



wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 07:53 PM BST

PDB ID : 4V7T
Title : Crystal structure of the E. coli ribosome bound to chloramphenicol.
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.
Deposited on : 2010-08-14
Resolution : 3.19 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

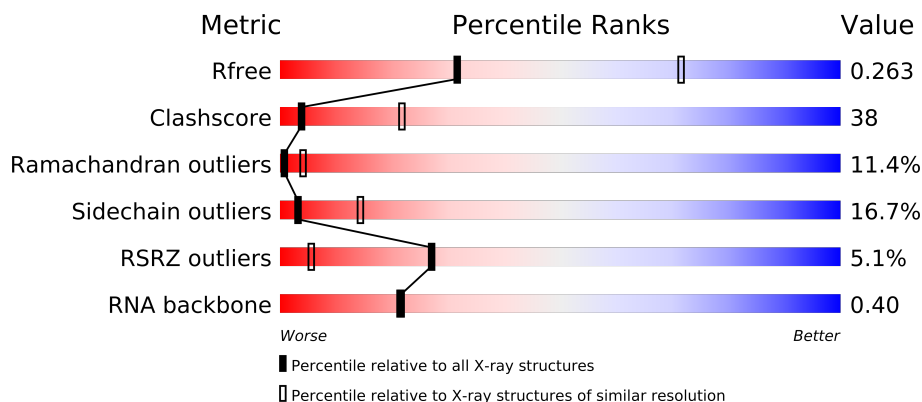
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.19 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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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

Mol	Chain	Length	Quality of chain
1	AA	1533	
2	AB	218	
2	CB	218	
3	AC	206	
3	CC	206	
4	AD	205	
4	CD	205	
5	AE	150	
5	CE	150	
6	AF	100	
6	CF	100	
7	AG	151	

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Mol	Chain	Length	Quality of chain
8	AH	129	
8	CH	129	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	117	
11	CK	117	
12	AL	123	
12	CL	123	
13	AM	114	
14	AN	100	
14	CN	100	
15	AO	88	
15	CO	88	
16	AP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
23	BB	118	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	
31	BJ	142	

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Mol	Chain	Length	Quality of chain
31	DJ	142	
32	BK	122	
32	DK	122	
33	BL	143	
33	DL	143	
34	BM	136	
34	DM	136	
35	BN	120	
35	DN	120	
36	BO	116	
36	DO	116	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	
44	BW	79	
44	DW	79	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	
52	B4	38	

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Mol	Chain	Length	Quality of chain
52	D4	38	
53	CA	1530	
54	CG	150	
55	CM	113	
56	CP	80	
57	DA	2904	
58	DB	117	
59	DF	178	

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

Mol	Type	Chain	Res	Geometry	Electron density
60	MG	AA	1614	-	X
60	MG	AA	1618	-	X
60	MG	AA	1621	-	X
60	MG	AA	1625	-	X
60	MG	AA	1626	-	X
60	MG	AA	1627	-	X
60	MG	AA	1640	-	X
60	MG	BA	3014	-	X
60	MG	BA	3018	-	X
60	MG	BA	3024	-	X
60	MG	BA	3029	-	X
60	MG	BA	3033	-	X
60	MG	BA	3035	-	X
60	MG	BA	3038	-	X
60	MG	BA	3039	-	X
60	MG	BA	3043	-	X
60	MG	BA	3054	-	X
60	MG	BA	3055	-	X
60	MG	BA	3056	-	X
60	MG	BA	3060	-	X
60	MG	BA	3069	-	X
60	MG	BA	3074	-	X
60	MG	BA	3075	-	X
60	MG	BA	3082	-	X
60	MG	BA	3086	-	X
60	MG	BA	3090	-	X
60	MG	BA	3096	-	X
60	MG	BA	3097	-	X
60	MG	BA	3103	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
60	MG	BA	3104	-	X
60	MG	BA	3107	-	X
60	MG	BA	3115	-	X
60	MG	BA	3118	-	X
60	MG	BA	3123	-	X
60	MG	BA	3124	-	X
60	MG	BA	3130	-	X
60	MG	BA	3132	-	X
60	MG	BA	3135	-	X
60	MG	BB	201	-	X
60	MG	CA	1612	-	X
60	MG	CA	1614	-	X
60	MG	CA	1615	-	X
60	MG	CA	1620	-	X
60	MG	CA	1626	-	X
60	MG	CA	1627	-	X
60	MG	CA	1640	-	X
60	MG	DA	3002	-	X
60	MG	DA	3003	-	X
60	MG	DA	3005	-	X
60	MG	DA	3007	-	X
60	MG	DA	3008	-	X
60	MG	DA	3010	-	X
60	MG	DA	3013	-	X
60	MG	DA	3014	-	X
60	MG	DA	3019	-	X
60	MG	DA	3025	-	X
60	MG	DA	3027	-	X
60	MG	DA	3034	-	X
60	MG	DA	3035	-	X
60	MG	DA	3046	-	X
60	MG	DA	3052	-	X
60	MG	DA	3057	-	X
60	MG	DA	3059	-	X
60	MG	DA	3061	-	X
60	MG	DA	3062	-	X
60	MG	DA	3063	-	X
60	MG	DA	3073	-	X
60	MG	DA	3074	-	X
60	MG	DA	3075	-	X
60	MG	DA	3077	-	X
60	MG	DA	3093	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
60	MG	DA	3096	-	X
60	MG	DA	3105	-	X
60	MG	DA	3107	-	X
60	MG	DA	3108	-	X
60	MG	DA	3114	-	X
60	MG	DA	3124	-	X
60	MG	DA	3127	-	X
60	MG	DA	3129	-	X
60	MG	DA	3130	-	X
60	MG	DE	301	-	X
60	MG	DJ	201	-	X

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 284499 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	CB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	CC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	CE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	CF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			
10	CJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
14	CN	95	Total	C	N	O	S	0	0	0
			769	480	159	127	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	CQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O		0	0	0
			456	288	86	82				
18	CR	55	Total	C	N	O		0	0	0
			456	288	86	82				

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	CS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			
21	CU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- 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			

- 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
			2083	1288	423	365	7			
24	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	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
			1411	899	249	257	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
			939	587	180	166	6			
32	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	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
			961	593	196	167	5			
35	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			739	466	139	132	2			
41	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	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
			780	492	146	142				
42	DU	102	Total	C	N	O		0	0	0
			780	492	146	142				

- 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			
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
			410	263	75	72			
49	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

- 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 protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	CG	150	Total	C	N	O	S	0	0	0
			1175	730	226	215	4			

- Molecule 55 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	CM	113	Total	C	N	O	S	0	0	0
			877	541	177	156	3			

- Molecule 56 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	CP	80	Total	C	N	O	S	0	0	0
			639	400	126	112	1			

- Molecule 57 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 58 is a RNA chain called 5S rRNA.

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

- Molecule 59 is a protein called 50S ribosomal protein L5.

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

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

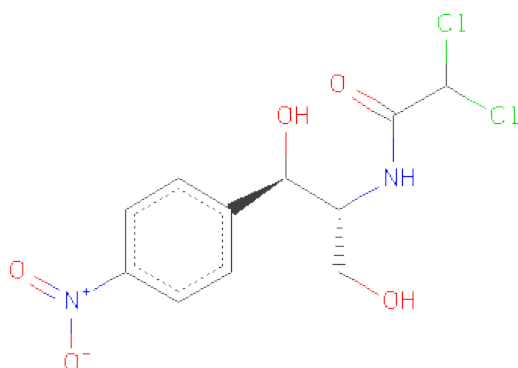
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BB	4	Total	Mg	0	0
			4	4		
60	DE	1	Total	Mg	0	0
			1	1		
60	BA	135	Total	Mg	0	0
			135	135		
60	CA	42	Total	Mg	0	0
			42	42		
60	DJ	1	Total	Mg	0	0
			1	1		
60	BL	1	Total	Mg	0	0
			1	1		
60	DA	133	Total	Mg	0	0
			133	133		
60	AA	42	Total	Mg	0	0
			42	42		
60	AN	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DC	1	Total	Mg	0	0
			1	1		
60	DB	1	Total	Mg	0	0
			1	1		

- Molecule 61 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	BA	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AA	197	Total	O	0	0
			197	197		
63	AL	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AN	6	Total 6	O 6	0	0
63	AT	2	Total 2	O 2	0	0
63	AU	1	Total 1	O 1	0	0
63	BA	608	Total 608	O 608	0	0
63	BB	19	Total 19	O 19	0	0
63	BC	8	Total 8	O 8	0	0
63	BD	2	Total 2	O 2	0	0
63	BE	1	Total 1	O 1	0	0
63	BL	4	Total 4	O 4	0	0
63	BN	2	Total 2	O 2	0	0
63	BQ	1	Total 1	O 1	0	0
63	BT	2	Total 2	O 2	0	0
63	BV	1	Total 1	O 1	0	0
63	B2	2	Total 2	O 2	0	0
63	B3	2	Total 2	O 2	0	0
63	B4	2	Total 2	O 2	0	0
63	CA	195	Total 195	O 195	0	0
63	CE	3	Total 3	O 3	0	0
63	CI	1	Total 1	O 1	0	0
63	CL	1	Total 1	O 1	0	0
63	CN	3	Total 3	O 3	0	0

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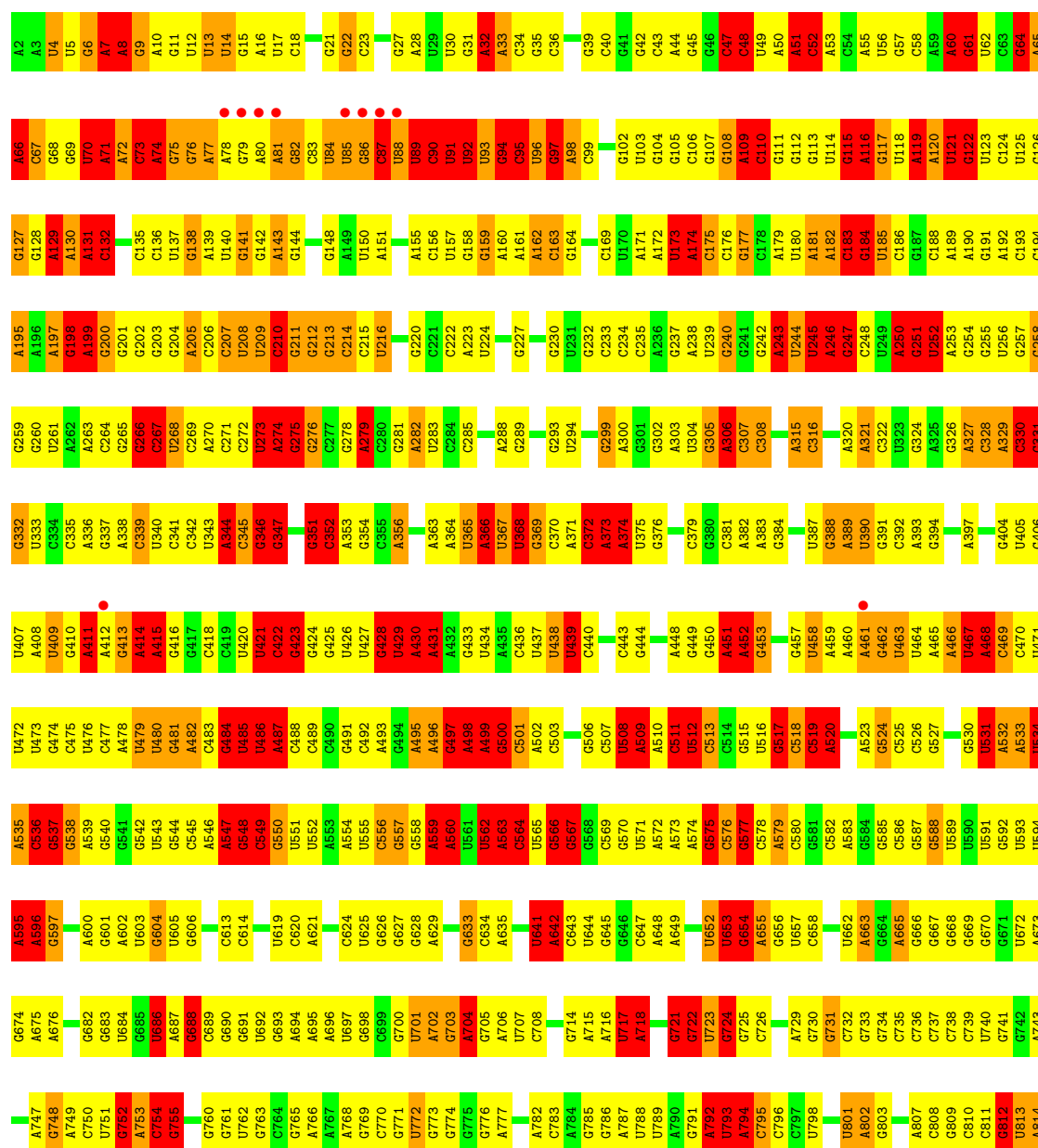
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	CT	2	Total 2	O 2	0	0
63	CU	2	Total 2	O 2	0	0
63	DA	603	Total 603	O 603	0	0
63	DB	4	Total 4	O 4	0	0
63	DC	10	Total 10	O 10	0	0
63	DD	1	Total 1	O 1	0	0
63	DE	3	Total 3	O 3	0	0
63	DJ	4	Total 4	O 4	0	0
63	DL	5	Total 5	O 5	0	0
63	DN	2	Total 2	O 2	0	0
63	DT	2	Total 2	O 2	0	0
63	DU	2	Total 2	O 2	0	0
63	DV	1	Total 1	O 1	0	0
63	D2	1	Total 1	O 1	0	0
63	D3	1	Total 1	O 1	0	0
63	D4	4	Total 4	O 4	0	0

