	206/233 (88%)	-0.35	3 (1%) 74 61	57, 83, 116, 147	0
2	CC	206/233 (88%)	0.39	13 (6%) 21 12	83, 129, 170, 188	0
3	AD	205/206 (99%)	-0.25	7 (3%) 46 30	50, 87, 137, 176	0
3	CD	205/206 (99%)	-0.37	3 (1%) 74 61	41, 63, 102, 148	0
4	AE	150/167 (89%)	-0.31	1 (0%) 87 80	51, 70, 116, 147	0
4	CE	150/167 (89%)	-0.06	1 (0%) 87 80	65, 87, 122, 144	0
5	AF	100/135 (74%)	-0.16	0 100 100	60, 90, 125, 142	0
5	CF	100/135 (74%)	0.05	0 100 100	65, 113, 147, 158	0
6	AG	151/179 (84%)	0.02	4 (2%) 56 41	69, 108, 139, 157	0
6	CG	150/179 (83%)	1.93	65 (43%) 0 0	98, 173, 223, 233	0
7	AH	129/130 (99%)	-0.52	2 (1%) 72 59	49, 71, 106, 133	0
7	CH	129/130 (99%)	-0.21	2 (1%) 72 59	63, 100, 133, 159	0
8	AI	127/130 (97%)	0.21	9 (7%) 17 10	56, 115, 166, 189	0
8	CI	127/130 (97%)	1.16	25 (19%) 1 1	127, 174, 225, 239	0
9	AJ	98/103 (95%)	0.07	6 (6%) 22 12	59, 97, 152, 160	0
9	CJ	98/103 (95%)	1.65	28 (28%) 1 1	122, 160, 189, 201	0
10	AK	117/129 (90%)	-0.13	1 (0%) 84 75	43, 88, 124, 137	0
10	CK	117/129 (90%)	-0.00	0 100 100	57, 99, 130, 151	0
11	AL	123/124 (99%)	-0.35	2 (1%) 72 59	33, 54, 96, 135	0
11	CL	123/124 (99%)	0.01	2 (1%) 72 59	47, 74, 110, 135	0
12	AM	114/118 (96%)	0.09	3 (2%) 56 41	70, 117, 155, 177	0
12	CM	113/118 (95%)	2.46	61 (53%) 0 0	220, 351, 413, 434	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/101 (95%)	-0.16	4 (4%) 37 24	59, 86, 136, 158	0
13	CN	95/101 (94%)	1.44	21 (22%) 1 1	102, 191, 256, 269	0
14	AO	88/89 (98%)	-0.43	1 (1%) 80 68	48, 75, 106, 128	0
14	CO	88/89 (98%)	0.11	1 (1%) 80 68	72, 109, 141, 167	0
15	AP	82/82 (100%)	-0.21	3 (3%) 42 27	55, 79, 129, 174	0
15	CP	80/82 (97%)	0.22	3 (3%) 41 27	64, 96, 133, 152	0
16	AQ	80/84 (95%)	0.15	4 (5%) 30 17	38, 73, 112, 144	0
16	CQ	80/84 (95%)	0.64	10 (12%) 4 3	54, 96, 117, 131	0
17	AR	55/75 (73%)	0.09	3 (5%) 26 15	56, 80, 129, 146	0
17	CR	55/75 (73%)	0.22	2 (3%) 43 28	57, 89, 131, 170	0
18	AS	79/92 (85%)	0.26	3 (3%) 41 27	79, 110, 152, 161	0
18	CS	79/92 (85%)	2.44	38 (48%) 0 0	250, 307, 359, 371	0
19	AT	85/87 (97%)	-0.22	1 (1%) 79 67	51, 81, 114, 133	0
19	CT	85/87 (97%)	0.66	7 (8%) 12 7	79, 125, 161, 177	0
20	AU	51/71 (71%)	0.27	1 (1%) 65 50	60, 104, 138, 148	0
20	CU	51/71 (71%)	0.09	1 (1%) 65 50	63, 97, 143, 153	0
21	AA	1533/1533 (100%)	-0.50	23 (1%) 74 61	34, 72, 169, 235	0
22	BA	2854/2903 (98%)	-0.47	66 (2%) 61 46	13, 33, 142, 320	0
22	DA	2841/2903 (97%)	0.42	149 (5%) 28 16	59, 119, 216, 320	0
23	BB	118/118 (100%)	-0.58	0 100 100	18, 47, 75, 99	0
24	BC	271/273 (99%)	-0.44	9 (3%) 47 31	20, 43, 83, 142	0
24	DC	271/273 (99%)	0.22	11 (4%) 38 25	63, 94, 128, 153	0
25	BD	209/209 (100%)	-0.69	0 100 100	13, 29, 72, 96	0
25	DD	209/209 (100%)	0.36	8 (3%) 41 27	68, 108, 141, 168	0
26	BE	201/201 (100%)	-0.64	0 100 100	15, 42, 87, 124	0
26	DE	201/201 (100%)	1.09	40 (19%) 1 1	89, 191, 252, 282	0
27	BF	177/179 (98%)	-0.31	0 100 100	32, 67, 116, 132	0
27	DF	178/179 (99%)	1.75	65 (36%) 0 0	125, 209, 220, 232	0
28	BG	176/177 (99%)	-0.43	0 100 100	27, 57, 103, 128	0