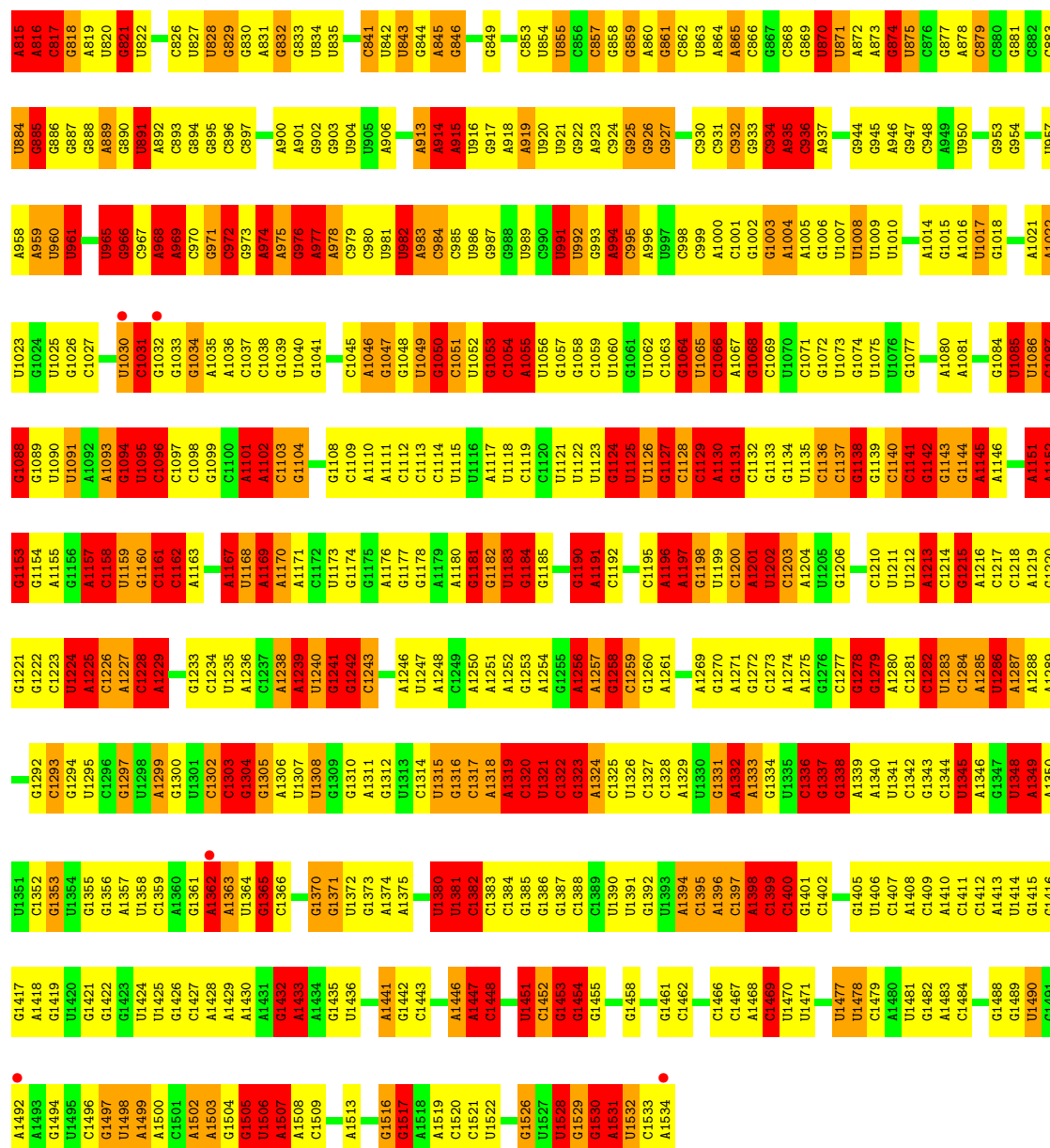
3 Residue-property plots

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

• Molecule 1: 16S rRNA

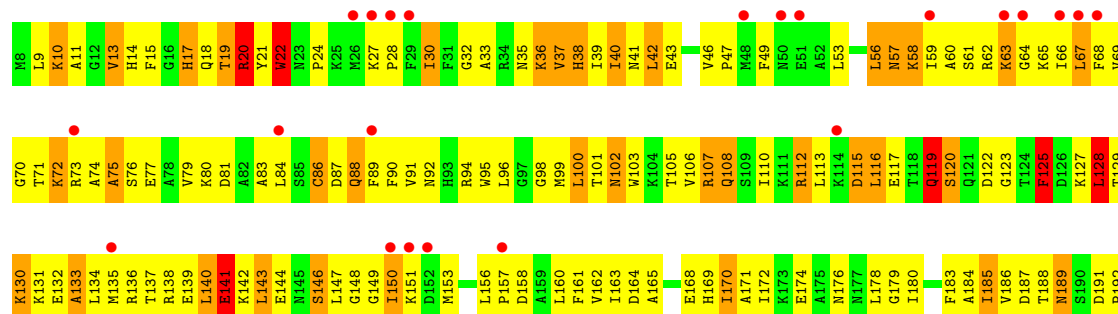
Chain AA: 





• Molecule 2: 30S ribosomal protein S2

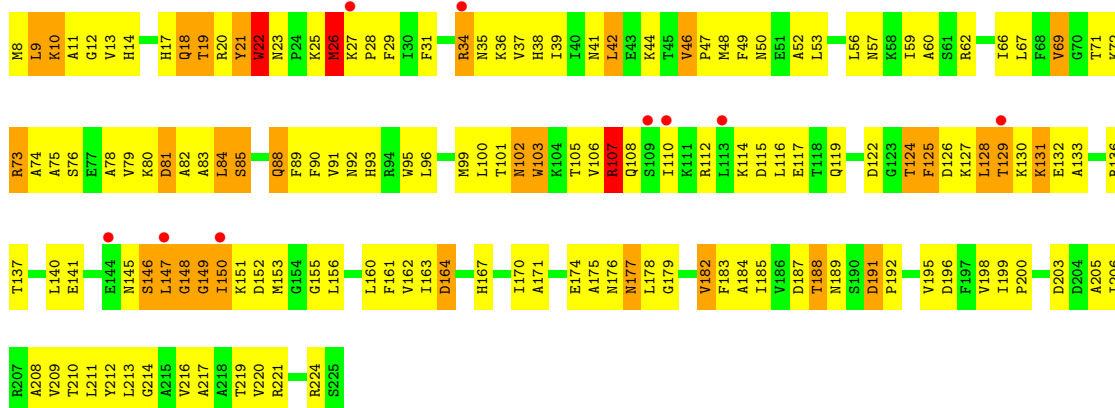
Chain AB:





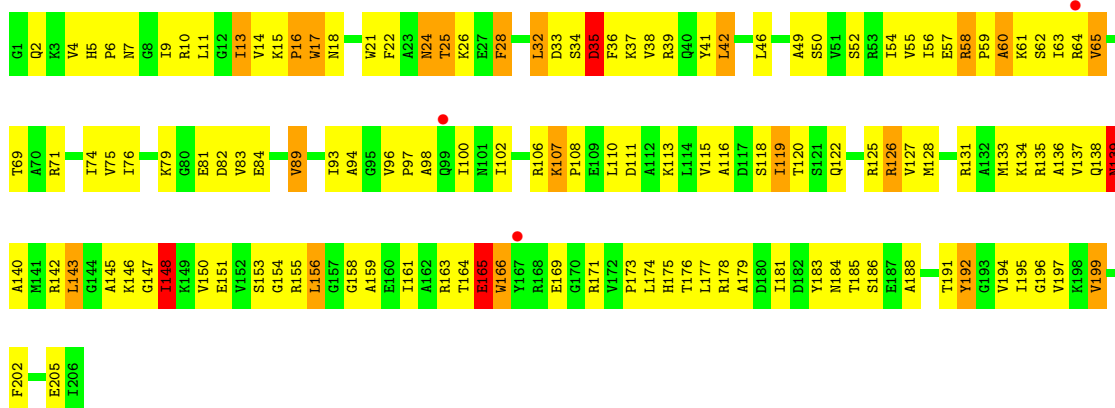
• Molecule 2: 30S ribosomal protein S2

Chain CB:



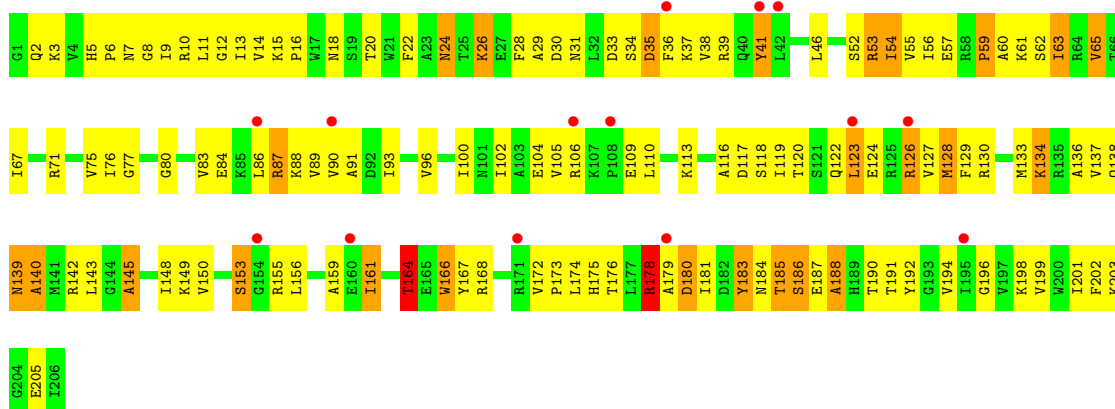
• Molecule 3: 30S ribosomal protein S3

Chain AC:



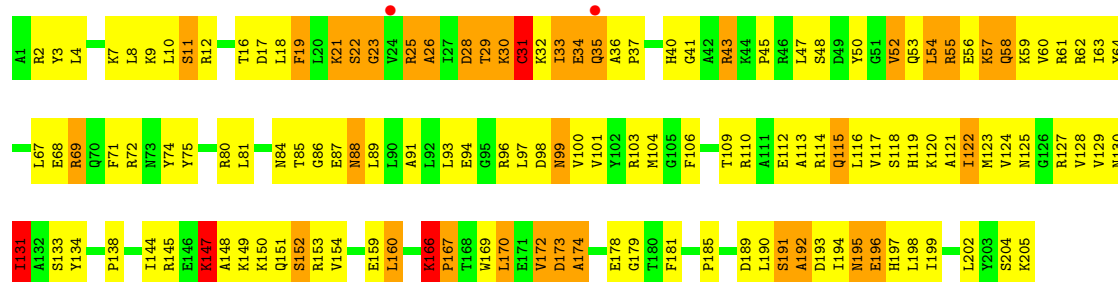
• Molecule 3: 30S ribosomal protein S3

Chain CC:



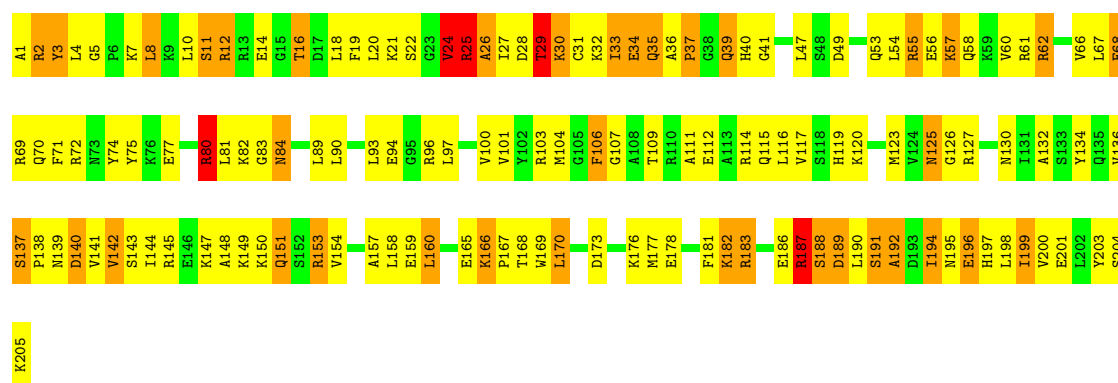
- Molecule 4: 30S ribosomal protein S4

Chain AD:



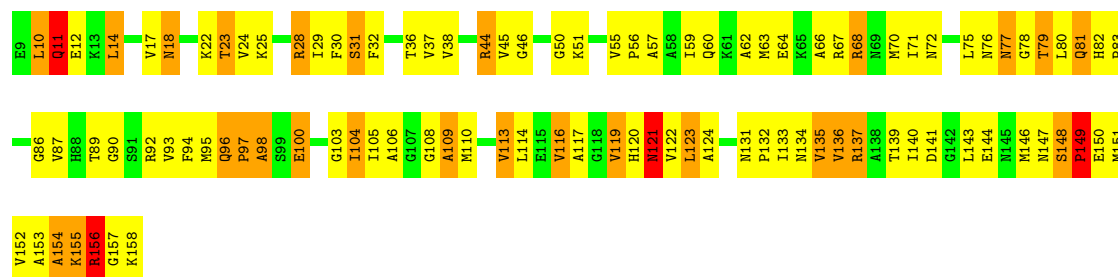
- Molecule 4: 30S ribosomal protein S4

Chain CD:



- Molecule 5: 30S ribosomal protein S5

Chain AE:



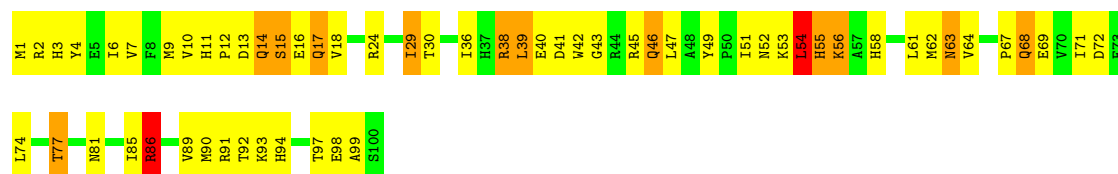
- Molecule 5: 30S ribosomal protein S5

Chain CE:



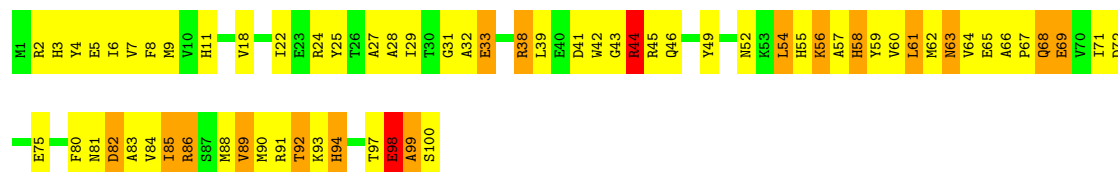
- Molecule 6: 30S ribosomal protein S6

Chain AF:



- Molecule 6: 30S ribosomal protein S6

Chain CF:



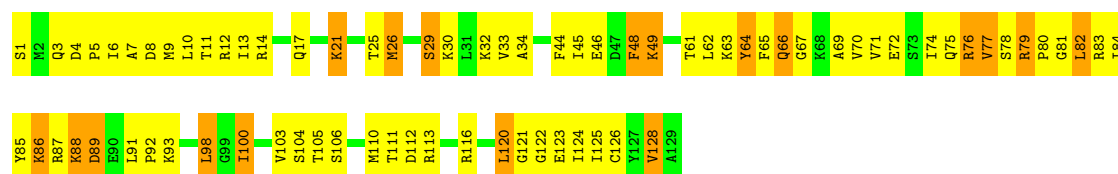
- Molecule 7: 30S ribosomal protein S7

Chain AG:



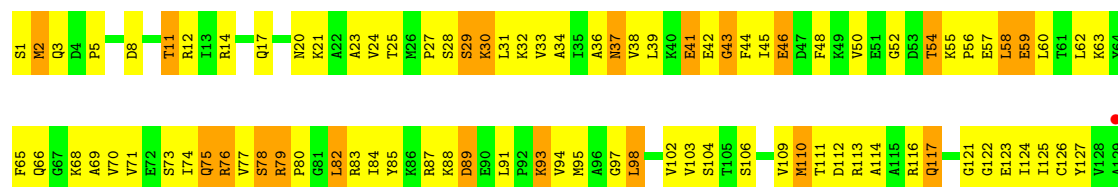
- Molecule 8: 30S ribosomal protein S8

Chain AH:



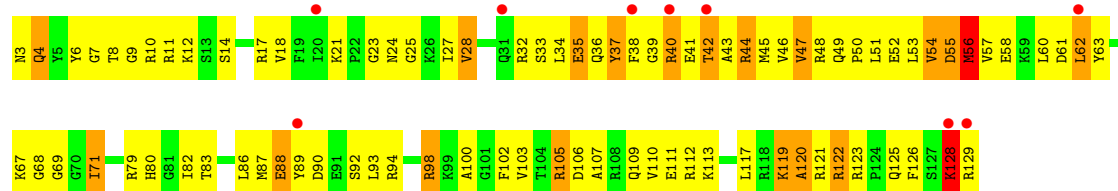
- Molecule 8: 30S ribosomal protein S8

Chain CH:



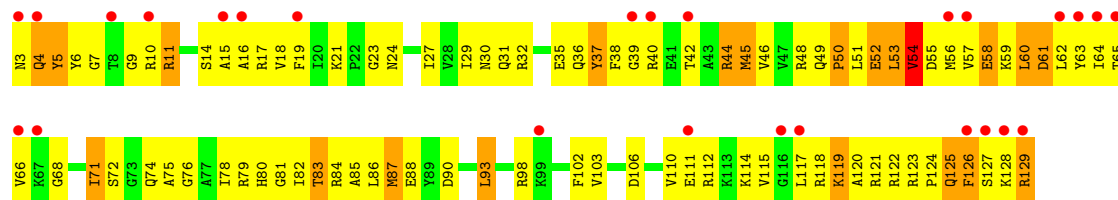
- Molecule 9: 30S ribosomal protein S9

Chain AI:



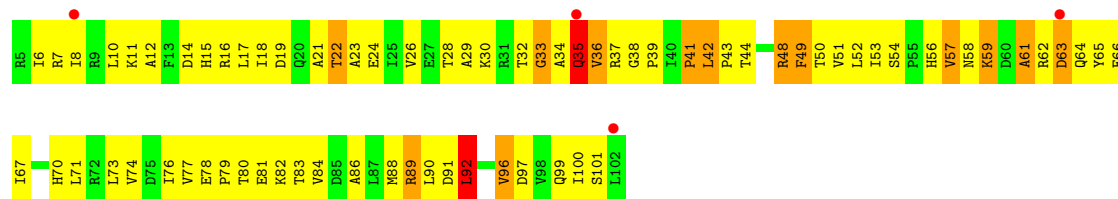
- Molecule 9: 30S ribosomal protein S9

Chain CI:



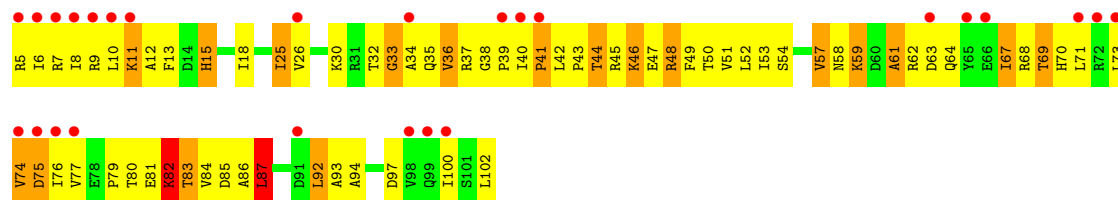
- Molecule 10: 30S ribosomal protein S10

Chain AJ:



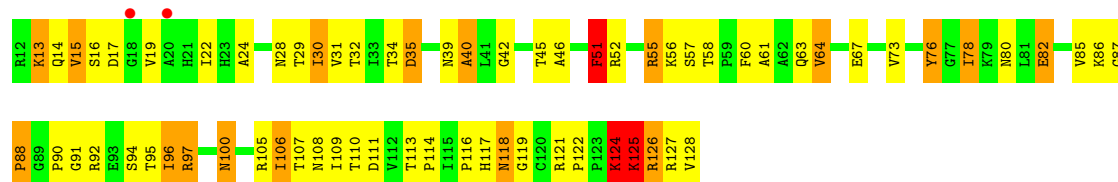
- Molecule 10: 30S ribosomal protein S10

Chain CJ:



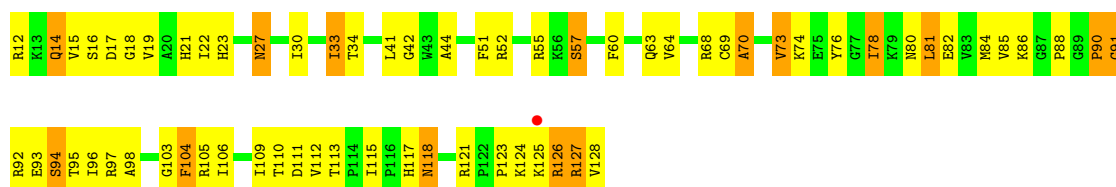
- Molecule 11: 30S ribosomal protein S11

Chain AK:



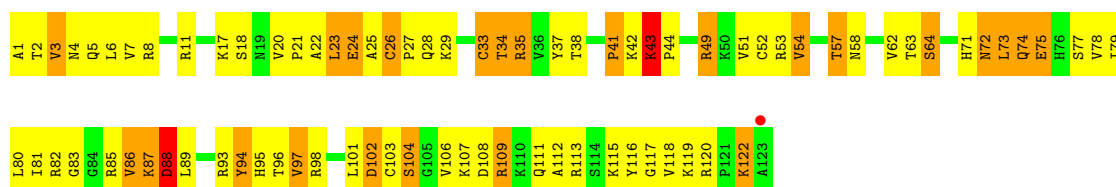
- Molecule 11: 30S ribosomal protein S11

Chain CK:



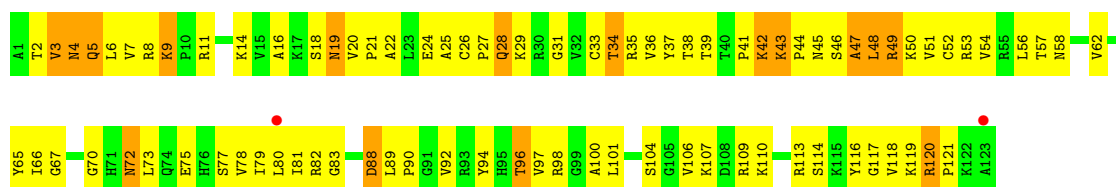
• Molecule 12: 30S ribosomal protein S12

Chain AL:



• Molecule 12: 30S ribosomal protein S12

Chain CL:



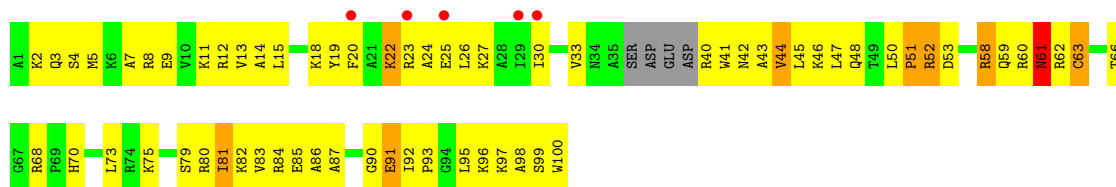
• Molecule 13: 30S ribosomal protein S13

Chain AM:



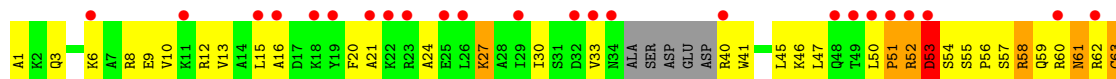
• Molecule 14: 30S ribosomal protein S14

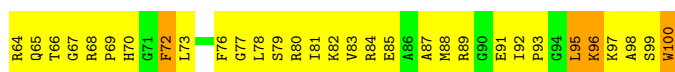
Chain AN:



• Molecule 14: 30S ribosomal protein S14

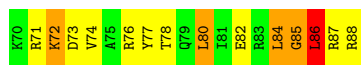
Chain CN:





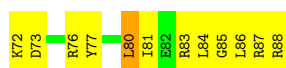
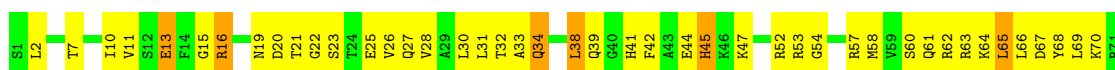
- Molecule 15: 30S ribosomal protein S15

Chain AO:



- Molecule 15: 30S ribosomal protein S15

Chain CO:



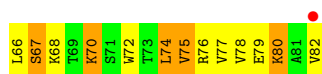
- Molecule 16: 30S ribosomal protein S16