28	DG	176/177 (99%)	1.28	41 (23%) 1 1	120, 165, 207, 220	0
29	BH	149/149 (100%)	2.08	59 (39%) 0 0	42, 178, 213, 217	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	DH	149/149 (100%)	2.48	55 (36%) 0 0	104, 173, 208, 219	0
30	BI	141/142 (99%)	2.89	76 (53%) 0 0	199, 245, 286, 294	0
30	DI	141/142 (99%)	5.02	117 (82%) 0 0	264, 305, 323, 331	0
31	BJ	142/142 (100%)	-0.68	0 100 100	12, 25, 57, 111	0
31	DJ	142/142 (100%)	0.20	4 (2%) 53 39	76, 110, 134, 153	0
32	BK	122/123 (99%)	-0.67	0 100 100	20, 32, 76, 121	0
32	DK	122/123 (99%)	0.10	3 (2%) 58 43	71, 93, 127, 142	0
33	BL	143/144 (99%)	-0.69	0 100 100	13, 38, 74, 100	0
33	DL	143/144 (99%)	1.09	28 (19%) 1 1	80, 150, 189, 202	0
34	BM	136/136 (100%)	-0.71	0 100 100	14, 30, 61, 99	0
34	DM	136/136 (100%)	0.12	1 (0%) 87 80	73, 117, 143, 161	0
35	BN	120/127 (94%)	-0.70	0 100 100	14, 28, 44, 97	0
35	DN	120/127 (94%)	0.56	7 (5%) 24 14	89, 121, 152, 171	0
36	BO	116/117 (99%)	-0.52	0 100 100	30, 46, 73, 101	0
36	DO	116/117 (99%)	1.52	40 (34%) 0 0	146, 178, 207, 216	0
37	BP	114/115 (99%)	-0.58	0 100 100	22, 39, 90, 131	0
37	DP	114/115 (99%)	0.36	9 (7%) 13 7	80, 108, 135, 143	0
38	BQ	117/118 (99%)	-0.68	1 (0%) 84 75	9, 22, 46, 96	0
38	DQ	117/118 (99%)	0.67	8 (6%) 18 10	87, 112, 154, 191	0
39	BR	103/103 (100%)	-0.60	1 (0%) 82 72	11, 33, 75, 91	0
39	DR	103/103 (100%)	1.22	28 (27%) 1 1	85, 135, 170, 190	0
40	BS	110/110 (100%)	-0.78	0 100 100	14, 23, 57, 118	0
40	DS	110/110 (100%)	0.81	16 (14%) 3 1	76, 120, 154, 170	0
41	BT	93/100 (93%)	-0.18	2 (2%) 62 48	28, 51, 112, 140	0
41	DT	93/100 (93%)	1.34	22 (23%) 1 1	132, 189, 223, 233	0
42	BU	102/104 (98%)	-0.26	3 (2%) 52 37	29, 54, 100, 155	0
42	DU	102/104 (98%)	2.19	54 (52%) 0 0	153, 202, 250, 283	0
43	BV	94/94 (100%)	-0.68	0 100 100	17, 39, 79, 105	0
43	DV	94/94 (100%)	0.45	6 (6%) 20 11	113, 143, 165, 179	0
44	BW	79/85 (92%)	-0.27	1 (1%) 77 65	18, 39, 94, 127	0
44	DW	79/85 (92%)	1.32	18 (22%) 1 1	99, 157, 191, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	BX	77/78 (98%)	-0.53	0 100 100	23, 43, 80, 104	0
45	DX	77/78 (98%)	0.57	5 (6%) 20 11	84, 124, 170, 177	0
46	BY	63/63 (100%)	-0.20	1 (1%) 72 59	41, 68, 113, 128	0
46	DY	63/63 (100%)	1.40	20 (31%) 0 0	180, 226, 268, 278	0
47	BZ	58/59 (98%)	-0.67	0 100 100	13, 27, 56, 97	0
47	DZ	58/59 (98%)	0.62	7 (12%) 5 3	97, 143, 180, 187	0
48	B0	56/57 (98%)	-0.80	0 100 100	12, 29, 61, 113	0
48	D0	56/57 (98%)	1.05	9 (16%) 2 1	84, 128, 163, 172	0
49	B1	50/55 (90%)	-0.20	1 (2%) 65 50	29, 50, 91, 116	0
49	D1	50/55 (90%)	1.64	16 (32%) 0 0	110, 143, 159, 168	0
50	B2	46/46 (100%)	-0.65	0 100 100	20, 30, 49, 131	0
50	D2	46/46 (100%)	0.76	1 (2%) 62 48	87, 115, 137, 147	0
51	B3	64/65 (98%)	-0.74	0 100 100	15, 30, 43, 62	0
51	D3	64/65 (98%)	1.16	14 (21%) 1 1	93, 126, 150, 169	0
52	B4	38/38 (100%)	-0.56	0 100 100	19, 33, 62, 87	0
52	D4	38/38 (100%)	0.91	7 (18%) 1 1	84, 127, 158, 161	0
53	CA	1530/1530 (100%)	0.14	82 (5%) 26 15	44, 100, 246, 325	0
54	DB	117/117 (100%)	0.51	8 (6%) 18 10	108, 175, 209, 221	0