Chain AP:



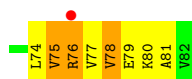
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



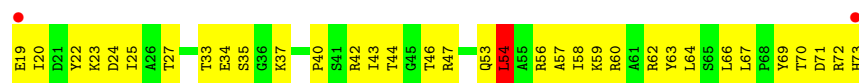
- Molecule 17: 30S ribosomal protein S17

Chain CQ:



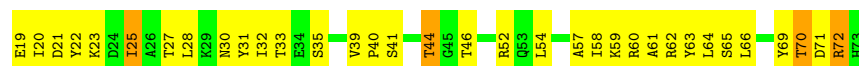
- Molecule 18: 30S ribosomal protein S18

Chain AR:



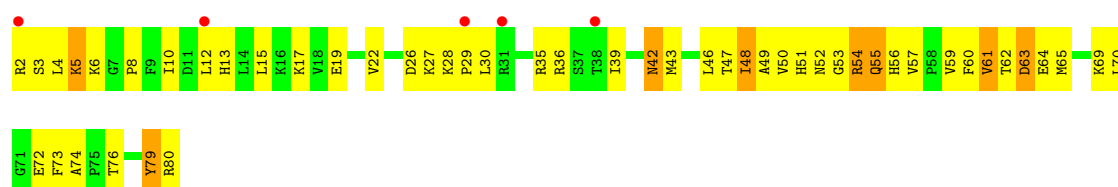
- Molecule 18: 30S ribosomal protein S18

Chain CR:



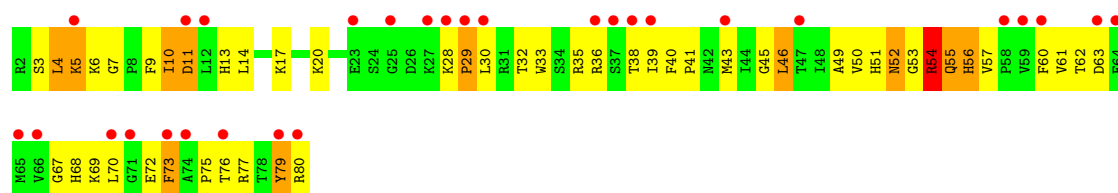
- Molecule 19: 30S ribosomal protein S19

Chain AS:



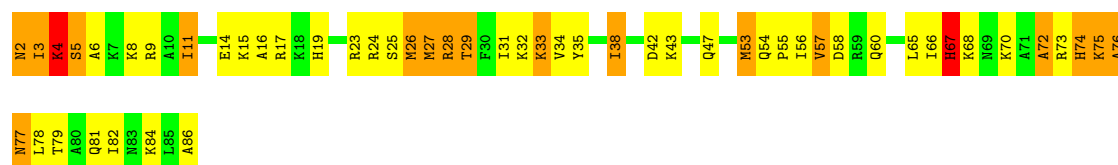
- Molecule 19: 30S ribosomal protein S19

Chain CS:



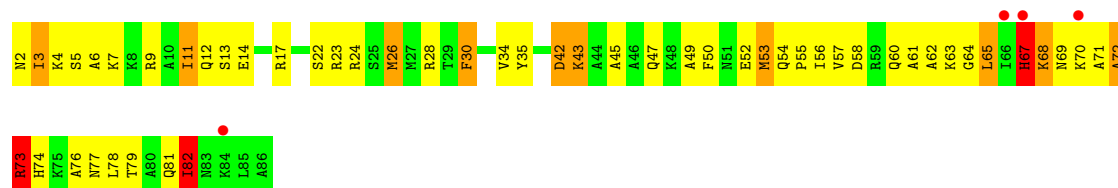
- Molecule 20: 30S ribosomal protein S20

Chain AT:



- Molecule 20: 30S ribosomal protein S20

Chain CT:



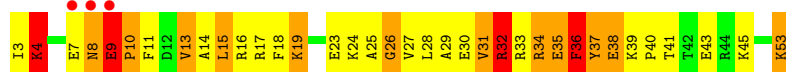
- Molecule 21: 30S ribosomal protein S21

Chain AU:



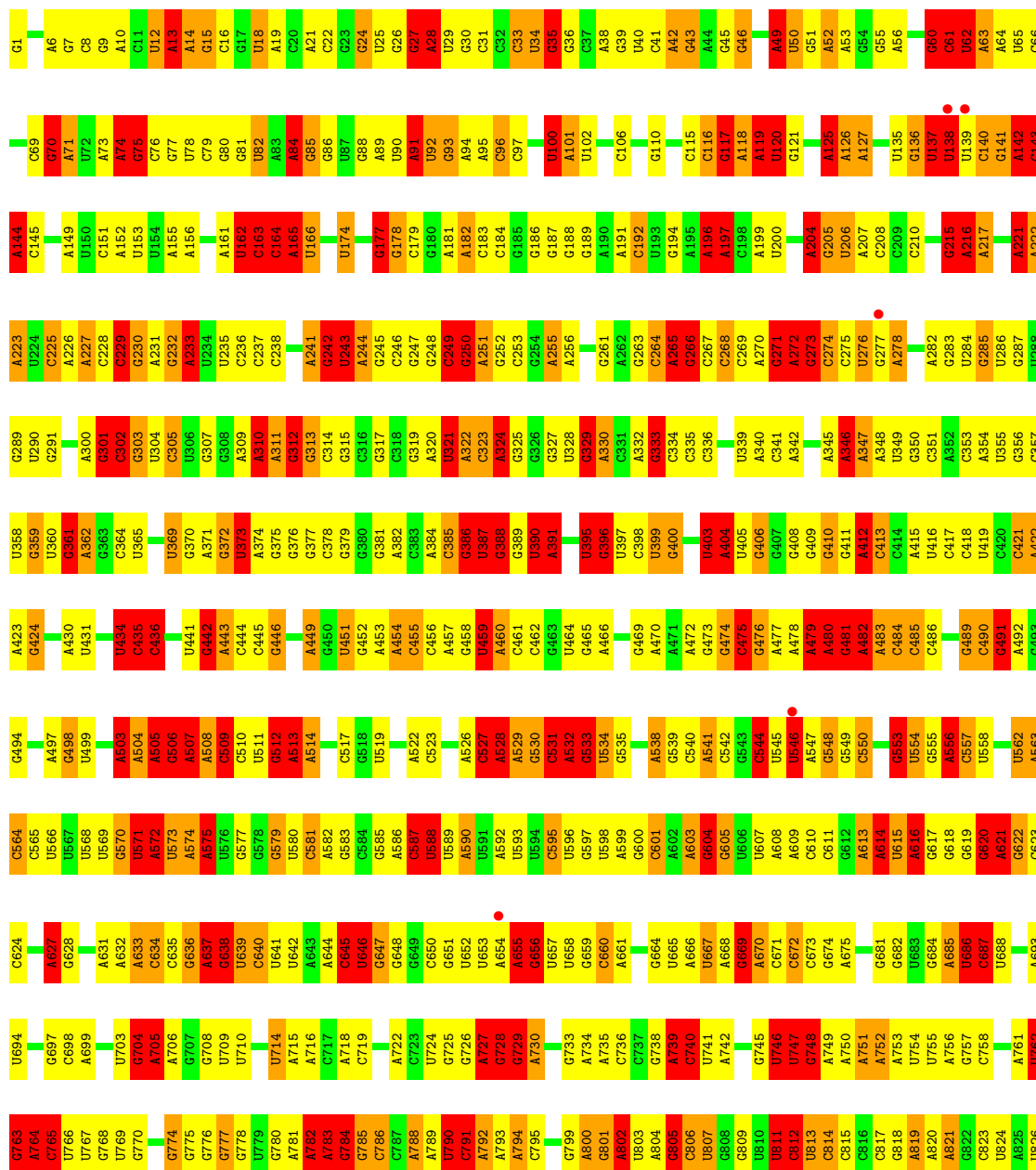
- Molecule 21: 30S ribosomal protein S21

Chain CU:



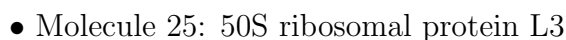
- Molecule 22: 23S rRNA

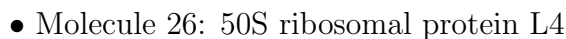
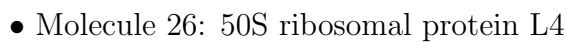
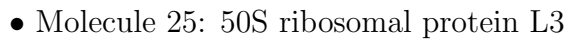
Chain BA:



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C1748	G1681	C1615	A1552	U1415	A1347	C1221	A1155	G1025	C965	C897	U828
G1753	G1682	A1616	A1553	C1416	A1348	U1222	A1156	G1026	C966	C898	G829
A1754	U1683	C1617	U1484	C1417	C1349	G1223	G1157	A1027	U967	A899	G830
A1755	G1684	A1618	U1485	A1418	C1350	U1224	U1158	A1028	C968	A900	G831
G1756	C1685	G1619	U1486	A1419	C1351	G1225	U1159	U1094	G969	C901	U832
A1757	C1686	G1622	U1487	A1420	C1352	A1226	G1160	G1031	U970	A833	A833
U1758	C1688	G1623	C1488	G1421	U1353	G1227	C1161	U1032	G971	G834	G834
A1759	U1689	U1624	A1489	G1422	A1354	G1228	G1162	U1033	A905	U839	U839
C1760	C1690	C1625	A1490	G1423	A1355	C1229	U1163	G1034	U906	U906	U906
A1761	U1693	G1626	G1491	G1424	G1356	A1230	C1164	U1035	G907	G907	G907
A1762	C1694	A1627	G1492	G1425	C1357	U1231	A1165	G1036	A908	C908	U842
G1763	G1695	G1628	A1493	C1426	G1358	G1232	G1166	G1037	G976	U909	G843
G1764	U1696	U1629	A1494	C1427	A1359	C1233	C1167	A1039	G977	A910	A844
U1765	G1697	G1630	A1495	G1428	G1360	U1234	G1168	A1040	U978	U913	U845
G1766	C1698	G1631	A1496	C1429	G1361	G1235	A1169	G1041	A980	G914	U846
A1769	A1699	G1632	C1498	G1430	U1372	U1236	C1170	G1042	A981	C915	U847
A1700	U1700	A1694	C1499	G1431	A1365	A1237	G1171	C1043	A982	C916	C948
A1701	G1701	U1695	G1500	A1432	A1366	G1238	C1172	C1044	C982	U916	C851
C1770	A1701	U1696	G1501	A1433	A1367	U1239	A1175	G1045	A983	A917	C851
A1773	C1706	U1697	G1502	A1434	A1368	U1240	U1176	A1046	A984	A918	C854
C1774	G1707	A1637	A1503	G1435	C1370	C1241	U1177	G1047	C985	U919	C854
U1775	U1708	C1638	A1504	C1436	G1371	C1242	G1178	A1048	C986	A920	G855
G1776	U1709	A1640	U1505	U1438	U1372	A1244	C1179	C1049	C987	C921	G856
U1777	C1709	A1641	U1506	A1439	A1373	G1245	U1180	A1050	A988	C922	G857
U1778	U1712	G1642	C1507	U1440	U1378	A1246	U1181	C989	C923	G923	G858
U1779	A1713	G1643	U1508	G1441	G1375	A1247	U1182	A990	G924	G924	G859
A1780	U1714	C1644	U1509	U1442	C1376	U1248	U1183	G1055	C991	C930	U860
U1781	G1715	G1645	G1510	U1443	G1377	U1249	U1184	A1057	C992	U931	G861
U1782	U1716	C1646	G1511	G1444	U1378	G1250	G1185	U1058	C993	U932	G862
A1717	A1717	U1647	C1512	C1445	U1379	C1251	G1186	G1059	C994	A933	C865
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A1785	A1785	G1649	G1514	C1447	G1381	A1253	U1188	U1061	A996	C935	A866
A1786	G1721	A1650	A1515	G1450	G1382	U1254	U1189	G1062	C997	U936	U867
A1787	U1722	G1651	C1451	C1451	A1383	U1255	G1190	G1063	C998	A936	U868
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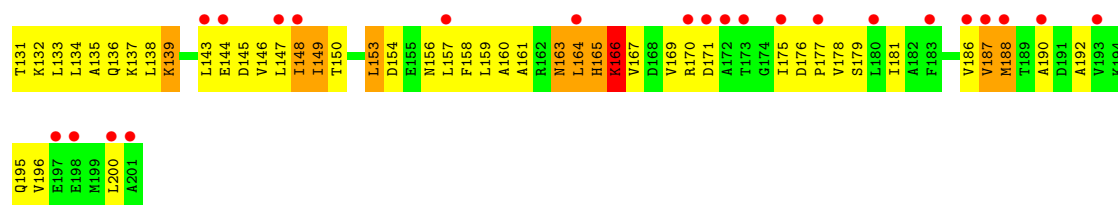
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				A2419		A2352	G2286	G2215		G2023			C1874
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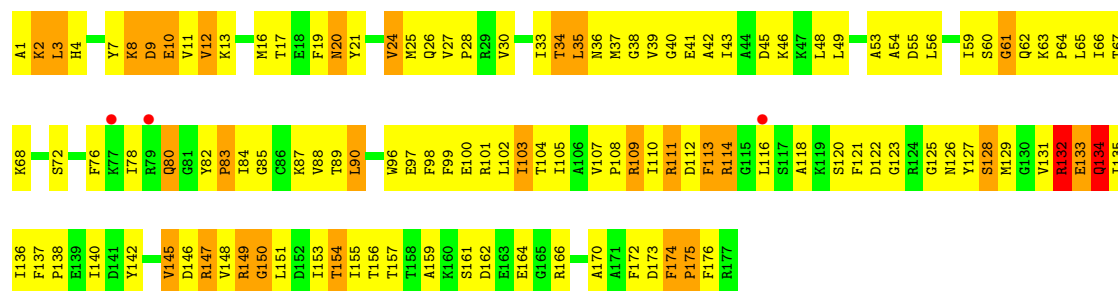
Response	Percentage
Yes	45%
No	55%