All	All	20431/21074 (96%)	0.16	1510 (7%) 15 9	9, 93, 219, 434	0

The worst 5 of 1510 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	DH	92	GLY	20.8
22	BA	2154	A	18.7
30	BI	2	LYS	16.8
30	DI	58	ILE	15.9
30	DI	4	VAL	14.9

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	BA	3132	1/1	0.92	0.39	20.34	202,202,202,202	0
55	MG	BA	3037	1/1	0.92	0.32	19.20	171,171,171,171	0
55	MG	BA	3072	1/1	0.94	0.36	18.19	94,94,94,94	0
55	MG	DA	3002	1/1	0.63	0.96	14.31	179,179,179,179	0
55	MG	BA	3125	1/1	0.98	0.68	13.30	162,162,162,162	0
55	MG	CA	1625	1/1	0.92	0.30	11.09	118,118,118,118	0
55	MG	BA	3058	1/1	0.89	0.22	10.26	164,164,164,164	0
55	MG	BA	3105	1/1	0.96	0.23	8.37	16,16,16,16	0
55	MG	BA	3137	1/1	0.91	0.36	8.15	188,188,188,188	0
55	MG	DA	3098	1/1	0.69	0.44	7.57	158,158,158,158	0
55	MG	CA	1628	1/1	0.92	1.05	7.37	204,204,204,204	0
55	MG	DA	3131	1/1	0.83	1.31	6.85	204,204,204,204	0
55	MG	BA	3038	1/1	0.98	0.18	6.47	30,30,30,30	0
55	MG	BA	3028	1/1	0.98	0.20	5.73	100,100,100,100	0
55	MG	BA	3110	1/1	0.99	0.21	5.17	11,11,11,11	0
55	MG	BA	3084	1/1	0.98	0.17	3.44	58,58,58,58	0
55	MG	DA	3109	1/1	0.66	0.39	3.36	165,165,165,165	0
55	MG	DA	3101	1/1	0.89	0.36	3.12	127,127,127,127	0
55	MG	DA	3116	1/1	0.91	0.27	3.07	154,154,154,154	0
55	MG	DA	3085	1/1	0.80	0.42	2.78	169,169,169,169	0
55	MG	DA	3070	1/1	0.80	0.35	2.24	209,209,209,209	0
55	MG	BA	3117	1/1	0.95	0.18	2.18	23,23,23,23	0
55	MG	BA	3098	1/1	0.95	0.19	1.68	60,60,60,60	0
55	MG	BA	3109	1/1	0.98	0.15	1.40	13,13,13,13	0
55	MG	BA	3106	1/1	0.98	0.16	1.34	37,37,37,37	0
55	MG	CA	1640	1/1	0.84	0.20	1.29	161,161,161,161	0
55	MG	DA	3104	1/1	0.90	0.20	1.24	109,109,109,109	0
55	MG	AA	1641	1/1	0.89	0.17	1.23	131,131,131,131	0
55	MG	AA	1622	1/1	0.98	0.14	1.11	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1637	1/1	0.95	0.20	1.10	100,100,100,100	0
55	MG	BA	3131	1/1	0.98	0.18	1.09	17,17,17,17	0
55	MG	BA	3108	1/1	0.99	0.17	1.04	30,30,30,30	0
55	MG	CA	1607	1/1	0.86	0.19	0.98	154,154,154,154	0
55	MG	BA	3041	1/1	0.98	0.15	0.90	19,19,19,19	0
55	MG	DA	3038	1/1	0.96	0.23	0.67	97,97,97,97	0
55	MG	CA	1631	1/1	0.96	0.18	0.57	92,92,92,92	0
55	MG	DA	3130	1/1	0.92	0.38	0.49	102,102,102,102	0
55	MG	DA	3135	1/1	0.75	0.25	0.48	162,162,162,162	0
55	MG	BA	3013	1/1	0.99	0.15	0.16	8,8,8,8	0
55	MG	DA	3107	1/1	0.67	0.26	0.07	169,169,169,169	0
55	MG	BA	3047	1/1	0.98	0.16	0.07	20,20,20,20	0
55	MG	BA	3029	1/1	0.93	0.16	-0.16	43,43,43,43	0
55	MG	AA	1629	1/1	0.95	0.17	-0.26	58,58,58,58	0
55	MG	BA	3133	1/1	0.99	0.20	-0.31	103,103,103,103	0
55	MG	DA	3096	1/1	0.88	0.19	-0.37	107,107,107,107	0
55	MG	CA	1616	1/1	0.68	0.29	-0.41	192,192,192,192	0
55	MG	DA	3017	1/1	0.90	0.23	-0.63	86,86,86,86	0
55	MG	BA	3012	1/1	0.97	0.15	-0.69	8,8,8,8	0
55	MG	CA	1621	1/1	0.90	0.15	-0.73	40,40,40,40	0
55	MG	CA	1617	1/1	0.85	0.23	-0.79	220,220,220,220	0
55	MG	AA	1633	1/1	0.99	0.10	-0.89	78,78,78,78	0
55	MG	CA	1611	1/1	0.89	0.17	-0.96	108,108,108,108	0
55	MG	BA	3130	1/1	0.96	0.13	-0.98	8,8,8,8	0
55	MG	DA	3084	1/1	0.72	0.16	-0.99	178,178,178,178	0
55	MG	DA	3028	1/1	0.87	0.16	-1.00	162,162,162,162	0
55	MG	CA	1618	1/1	0.91	0.14	-1.01	90,90,90,90	0
55	MG	DA	3025	1/1	0.94	0.17	-1.01	108,108,108,108	0
56	ZN	D4	101	1/1	0.92	0.07	-1.02	156,156,156,156	0
55	MG	DA	3106	1/1	0.94	0.17	-1.12	69,69,69,69	0
55	MG	AA	1602	1/1	0.95	0.12	-1.16	121,121,121,121	0
55	MG	CA	1639	1/1	0.91	0.16	-1.17	149,149,149,149	0
55	MG	AA	1612	1/1	0.98	0.10	-1.18	60,60,60,60	0
55	MG	BA	3025	1/1	0.99	0.12	-1.23	21,21,21,21	0
55	MG	BA	3024	1/1	0.97	0.13	-1.26	16,16,16,16	0
55	MG	AA	1618	1/1	0.83	0.12	-1.27	68,68,68,68	0
55	MG	DA	3045	1/1	0.95	0.16	-1.32	102,102,102,102	0
55	MG	AA	1620	1/1	0.95	0.10	-1.33	107,107,107,107	0
55	MG	DA	3105	1/1	0.91	0.17	-1.36	62,62,62,62	0
55	MG	DA	3012	1/1	0.98	0.20	-1.39	75,75,75,75	0
55	MG	DA	3125	1/1	0.68	0.18	-1.44	77,77,77,77	0
55	MG	BA	3008	1/1	0.99	0.12	-1.44	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1629	1/1	0.72	0.10	-1.45	174,174,174,174	0
55	MG	DA	3041	1/1	0.87	0.17	-1.48	77,77,77,77	0
55	MG	DA	3052	1/1	0.79	0.15	-1.49	110,110,110,110	0
55	MG	BA	3135	1/1	0.99	0.12	-1.74	12,12,12,12	0
55	MG	BA	3063	1/1	0.91	0.11	-1.74	42,42,42,42	0
55	MG	AA	1607	1/1	0.96	0.11	-1.76	62,62,62,62	0
55	MG	DB	201	1/1	0.92	0.08	-1.79	117,117,117,117	0
56	ZN	B4	101	1/1	0.96	0.09	-1.91	51,51,51,51	0
55	MG	DA	3049	1/1	0.83	0.14	-1.92	99,99,99,99	0
55	MG	BB	202	1/1	0.93	0.10	-1.97	67,67,67,67	0
55	MG	DA	3053	1/1	0.91	0.14	-2.13	59,59,59,59	0
55	MG	DA	3036	1/1	0.92	0.09	-2.14	97,97,97,97	0
55	MG	BA	3023	1/1	0.97	0.11	-2.15	11,11,11,11	0
55	MG	BA	3017	1/1	0.98	0.12	-2.16	9,9,9,9	0
55	MG	BA	3119	1/1	0.94	0.12	-2.20	88,88,88,88	0
55	MG	DA	3023	1/1	0.90	0.13	-2.27	71,71,71,71	0
55	MG	BA	3050	1/1	0.98	0.12	-2.44	16,16,16,16	0
55	MG	DA	3040	1/1	0.79	0.17	-2.50	117,117,117,117	0
55	MG	BA	3022	1/1	0.98	0.06	-2.54	37,37,37,37	0
55	MG	DA	3066	1/1	0.91	0.10	-2.56	94,94,94,94	0
55	MG	AA	1608	1/1	0.90	0.11	-2.57	106,106,106,106	0
55	MG	BA	3115	1/1	0.98	0.13	-2.72	49,49,49,49	0
55	MG	DA	3051	1/1	0.83	0.13	-2.78	140,140,140,140	0
55	MG	DA	3067	1/1	0.95	0.09	-2.84	70,70,70,70	0
55	MG	BA	3051	1/1	0.96	0.09	-2.89	71,71,71,71	0
55	MG	BA	3048	1/1	0.80	0.10	-2.89	144,144,144,144	0
55	MG	BA	3074	1/1	0.98	0.07	-2.95	59,59,59,59	0
55	MG	DA	3102	1/1	0.94	0.18	-2.96	83,83,83,83	0
55	MG	DA	3113	1/1	0.96	0.08	-2.99	59,59,59,59	0
55	MG	CA	1641	1/1	0.96	0.08	-3.00	68,68,68,68	0
55	MG	DA	3080	1/1	0.83	0.09	-3.30	74,74,74,74	0
55	MG	BA	3113	1/1	0.92	0.09	-3.36	60,60,60,60	0
55	MG	CA	1642	1/1	0.96	0.06	-3.42	78,78,78,78	0
55	MG	DA	3062	1/1	0.85	0.08	-3.49	113,113,113,113	0
55	MG	BA	3066	1/1	0.99	0.10	-3.62	18,18,18,18	0
55	MG	BA	3054	1/1	0.99	0.09	-3.64	14,14,14,14	0
55	MG	CA	1604	1/1	0.96	0.07	-3.75	71,71,71,71	0
55	MG	BA	3002	1/1	0.95	0.11	-3.80	81,81,81,81	0
55	MG	BA	3018	1/1	0.98	0.08	-3.84	35,35,35,35	0
55	MG	AA	1614	1/1	0.94	0.06	-3.91	55,55,55,55	0
55	MG	BA	3059	1/1	0.99	0.07	-4.03	36,36,36,36	0
55	MG	BA	3121	1/1	0.95	0.10	-4.09	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3069	1/1	0.95	0.07	-4.16	79,79,79,79	0