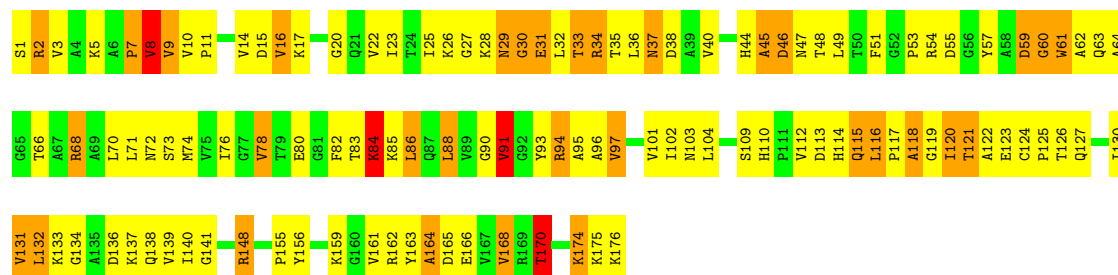
• Molecule 27: 50S ribosomal protein L5

Chain BF:



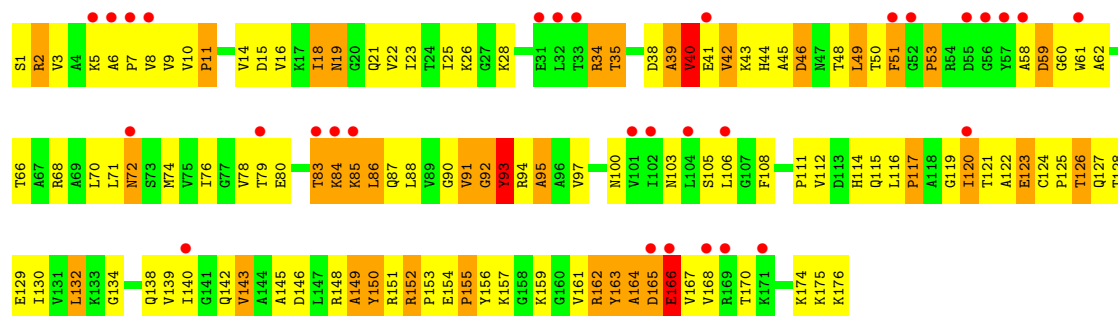
• Molecule 28: 50S ribosomal protein L6

Chain BG:



• Molecule 28: 50S ribosomal protein L6

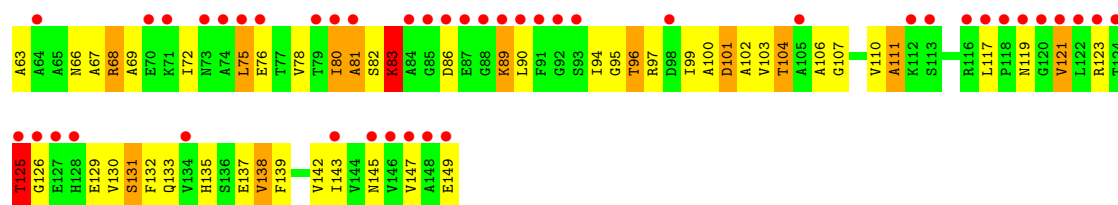
Chain DG:



• Molecule 29: 50S ribosomal protein L9

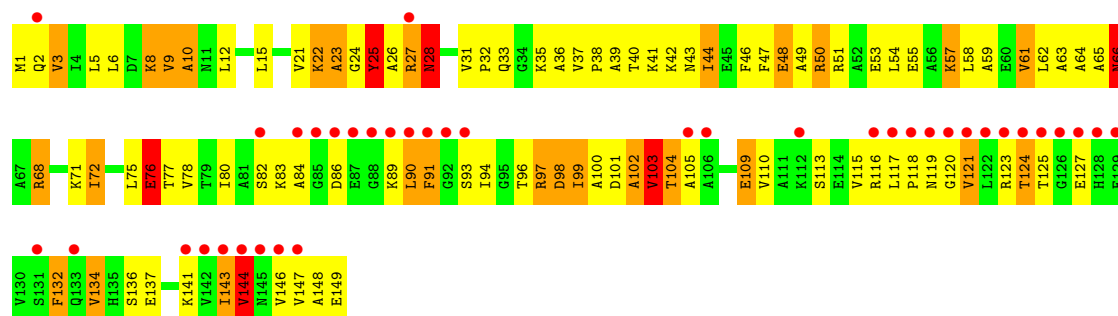
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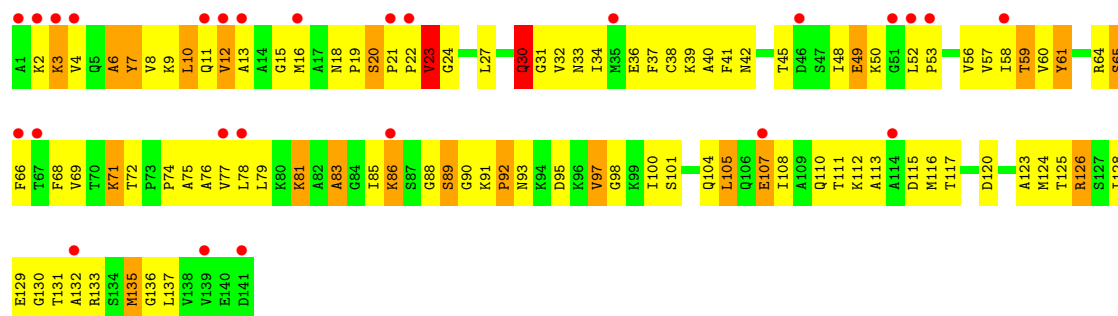
• Molecule 29: 50S ribosomal protein L9

Chain DH:



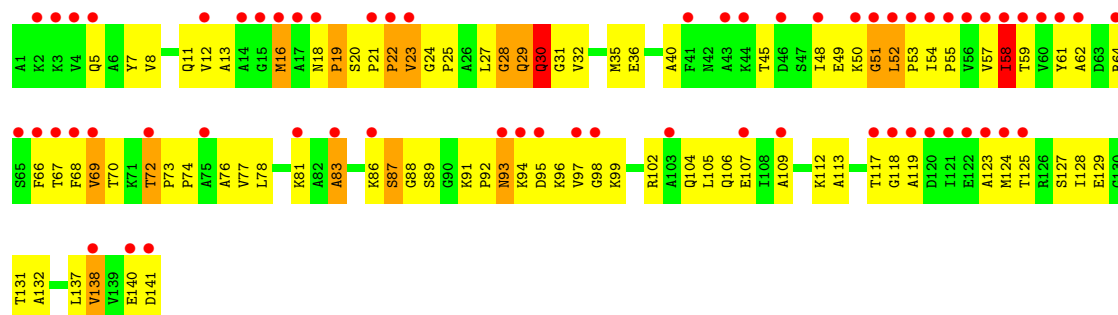
• Molecule 30: 50S ribosomal protein L11

Chain BI:



• Molecule 30: 50S ribosomal protein L11

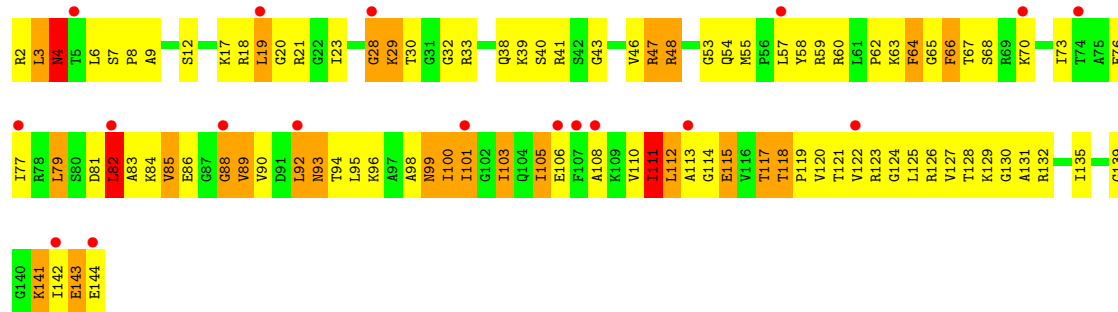
Chain DI:



• Molecule 31: 50S ribosomal protein L13

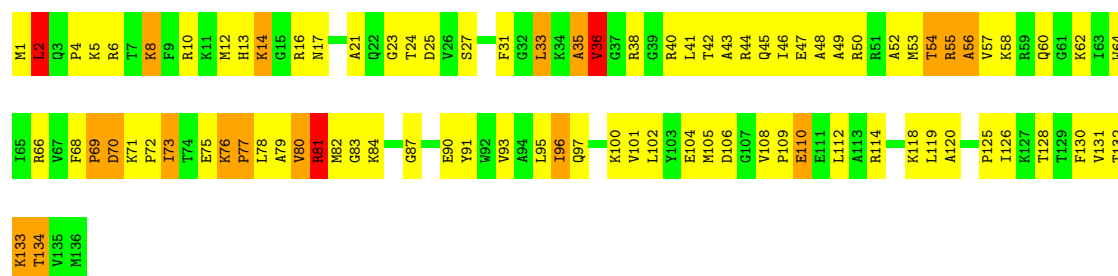
Chain BJ:

Chain DL: 



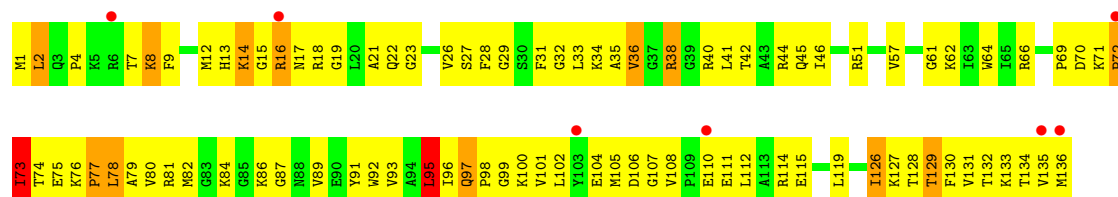
- Molecule 34: 50S ribosomal protein L16

Chain BM: 



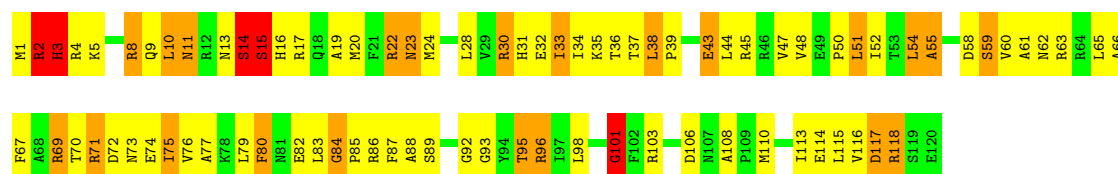
- Molecule 34: 50S ribosomal protein L16

Chain DM: 



- Molecule 35: 50S ribosomal protein L17

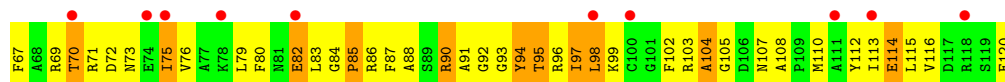
Chain BN: 



- Molecule 35: 50S ribosomal protein L17

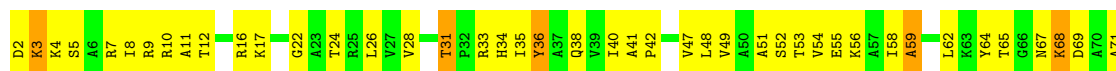
Chain DN: 





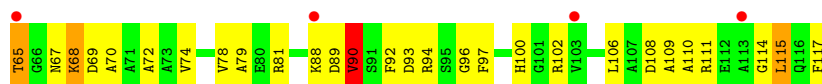
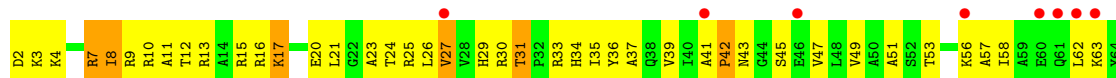
- Molecule 36: 50S ribosomal protein L18