55	MG	BA	3102	1/1	0.99	0.08	-4.20	36,36,36,36	0
55	MG	AA	1643	1/1	0.95	0.05	-4.23	35,35,35,35	0
55	MG	AA	1631	1/1	0.96	0.06	-4.33	165,165,165,165	0
55	MG	DA	3024	1/1	0.94	0.04	-4.39	85,85,85,85	0
55	MG	DA	3056	1/1	0.97	0.14	-4.92	103,103,103,103	0
55	MG	AA	1605	1/1	0.95	0.06	-5.17	123,123,123,123	0
55	MG	AA	1610	1/1	0.99	0.07	-5.23	33,33,33,33	0
55	MG	BA	3064	1/1	0.99	0.08	-5.45	38,38,38,38	0
55	MG	BA	3005	1/1	0.96	0.09	-5.55	86,86,86,86	0
55	MG	BA	3069	1/1	0.95	0.07	-5.74	14,14,14,14	0
55	MG	CA	1613	1/1	0.93	0.08	-5.92	96,96,96,96	0
55	MG	CA	1606	1/1	0.93	0.11	-6.40	64,64,64,64	0
55	MG	AA	1625	1/1	0.97	0.05	-6.40	67,67,67,67	0
55	MG	CA	1609	1/1	0.98	0.12	-6.51	83,83,83,83	0
55	MG	BA	3094	1/1	0.90	0.06	-6.73	37,37,37,37	0
55	MG	AA	1634	1/1	0.98	0.08	-7.04	59,59,59,59	0
55	MG	DA	3133	1/1	0.94	0.09	-7.47	84,84,84,84	0
55	MG	AA	1617	1/1	0.96	0.10	-7.57	83,83,83,83	0
55	MG	BA	3097	1/1	0.99	0.07	-8.27	18,18,18,18	0
55	MG	BA	3111	1/1	0.96	0.06	-8.99	47,47,47,47	0
55	MG	BA	3080	1/1	0.90	0.08	-9.88	31,31,31,31	0
55	MG	BA	3039	1/1	0.96	0.08	-14.76	9,9,9,9	0
55	MG	BB	203	1/1	0.94	0.10	-	37,37,37,37	0
55	MG	BA	3128	1/1	0.99	0.10	-	18,18,18,18	0
55	MG	DA	3008	1/1	0.83	0.11	-	100,100,100,100	0
55	MG	CA	1623	1/1	0.86	0.21	-	96,96,96,96	0
55	MG	BA	3120	1/1	0.94	0.26	-	156,156,156,156	0
55	MG	DA	3019	1/1	0.96	0.14	-	161,161,161,161	0
55	MG	DA	3087	1/1	0.86	0.16	-	87,87,87,87	0
55	MG	BA	3087	1/1	0.95	0.12	-	13,13,13,13	0
55	MG	DA	3059	1/1	0.85	0.53	-	188,188,188,188	0
55	MG	BA	3016	1/1	0.96	0.05	-	64,64,64,64	0
55	MG	BA	3118	1/1	0.98	0.07	-	13,13,13,13	0
55	MG	BA	3019	1/1	0.95	0.07	-	39,39,39,39	0
55	MG	DA	3097	1/1	0.93	0.16	-	110,110,110,110	0
55	MG	AA	1630	1/1	0.90	0.11	-	163,163,163,163	0
55	MG	CA	1627	1/1	0.86	0.23	-	166,166,166,166	0
55	MG	CA	1619	1/1	0.78	0.44	-	180,180,180,180	0
55	MG	BA	3089	1/1	0.91	0.15	-	134,134,134,134	0
55	MG	DA	3009	1/1	0.97	0.18	-	107,107,107,107	0
55	MG	DA	3014	1/1	0.89	0.24	-	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3048	1/1	0.80	0.17	-	128,128,128,128	0
55	MG	DA	3095	1/1	0.95	0.14	-	114,114,114,114	0
55	MG	AA	1609	1/1	0.98	0.19	-	71,71,71,71	0
55	MG	BA	3068	1/1	0.98	0.11	-	11,11,11,11	0
55	MG	BA	3070	1/1	0.88	0.12	-	164,164,164,164	0
55	MG	DA	3094	1/1	0.70	0.20	-	172,172,172,172	0
55	MG	DA	3129	1/1	0.72	1.28	-	194,194,194,194	0
55	MG	BA	3100	1/1	0.92	0.11	-	47,47,47,47	0
55	MG	AA	1606	1/1	0.96	0.15	-	38,38,38,38	0
55	MG	DA	3042	1/1	0.66	0.36	-	139,139,139,139	0
55	MG	AA	1637	1/1	0.97	0.08	-	85,85,85,85	0
55	MG	BA	3075	1/1	0.97	0.25	-	119,119,119,119	0
55	MG	DA	3020	1/1	0.71	0.70	-	207,207,207,207	0
55	MG	BA	3036	1/1	0.98	0.14	-	11,11,11,11	0
55	MG	DA	3124	1/1	0.91	0.32	-	165,165,165,165	0
55	MG	BA	3004	1/1	0.83	0.16	-	155,155,155,155	0
55	MG	BA	3077	1/1	0.93	0.22	-	90,90,90,90	0
55	MG	DA	3029	1/1	0.82	0.56	-	205,205,205,205	0
55	MG	DA	3088	1/1	0.92	0.17	-	160,160,160,160	0
55	MG	DA	3132	1/1	0.32	0.77	-	216,216,216,216	0
55	MG	BA	3085	1/1	0.97	0.14	-	116,116,116,116	0