Chain BO:



- Molecule 36: 50S ribosomal protein L18

Chain DO:



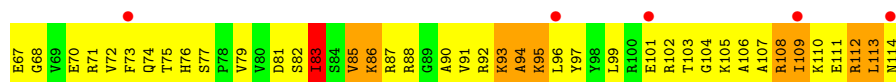
- Molecule 37: 50S ribosomal protein L19

Chain BP:



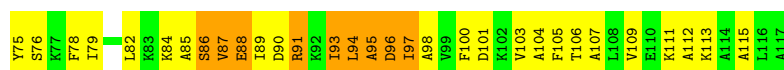
- Molecule 37: 50S ribosomal protein L19

Chain DP:



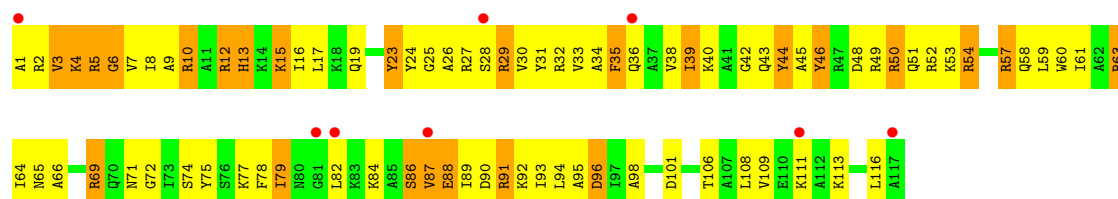
- Molecule 38: 50S ribosomal protein L20

Chain BQ:



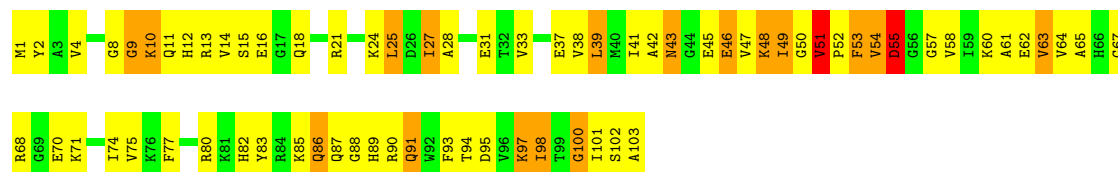
- Molecule 38: 50S ribosomal protein L20

Chain DQ:



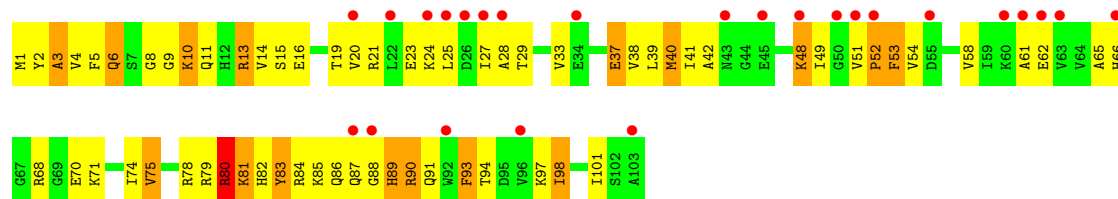
- Molecule 39: 50S ribosomal protein L21

Chain BR:



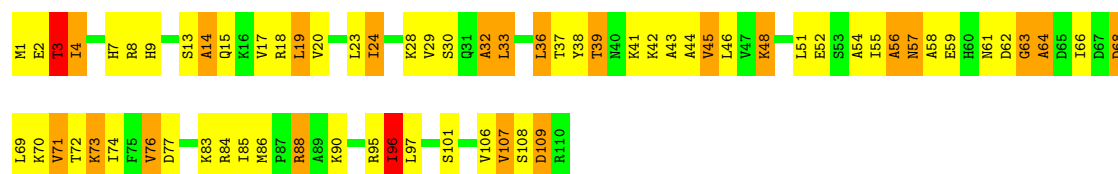
- Molecule 39: 50S ribosomal protein L21

Chain DR:



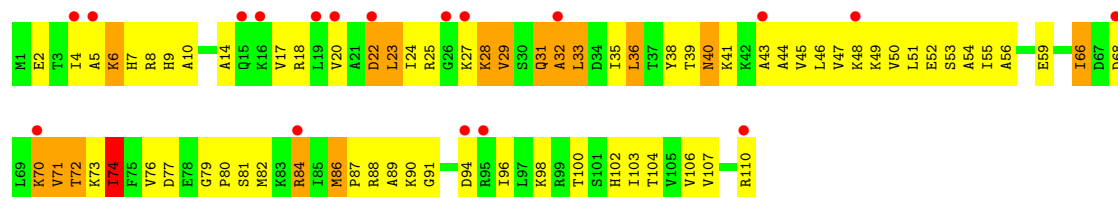
- Molecule 40: 50S ribosomal protein L22

Chain BS:



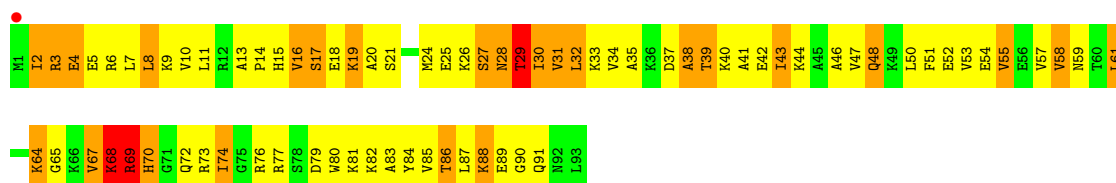
- Molecule 40: 50S ribosomal protein L22

Chain DS:



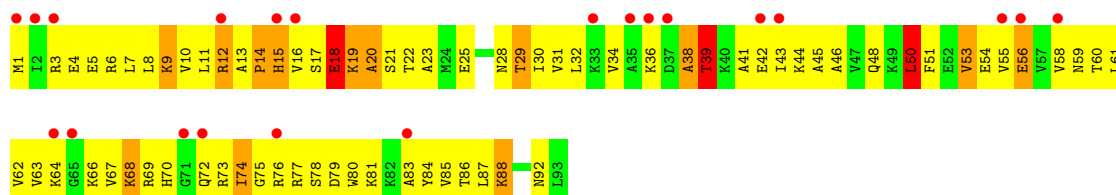
- Molecule 41: 50S ribosomal protein L23

Chain BT:



• Molecule 41: 50S ribosomal protein L23

Chain DT:



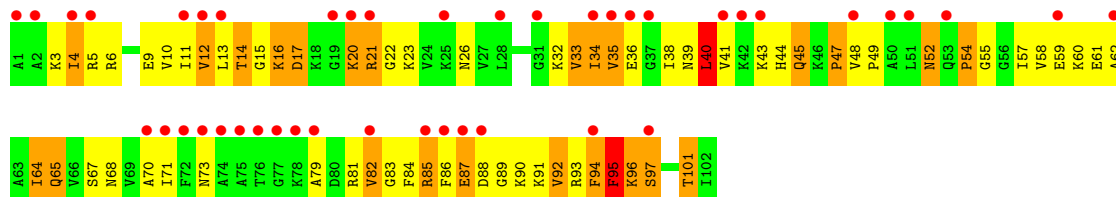
• Molecule 42: 50S ribosomal protein L24

Chain BU:



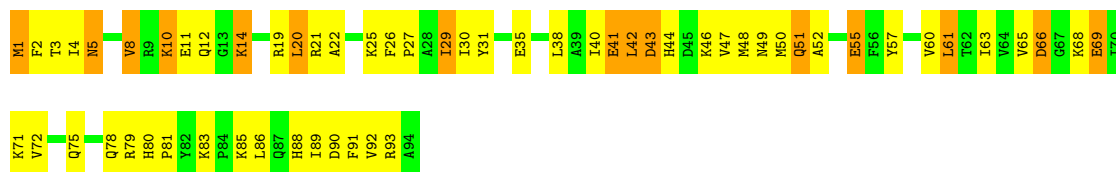
• Molecule 42: 50S ribosomal protein L24

Chain DU:



• Molecule 43: 50S ribosomal protein L25

Chain BV:



• Molecule 43: 50S ribosomal protein L25

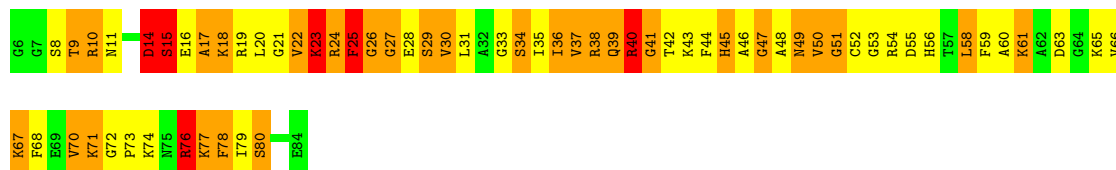
Chain DV:





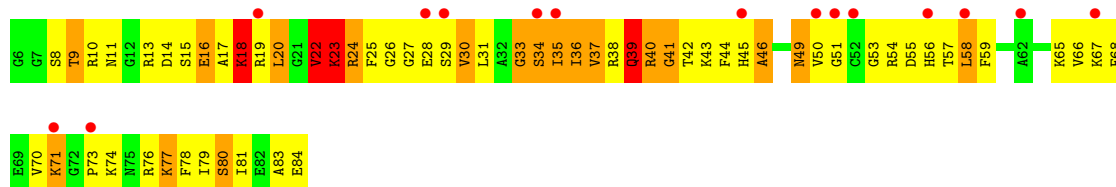
- Molecule 44: 50S ribosomal protein L27

Chain BW:



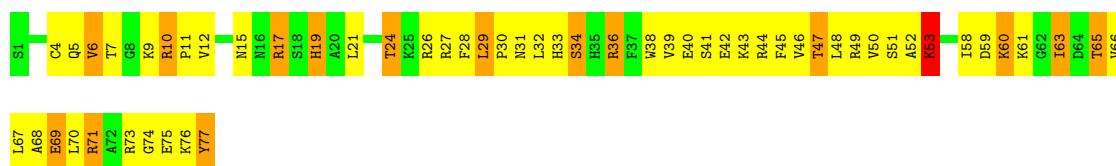
- Molecule 44: 50S ribosomal protein L27

Chain DW:



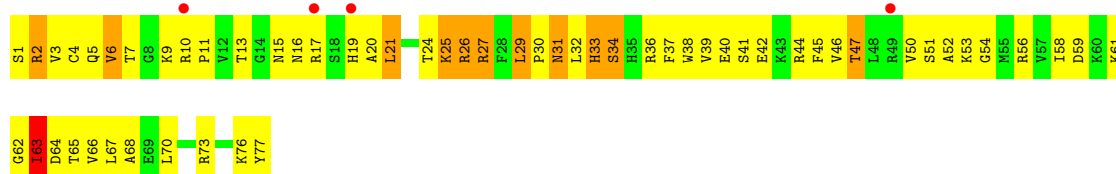
- Molecule 45: 50S ribosomal protein L28

Chain BX:



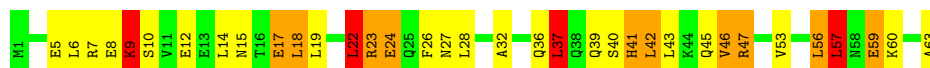
- Molecule 45: 50S ribosomal protein L28

Chain DX:



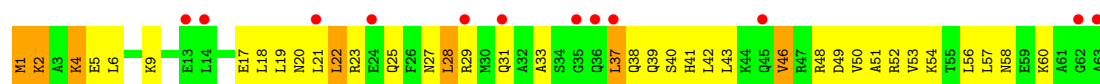
- Molecule 46: 50S ribosomal protein L29

Chain BY:



- Molecule 46: 50S ribosomal protein L29

Chain DY:



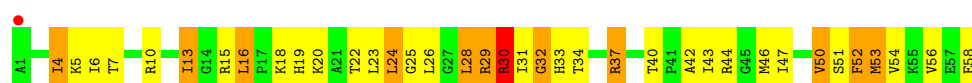
- Molecule 47: 50S ribosomal protein L30

Chain BZ:



- Molecule 47: 50S ribosomal protein L30

Chain DZ:



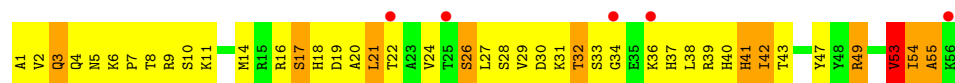
- Molecule 48: 50S ribosomal protein L32

Chain B0:



- Molecule 48: 50S ribosomal protein L32

Chain D0:



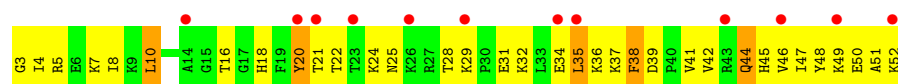
- Molecule 49: 50S ribosomal protein L33