55	MG	DA	3078	1/1	0.98	0.19	-	68,68,68,68	0
55	MG	DA	3068	1/1	0.94	0.08	-	65,65,65,65	0
55	MG	DA	3043	1/1	0.91	0.15	-	104,104,104,104	0
55	MG	DA	3112	1/1	0.94	0.11	-	148,148,148,148	0
55	MG	AA	1616	1/1	0.87	0.08	-	126,126,126,126	0
55	MG	DA	3090	1/1	0.97	0.12	-	90,90,90,90	0
55	MG	DA	3108	1/1	0.77	0.12	-	103,103,103,103	0
55	MG	AA	1603	1/1	0.83	0.13	-	124,124,124,124	0
55	MG	CA	1634	1/1	0.87	0.11	-	112,112,112,112	0
55	MG	CA	1601	1/1	0.91	0.10	-	124,124,124,124	0
55	MG	DA	3061	1/1	0.86	0.42	-	160,160,160,160	0
55	MG	BA	3030	1/1	0.96	0.09	-	57,57,57,57	0
55	MG	DA	3081	1/1	0.95	0.15	-	141,141,141,141	0
55	MG	BA	3095	1/1	0.98	0.09	-	38,38,38,38	0
55	MG	AA	1611	1/1	0.62	0.23	-	176,176,176,176	0
55	MG	DA	3021	1/1	0.97	0.23	-	66,66,66,66	0
55	MG	BA	3055	1/1	0.98	0.09	-	25,25,25,25	0
55	MG	BA	3086	1/1	0.94	0.12	-	45,45,45,45	0
55	MG	DA	3079	1/1	0.90	0.47	-	184,184,184,184	0
55	MG	DA	3118	1/1	0.93	0.14	-	77,77,77,77	0
55	MG	BA	3114	1/1	0.97	0.13	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3082	1/1	0.94	0.12	-	83,83,83,83	0
55	MG	DA	3016	1/1	0.93	0.16	-	169,169,169,169	0
55	MG	DA	3006	1/1	0.47	0.20	-	200,200,200,200	0
55	MG	BA	3071	1/1	0.97	0.35	-	132,132,132,132	0
55	MG	CA	1632	1/1	0.84	0.16	-	160,160,160,160	0
55	MG	BA	3043	1/1	0.99	0.05	-	17,17,17,17	0
55	MG	DA	3086	1/1	0.94	0.23	-	122,122,122,122	0
55	MG	DA	3122	1/1	0.91	0.17	-	113,113,113,113	0
55	MG	AA	1628	1/1	0.94	0.33	-	96,96,96,96	0
55	MG	DA	3037	1/1	0.88	0.21	-	176,176,176,176	0
55	MG	DA	3077	1/1	0.83	0.20	-	159,159,159,159	0
55	MG	CA	1620	1/1	0.92	0.31	-	172,172,172,172	0
55	MG	BA	3107	1/1	0.99	0.13	-	11,11,11,11	0
55	MG	CA	1636	1/1	0.59	0.26	-	171,171,171,171	0
55	MG	DA	3091	1/1	0.96	0.13	-	95,95,95,95	0
55	MG	DA	3103	1/1	0.96	0.12	-	62,62,62,62	0
55	MG	DA	3100	1/1	0.72	0.18	-	171,171,171,171	0
55	MG	DA	3018	1/1	0.66	0.19	-	194,194,194,194	0
55	MG	AA	1627	1/1	0.98	0.24	-	86,86,86,86	0
55	MG	DA	3092	1/1	0.89	0.19	-	157,157,157,157	0
55	MG	BA	3127	1/1	0.98	0.18	-	43,43,43,43	0
55	MG	DA	3114	1/1	0.93	0.09	-	95,95,95,95	0
55	MG	BA	3045	1/1	0.97	0.19	-	21,21,21,21	0
55	MG	DA	3015	1/1	0.81	0.84	-	183,183,183,183	0
55	MG	BA	3065	1/1	0.95	0.08	-	26,26,26,26	0
55	MG	DA	3005	1/1	0.54	0.89	-	208,208,208,208	0
55	MG	BA	3067	1/1	0.96	0.10	-	21,21,21,21	0
55	MG	BA	3020	1/1	0.99	0.29	-	16,16,16,16	0
55	MG	AA	1604	1/1	0.95	0.10	-	98,98,98,98	0
55	MG	BA	3112	1/1	0.93	0.15	-	121,121,121,121	0
55	MG	BA	3009	1/1	1.00	0.09	-	13,13,13,13	0
55	MG	DA	3126	1/1	0.83	0.42	-	164,164,164,164	0
55	MG	AA	1619	1/1	0.88	0.45	-	165,165,165,165	0
55	MG	AA	1638	1/1	0.97	0.08	-	29,29,29,29	0
55	MG	BA	3099	1/1	0.98	0.10	-	82,82,82,82	0
55	MG	DA	3115	1/1	0.86	0.22	-	151,151,151,151	0
55	MG	DA	3119	1/1	0.82	0.09	-	86,86,86,86	0
55	MG	DA	3035	1/1	0.94	0.15	-	87,87,87,87	0
55	MG	DA	3039	1/1	0.55	0.46	-	220,220,220,220	0
55	MG	BA	3046	1/1	0.91	0.13	-	23,23,23,23	0
55	MG	BA	3027	1/1	0.99	0.11	-	31,31,31,31	0
55	MG	BA	3092	1/1	0.92	0.18	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1624	1/1	0.88	0.11	-	101,101,101,101	0