Chain B1:



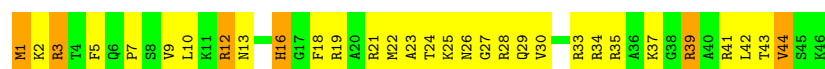
- Molecule 49: 50S ribosomal protein L33

Chain D1:



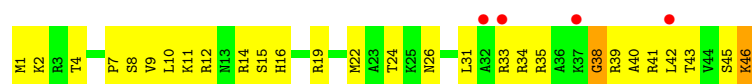
- Molecule 50: 50S ribosomal protein L34

Chain B2:



- Molecule 50: 50S ribosomal protein L34

Chain D2:



- Molecule 51: 50S ribosomal protein L35

Chain B3:



- Molecule 51: 50S ribosomal protein L35

Chain D3:



- Molecule 52: 50S ribosomal protein L36

Chain B4:



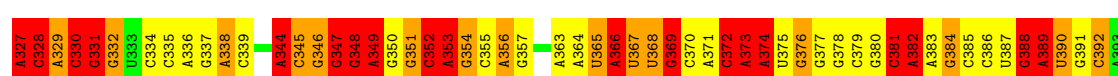
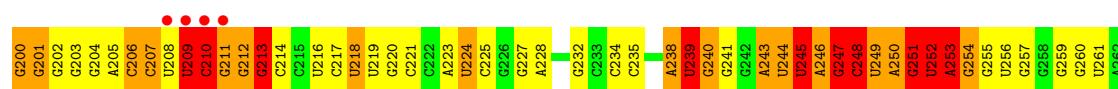
- Molecule 52: 50S ribosomal protein L36

Chain D4:

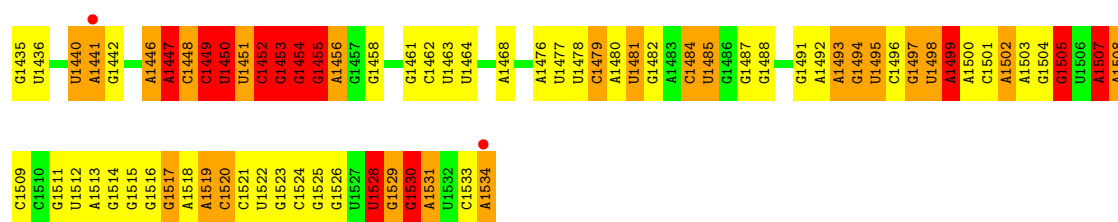


- Molecule 53: 16S rRNA

Chain CA:

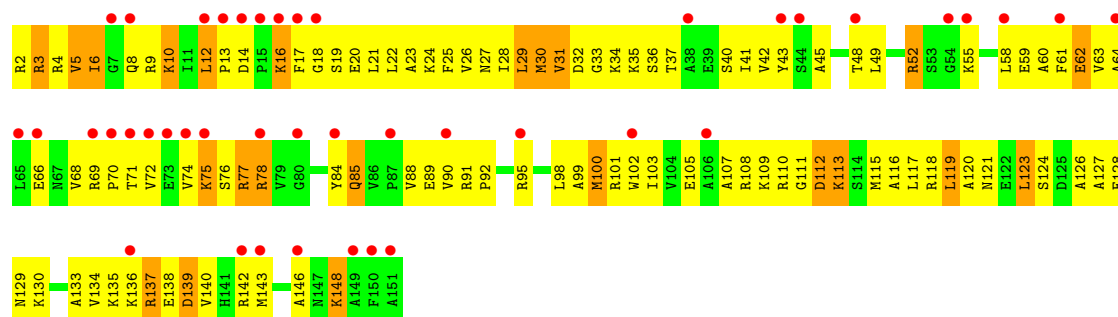






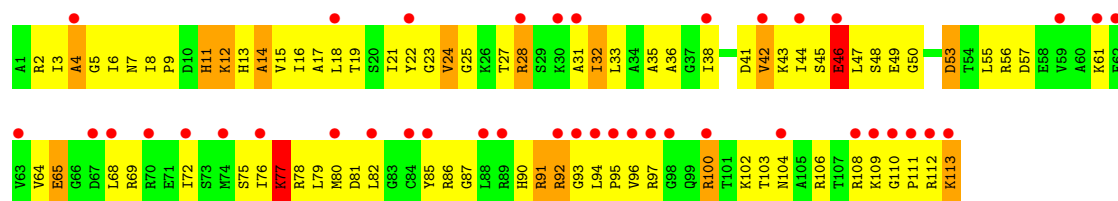
• Molecule 54: 30S ribosomal protein S7

Chain CG:



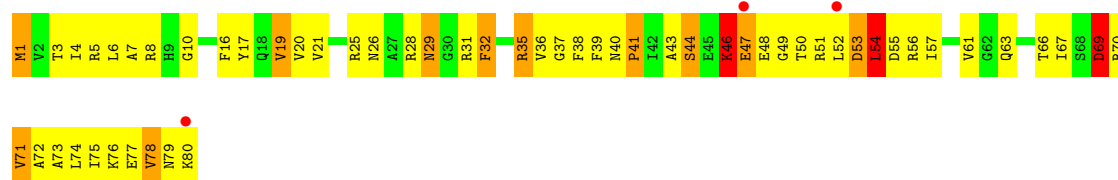
• Molecule 55: 30S ribosomal protein S13

Chain CM:



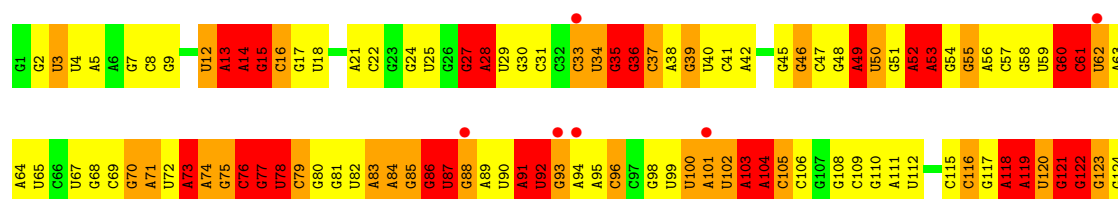
• Molecule 56: 30S ribosomal protein S16

Chain CP:



• Molecule 57: 23S rRNA

Chain DA:



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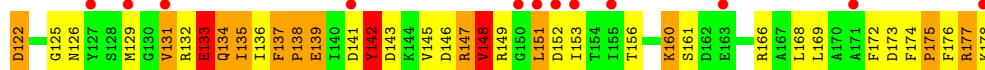
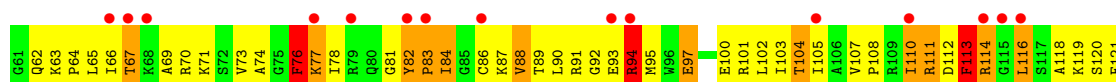
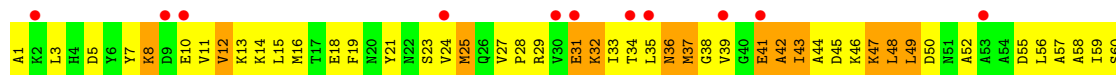
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A2670	G2671	U2672	G2673	G2674	G2675	G2676	G2677	G2678	A2679	G2680	G2681	A2682	G2683	U2684	G2685	G2686	G2687	G2688	U2689	G2690	G2691	G2692	G2693	G2694	U2695	G2696	G2697	G2698	G2699	G2700	G2701	G2702	G2703	G2704	G2705	G2706	G2707	G2708	G2709	G2710	A2711	G2712	G2713	G2714	G2715	G2716	G2717	G2718	G2719	G2720	A2721	G2722	G2723	G2724	A2725	A2726	G2727	U2728	G2729	G2730	G2731	G2732	A2733	G2734	G2735	G2736	G2737	G2738	G2739	G2740	G2741	G2742	G2743	G2744	G2745	G2746	G2747	G2748	G2749	G2750	G2751	G2752	G2753	G2754	G2755	G2756	G2757	G2758	G2759	G2760	G2761	G2762	G2763	G2764	G2765	G2766	G2767	G2768	G2769	G2770	G2771	G2772	G2773	G2774	G2775	G2776	G2777	G2778	G2779	G2780	G2781	G2782	G2783	G2784	G2785	G2786	G2787	G2788	G2789	G2790	G2791	G2792	G2793	G2794	G2795	G2796	G2797	G2798	G2799	G2800	G2801	G2802	G2803	G2804	G2805	G2806	G2807	G2808	G2809	G2810	G2811	G2812	G2813	G2814	G2815	G2816	G2817	G2818	G2819	G2820	G2821	G2822	G2823	G2824	G2825	G2826	G2827	G2828	G2829	G2830	G2831	G2832	G2833	G2834	G2835	G2836	G2837	G2838	G2839	G2840	G2841	G2842	G2843	G2844	G2845	G2846	G2847	G2848	G2849	G2850	G2851	G2852	G2853	G2854	G2855	G2856	G2857	G2858	G2859	G2860	G2861	G2862	G2863	G2864	G2865	G2866	G2867	G2868	G2869																																																																																																																															
G2543	G2544	G2545	U2546	U2547	U2548	G2549	G2550	G2551	U2552	U2553	U2554	G2555	G2556	G2557	G2558	G2559	A2560	U2561	U2562	U2563	A2564	A2565	A2566	U2567	U2568	G2569	G2570	U2571	A2572	G2573	G2574	G2575	G2576	A2577	G2578	G2579	G2580	G2581	G2582	G2583	U2584	U2585	U2586	A2587	G2588	A2589	A2590	G2591	G2592	U2593	G2594	G2595	U2596	G2597	A2598	G2599	A2600	G2601	G2602	U2603	G2604	G2605	G2606	G2607	G2608	G2609	G2610	G2611	G2612	G2613	G2614	G2615	G2616	G2617	G2618	G2619	G2620	G2621	G2622	G2623	G2624	G2625	G2626	G2627	G2628	G2629	G2630	G2631	A2632	G2633	G2634	G2635	G2636	G2637	G2638	G2639	G2640	G2641	G2642	G2643	G2644	G2645	G2646	U2647	G2648	G2649	G2650	G2651	G2652	G2653	G2654	G2655	G2656	A2657	G2658	G2659	A2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	G2668	G2669																																																																																																																																																																																																								
U2477	A2478	U2479	G2480	A2481	A2482	G2483	G2484	G2485	G2486	G2487	A2488	U2489	G2490	U2491	U2492	U2493	U2494	G2495	G2496	A2497	A2498	G2499	G2500	G2501	G2502	A2503	U2504	G2505	U2506	G2507	G2508	G2509	G2510	U2511	G2512	A2513	U2514	G2515	A2516	G2517	U2518	U2519	G2520	G2521	G2522	G2523	G2524	G2525	G2526	A2527	U2528	G2529	A2530	U2531	U2532	U2533	U2534	U2535	U2536	U2537	U2538	U2539	U2540	U2541	U2542	U2543	U2544	U2545	U2546	U2547	U2548	U2549	U2550	U2551	U2552	U2553	U2554	U2555	U2556	U2557	U2558	U2559	U2560	U2561	U2562	U2563	U2564	U2565	U2566	U2567	U2568	U2569	U2570	U2571	U2572	U2573	U2574	U2575	U2576	U2577	U2578	U2579	U2580	U2581	U2582	U2583	U2584	U2585	U2586	U2587	U2588	U2589	U2590	U2591	U2592	U2593	U2594	U2595	U2596	U2597	U2598	U2599	U2600	U2601	U2602	U2603	U2604	U2605	U2606	U2607	U2608	U2609	U2610	U2611	U2612	U2613	U2614	U2615	U2616	U2617	U2618	U2619	U2620	U2621	U2622	U2623	U2624	U2625	U2626	U2627	U2628	U2629	U2630	U2631	U2632	U2633	U2634	U2635	U2636	U2637	U2638	U2639	U2640	U2641	U2642	U2643	U2644	U2645	U2646	U2647	U2648	U2649	U2650	U2651	U2652	U2653	U2654	U2655	U2656	U2657	U2658	U2659	U2660	U2661	U2662	U2663	U2664	U2665	U2666	U2667	U2668	U2669																																																																																																																																						
U2343	U2344	G2345	G2346	U2347	U2348	G2349	G2350	G2351	A2352	G2353	G2354	U2355	U2356	U2357	G2358	G2359	G2360	G2361	G2362	G2363	G2364	G2365	A2366	G2367	G2368	G2369	G2370	G2371	U2372	G2373	G2374	G2375	G2376	G2377	G2378	G2379	G2380	A2381	G2382	U2383	U2384	A2385	A2386	U2387	U2388	U2389	U2390	U2391	A2392	U2393	U2394	G2395	G2396	G2397	U2398	U2399	U2400	U2401	U2402	U2403	U2404	G2405	U2406	U2407	U2408	U2409	U2410	U2411	U2412	U2413	U2414	U2415	U2416	U2417	U2418	U2419	U2420	U2421	U2422	U2423	U2424	U2425	U2426	U2427	U2428	U2429	U2430	U2431	U2432	U2433	U2434	U2435	U2436	U2437	U2438	U2439	U2440	U2441	U2442	U2443	U2444	U2445	U2446	U2447	U2448	U2449	U2450	U2451	U2452	U2453	U2454	U2455	U2456	U2457	U2458	U2459	U2460	A2461	U2462	U2463	U2464	U2465	U2466	U2467	U2468	U2469	U2470	U2471	U2472	U2473	U2474	U2475	U2476	U2477	U2478	U2479	U2480	U2481	U2482	U2483	U2484	U2485	U2486	U2487	U2488	U2489	U2490	U2491	U2492	U2493	U2494	U2495	U2496	U2497	U2498	U2499	U2500	U2501	U2502	U2503	U2504	U2505	U2506	U2507	U2508	U2509	U2510	U2511	U2512	U2513	U2514	U2515	U2516	U2517	U2518	U2519	U2520	U2521	U2522	U2523	U2524	U2525	U2526	U2527	U2528	U2529	U2530	U2531	U2532	U2533	U2534	U2535	U2536	U2537	U2538	U2539	U2540	U2541	U2542	U2543	U2544	U2545	U2546	U2547	U2548	U2549	U2550	U2551	U2552	U2553	U2554	U2555	U2556	U2557	U2558	U2559	U2560	U2561	U2562	U2563	U2564	U2565	U2566	U2567	U2568	U2569	U2570	U2571	U2572	U2573	U2574	U2575	U2576	U2577	U2578	U2579	U2580	U2581	U2582	U2583	U2584	U2585	U2586	U2587	U2588	U2589	U2590	U2591	U2592	U2593	U2594	U2595	U2596	U2597	U2598	U2599	U2600	U2601	U2602	U2603	U2604	U2605	U2606	U2607	U2608	U2609	U2610	U2611	U2612	U2613	U2614	U2615	U2616	U2617	U2618	U2619	U2620	U2621	U2622	U2623	U2624	U2625	U2626	U2627	U2628	U2629	U2630	U2631	U2632	U2633	U2634	U2635	U2636	U2637	U2638	U2639	U2640	U2641	U2642	U2643	U2644	U2645	U2646	U2647	U2648	U2649	U2650	U2651	U2652	U2653	U2654	U2655	U2656	U2657	U2658	U2659	U2660	U2661	U2662	U2663	U2664	U2665	U2666	U2667	U2668	U2669
U2280	A2281	G2282	G2283	A2284	G2285	G2286	A2287	A2288	G2289	G2290	G2291	U2292	G2293	U2294	U2295	U2296	U2297	A2298	U2299	G2300	G2301	G2302	G2303	G2304	U2305	G2306	G2307	G2308	G2309	G2310	A2311	U2312	G2313	A2314	G2315	G2316	A2317	G2318	G2319	U2320	U2321	A2322	G2323	U2324	G2325	U2326	G2327	U2328	U2329	U2330	U2331	U2332	U2333	U2334	U2335	U2336	U2337	U2338	U2339	U2340	U2341	U2342	U2343	U2344	U2345	U2346	U2347	U2348	U2349	U2350	U2351	U2352	U2353	U2354	U2355	U2356	U2357	U2358	U2359	U2360	U2361	U2362	U2363	U2364	U2365	U2366	U2367	U2368	U2369	U2370	U2371	U2372	U2373	U2374	U2375	U2376	U2377	U2378	U2379	U2380	U2381	U2382	U2383	U2384	U2385	U2386	U2387	U2388	U2389	U2390	U2391	U2392	U2393	U2394	U2395	U2396	U2397	U2398	U2399	U2400	U2401	U2402	U2403	U2404	U2405	U2406	U2407	U2408	U2409	U2410	U2411	U2412	U2413	U2414	U2415	U2416	U2417	U2418	U2419	U2420	U2421	U2422	U2423	U2424	U2425	U2426	U2427	U2428	U2429	U2430	U2431	U2432	U2433	U2434	U2435	U2436	U2437	U2438	U2439	U2440	U2441	U2442	U2443	U2444	U2445	U2446	U2447	U2448	U2449	U2450	U2451	U2452	U2453	U2454	U2455	U2456	U2457	U2458	U2459	U2460	A2461	U2462	U2463	U2464	U2465	U2466	U2467	U2468	U2469	U2470	U2471	U2472	U2473	U2474	U2475	U2476	U2477	U2478	U2479	U2480	U2481	U2482	U2483	U2484	U2485	U2486	U2487	U2488	U2																																																																																																																					