55	MG	DA	3030	1/1	0.94	0.18	-	144,144,144,144	0
55	MG	DA	3060	1/1	0.70	0.33	-	198,198,198,198	0
55	MG	DA	3050	1/1	0.52	0.20	-	209,209,209,209	0
55	MG	DA	3046	1/1	0.72	0.14	-	173,173,173,173	0
55	MG	AA	1636	1/1	0.83	0.62	-	164,164,164,164	0
55	MG	BA	3026	1/1	0.94	0.58	-	152,152,152,152	0
55	MG	DA	3047	1/1	0.89	0.11	-	82,82,82,82	0
55	MG	BA	3073	1/1	0.97	0.12	-	12,12,12,12	0
55	MG	BA	3078	1/1	0.98	0.07	-	26,26,26,26	0
55	MG	DA	3075	1/1	0.82	1.60	-	207,207,207,207	0
55	MG	AA	1601	1/1	0.96	0.09	-	82,82,82,82	0
55	MG	DA	3127	1/1	0.74	0.33	-	97,97,97,97	0
55	MG	BA	3031	1/1	0.95	0.13	-	11,11,11,11	0
55	MG	BA	3034	1/1	0.98	0.14	-	8,8,8,8	0
55	MG	CA	1635	1/1	0.86	0.14	-	76,76,76,76	0
55	MG	DA	3111	1/1	0.83	0.19	-	166,166,166,166	0
55	MG	BA	3003	1/1	0.91	0.10	-	63,63,63,63	0
55	MG	DA	3054	1/1	0.94	0.10	-	75,75,75,75	0
55	MG	DA	3064	1/1	0.42	3.06	-	204,204,204,204	0
55	MG	CA	1622	1/1	0.87	0.09	-	169,169,169,169	0
55	MG	BA	3082	1/1	0.97	0.07	-	30,30,30,30	0
55	MG	BA	3096	1/1	0.98	0.04	-	40,40,40,40	0
55	MG	BA	3049	1/1	0.85	0.16	-	104,104,104,104	0
55	MG	CA	1614	1/1	0.91	0.58	-	178,178,178,178	0
55	MG	DA	3089	1/1	0.69	0.14	-	169,169,169,169	0
55	MG	BA	3090	1/1	0.98	0.05	-	28,28,28,28	0
55	MG	DJ	201	1/1	-0.26	3.52	-	242,242,242,242	0
55	MG	BA	3088	1/1	0.92	0.19	-	81,81,81,81	0
55	MG	AA	1642	1/1	0.99	0.14	-	40,40,40,40	0
55	MG	BA	3052	1/1	0.99	0.09	-	25,25,25,25	0
55	MG	BA	3040	1/1	0.98	0.15	-	27,27,27,27	0
55	MG	CA	1615	1/1	0.90	0.25	-	136,136,136,136	0
55	MG	DA	3003	1/1	0.46	1.03	-	210,210,210,210	0
55	MG	BA	3091	1/1	0.88	0.08	-	47,47,47,47	0
55	MG	AA	1635	1/1	0.95	0.13	-	64,64,64,64	0
55	MG	CA	1630	1/1	0.89	0.11	-	121,121,121,121	0
55	MG	AA	1632	1/1	0.97	0.07	-	81,81,81,81	0
55	MG	DA	3093	1/1	0.86	0.16	-	121,121,121,121	0
55	MG	BA	3001	1/1	0.90	0.12	-	109,109,109,109	0
55	MG	DA	3010	1/1	0.68	1.13	-	200,200,200,200	0
55	MG	BA	3129	1/1	0.98	0.10	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	3033	1/1	0.98	0.09	-	9,9,9,9	0
55	MG	BA	3061	1/1	0.98	0.21	-	171,171,171,171	0
55	MG	BA	3057	1/1	0.80	0.51	-	219,219,219,219	0
55	MG	CA	1605	1/1	0.85	0.16	-	48,48,48,48	0
55	MG	DA	3076	1/1	0.98	0.24	-	167,167,167,167	0
55	MG	CA	1608	1/1	0.89	0.16	-	60,60,60,60	0
55	MG	DA	3007	1/1	0.64	0.30	-	198,198,198,198	0
55	MG	BA	3076	1/1	0.98	0.15	-	16,16,16,16	0
55	MG	CA	1638	1/1	0.86	0.15	-	155,155,155,155	0
55	MG	DA	3027	1/1	0.60	1.20	-	195,195,195,195	0
55	MG	DA	3055	1/1	0.92	0.07	-	75,75,75,75	0
55	MG	DA	3004	1/1	0.89	0.17	-	118,118,118,118	0
55	MG	DA	3033	1/1	0.71	0.14	-	113,113,113,113	0
55	MG	BA	3079	1/1	0.96	0.07	-	99,99,99,99	0
55	MG	BB	204	1/1	0.97	0.10	-	40,40,40,40	0
55	MG	DA	3031	1/1	0.86	0.13	-	113,113,113,113	0
55	MG	DA	3065	1/1	0.08	2.46	-	221,221,221,221	0
55	MG	BA	3123	1/1	0.98	0.14	-	10,10,10,10	0
55	MG	DA	3134	1/1	0.61	0.42	-	198,198,198,198	0
55	MG	DA	3022	1/1	0.97	0.23	-	155,155,155,155	0
55	MG	BA	3021	1/1	0.99	0.06	-	17,17,17,17	0
55	MG	CA	1602	1/1	0.75	0.15	-	120,120,120,120	0
55	MG	DA	3117	1/1	0.88	0.13	-	67,67,67,67	0
55	MG	AA	1613	1/1	0.90	0.12	-	102,102,102,102	0
55	MG	BB	201	1/1	0.80	0.44	-	187,187,187,187	0
55	MG	DA	3073	1/1	0.93	0.13	-	141,141,141,141	0
55	MG	DA	3057	1/1	0.88	0.15	-	104,104,104,104	0
55	MG	AA	1621	1/1	0.96	0.08	-	139,139,139,139	0
55	MG	CA	1610	1/1	0.85	0.18	-	145,145,145,145	0
55	MG	BA	3007	1/1	0.93	0.09	-	67,67,67,67	0
55	MG	DA	3058	1/1	0.83	0.36	-	171,171,171,171	0
55	MG	DA	3013	1/1	0.23	0.57	-	211,211,211,211	0
55	MG	AA	1626	1/1	0.95	0.18	-	39,39,39,39	0
55	MG	BA	3035	1/1	0.88	0.35	-	168,168,168,168	0
55	MG	DA	3121	1/1	0.64	0.22	-	97,97,97,97	0
55	MG	BA	3093	1/1	0.90	0.16	-	110,110,110,110	0
55	MG	BA	3060	1/1	0.92	0.34	-	129,129,129,129	0
55	MG	BA	3122	1/1	0.98	0.06	-	64,64,64,64	0
55	MG	BA	3081	1/1	0.98	0.08	-	32,32,32,32	0
55	MG	BA	3044	1/1	0.97	0.09	-	34,34,34,34	0
55	MG	DA	3128	1/1	0.95	0.21	-	153,153,153,153	0
55	MG	BA	3124	1/1	0.94	0.09	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1639	1/1	0.94	0.10	-	96,96,96,96	0
55	MG	BA	3083	1/1	0.98	0.11	-	42,42,42,42	0
55	MG	CA	1612	1/1	0.88	0.33	-	117,117,117,117	0
55	MG	BA	3126	1/1	0.96	0.14	-	21,21,21,21	0
55	MG	AA	1623	1/1	0.95	0.16	-	70,70,70,70	0
55	MG	DA	3123	1/1	0.82	0.09	-	99,99,99,99	0
55	MG	DA	3083	1/1	0.86	0.14	-	144,144,144,144	0
55	MG	CA	1624	1/1	0.48	0.74	-	120,120,120,120	0
55	MG	DA	3032	1/1	0.89	0.17	-	71,71,71,71	0
55	MG	BA	3042	1/1	0.99	0.15	-	18,18,18,18	0
55	MG	BA	3101	1/1	0.99	0.12	-	27,27,27,27	0
55	MG	AA	1640	1/1	0.93	0.12	-	109,109,109,109	0
55	MG	BA	3116	1/1	0.95	0.13	-	133,133,133,133	0
55	MG	DA	3044	1/1	0.79	0.13	-	138,138,138,138	0
55	MG	BA	3014	1/1	0.98	0.20	-	64,64,64,64	0
55	MG	BA	3010	1/1	0.96	0.07	-	29,29,29,29	0
55	MG	DA	3011	1/1	0.90	0.16	-	126,126,126,126	0
55	MG	BA	3006	1/1	0.99	0.06	-	32,32,32,32	0
55	MG	CA	1603	1/1	0.67	0.23	-	169,169,169,169	0
55	MG	BA	3104	1/1	0.99	0.10	-	22,22,22,22	0
55	MG	DA	3063	1/1	0.52	1.14	-	191,191,191,191	0
55	MG	BA	3134	1/1	0.95	0.52	-	137,137,137,137	0
55	MG	DA	3072	1/1	0.87	0.24	-	80,80,80,80	0
55	MG	DA	3120	1/1	0.91	0.12	-	84,84,84,84	0
55	MG	BA	3056	1/1	0.54	0.34	-	187,187,187,187	0
55	MG	BA	3015	1/1	0.64	0.37	-	221,221,221,221	0
55	MG	DA	3071	1/1	0.94	0.11	-	64,64,64,64	0
55	MG	DA	3034	1/1	0.80	0.23	-	105,105,105,105	0
55	MG	DA	3099	1/1	0.66	0.15	-	142,142,142,142	0
55	MG	AA	1615	1/1	0.92	0.18	-	164,164,164,164	0
55	MG	BA	3032	1/1	0.96	0.11	-	31,31,31,31	0
55	MG	DA	3026	1/1	0.87	0.17	-	145,145,145,145	0
55	MG	DA	3074	1/1	0.50	0.15	-	194,194,194,194	0
55	MG	CA	1633	1/1	0.96	0.07	-	61,61,61,61	0
55	MG	BA	3062	1/1	0.96	0.35	-	193,193,193,193	0
55	MG	CA	1626	1/1	0.91	0.19	-	40,40,40,40	0
55	MG	DA	3001	1/1	0.90	0.08	-	109,109,109,109	0
55	MG	DA	3110	1/1	0.54	1.28	-	181,181,181,181	0
55	MG	BA	3011	1/1	0.96	0.19	-	120,120,120,120	0
55	MG	BA	3103	1/1	0.99	0.14	-	60,60,60,60	0
55	MG	BA	3053	1/1	0.93	0.10	-	30,30,30,30	0
55	MG	BA	3136	1/1	0.92	0.17	-	150,150,150,150	0

6.5 Other polymers [i](#)

There are no such residues in this entry.