• Molecule 59: 50S ribosomal protein L5

Chain DF:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.46Å 434.08Å 621.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.15 – 3.19 82.15 – 3.19	Depositor EDS
% Data completeness (in resolution range)	75.8 (82.15-3.19) 75.8 (82.15-3.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.191 , 0.252 0.204 , 0.263	Depositor DCC
R_{free} test set	14299 reflections (2.06%)	DCC
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 759111 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	284499	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLM, 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	AA	0.50	6/36834 (0.0%)	1.27	532/57462 (0.9%)
2	AB	0.40	2/1736 (0.1%)	0.57	4/2338 (0.2%)
2	CB	0.37	2/1736 (0.1%)	0.54	4/2338 (0.2%)
3	AC	0.26	0/1652	0.50	0/2225
3	CC	0.23	0/1652	0.44	0/2225
4	AD	0.29	0/1665	0.52	0/2227
4	CD	0.34	0/1665	0.57	0/2227
5	AE	0.37	1/1119 (0.1%)	0.59	0/1504
5	CE	0.31	0/1119	0.55	0/1504
6	AF	0.28	0/836	0.49	0/1128
6	CF	0.27	0/836	0.50	0/1128
7	AG	0.23	0/1196	0.46	0/1602
8	AH	0.29	0/989	0.54	0/1326
8	CH	0.26	0/989	0.49	0/1326
9	AI	0.23	0/1034	0.47	0/1375
9	CI	0.22	0/1034	0.42	0/1375
10	AJ	0.24	0/797	0.49	0/1077
10	CJ	0.22	0/797	0.47	0/1077
11	AK	0.27	0/893	0.52	0/1205
11	CK	0.25	0/893	0.51	0/1205
12	AL	0.36	0/969	0.67	0/1300
12	CL	0.40	1/969 (0.1%)	0.56	0/1300
13	AM	0.22	0/893	0.47	0/1193
14	AN	0.25	0/785	0.49	0/1043
14	CN	0.21	0/780	0.39	0/1036
15	AO	0.27	0/722	0.47	0/964
15	CO	0.25	0/722	0.45	0/964
16	AP	0.28	0/659	0.49	0/884
17	AQ	0.35	0/658	0.56	0/881
17	CQ	0.27	0/658	0.51	0/881
18	AR	0.28	0/463	0.50	0/621
18	CR	0.28	0/463	0.46	0/621

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	AS	0.23	0/653	0.47	0/877
19	CS	0.21	0/653	0.42	0/877
20	AT	0.30	0/671	0.57	0/888
20	CT	0.25	0/671	0.50	0/888
21	AU	0.28	0/431	0.49	0/570
21	CU	0.31	0/431	0.60	0/570
22	BA	0.71	8/68626 (0.0%)	1.50	1274/107056 (1.2%)
23	BB	0.64	0/2828	1.43	38/4410 (0.9%)
24	BC	0.41	0/2122	0.69	1/2852 (0.0%)
24	DC	0.29	0/2122	0.53	0/2852
25	BD	0.48	0/1586	0.76	2/2134 (0.1%)
25	DD	0.28	0/1586	0.57	0/2134
26	BE	0.40	0/1571	0.66	1/2113 (0.0%)
26	DE	0.25	0/1571	0.47	0/2113
27	BF	0.31	0/1435	0.54	0/1926
28	BG	0.33	0/1343	0.60	0/1816
28	DG	0.22	0/1343	0.46	0/1816
29	BH	0.30	0/1122	0.50	0/1515
29	DH	0.34	1/1122 (0.1%)	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	0.51	0/1152	0.75	0/1551
31	DJ	0.26	0/1152	0.57	1/1551 (0.1%)
32	BK	0.46	0/948	0.78	0/1268
32	DK	0.29	0/948	0.55	0/1268
33	BL	0.42	0/1054	0.75	1/1403 (0.1%)
33	DL	0.24	0/1054	0.51	0/1403
34	BM	0.44	0/1093	0.67	0/1460
34	DM	0.27	0/1093	0.48	0/1460
35	BN	0.45	0/974	0.70	1/1301 (0.1%)
35	DN	0.27	0/974	0.51	0/1301
36	BO	0.38	0/902	0.60	0/1209
36	DO	0.22	0/902	0.42	0/1209
37	BP	0.43	0/929	0.71	0/1242
37	DP	0.28	0/929	0.49	0/1242
38	BQ	0.52	0/960	0.76	0/1278
38	DQ	0.26	0/960	0.44	0/1278
39	BR	0.54	0/829	0.77	1/1107 (0.1%)
39	DR	0.25	0/829	0.48	0/1107
40	BS	0.50	0/864	0.73	0/1156
40	DS	0.27	0/864	0.51	0/1156
41	BT	0.43	0/745	0.71	0/994
41	DT	0.22	0/745	0.48	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
42	BU	0.39	0/788	0.70	0/1051
42	DU	0.23	0/788	0.46	0/1051
43	BV	0.39	0/766	0.61	0/1025
43	DV	0.23	0/766	0.43	0/1025
44	BW	0.53	0/603	0.82	0/797
44	DW	0.25	0/603	0.49	0/797
45	BX	0.37	0/635	0.66	0/848
45	DX	0.27	0/635	0.56	0/848
46	BY	0.33	0/510	0.62	0/677
46	DY	0.21	0/510	0.43	0/677
47	BZ	0.45	0/453	0.80	0/605
47	DZ	0.25	0/453	0.50	0/605
48	B0	0.43	0/450	0.71	0/599
48	D0	0.26	0/450	0.50	0/599
49	B1	0.31	0/417	0.57	0/554
49	D1	0.24	0/417	0.45	0/554
50	B2	0.41	0/380	0.71	0/498
50	D2	0.26	0/380	0.51	0/498
51	B3	0.43	0/513	0.66	0/676
51	D3	0.27	0/513	0.52	0/676
52	B4	0.39	0/303	0.69	0/397
52	D4	0.43	0/303	0.54	0/397
53	CA	0.47	6/36762 (0.0%)	1.24	525/57350 (0.9%)
54	CG	0.22	0/1188	0.44	0/1591
55	CM	0.19	0/885	0.41	0/1181
56	CP	0.28	0/649	0.52	0/870
57	DA	0.46	0/68314	1.28	1097/106569 (1.0%)
58	DB	0.51	1/2803 (0.0%)	1.21	38/4371 (0.9%)
59	DF	0.23	0/1444	0.48	0/1937
All	All	0.50	28/306773 (0.0%)	1.19	3520/458565 (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
2	CB	0	1
25	BD	0	1
35	BN	0	1
All	All	0	3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	DB	69	G	O3'-P	-16.79	1.41	1.61
1	AA	1047	G	O3'-P	-14.49	1.43	1.61
2	AB	107	ARG	C-N	11.33	1.60	1.34
53	CA	1396	A	O3'-P	-11.26	1.47	1.61
2	CB	146	SER	C-N	10.14	1.57	1.34

The worst 5 of 3520 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	CA	1396	A	P-O3'-C3'	16.36	139.33	119.70
57	DA	2586	U	N1-C1'-C2'	-15.75	93.52	114.00
22	BA	2283	C	N1-C1'-C2'	-15.29	94.12	114.00
57	DA	1997	C	N1-C1'-C2'	-14.86	94.69	114.00
23	BB	90	C	N1-C1'-C2'	-14.66	94.94	114.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	BD	9	VAL	Peptide
35	BN	101	GLY	Peptide
2	CB	107	ARG	Mainchain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32895	0	16553	1473	0
2	AB	1705	0	1732	195	0
2	CB	1705	0	1732	176	0
3	AC	1625	0	1699	121	0
3	CC	1625	0	1699	127	0
4	AD	1643	0	1710	166	0
4	CD	1643	0	1710	177	0
5	AE	1106	0	1147	146	0
5	CE	1106	0	1148	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AF	818	0	808	76	0
6	CF	818	0	808	74	0
7	AG	1182	0	1240	89	0
8	AH	979	0	1034	102	0
8	CH	979	0	1034	115	0
9	AI	1022	0	1070	91	0
9	CI	1022	0	1070	108	0
10	AJ	787	0	828	83	0
10	CJ	787	0	828	93	0
11	AK	877	0	887	91	0
11	CK	877	0	887	79	0
12	AL	955	0	1019	92	0
12	CL	955	0	1019	100	0
13	AM	884	0	944	70	0
14	AN	774	0	827	81	0
14	CN	769	0	822	85	0
15	AO	714	0	737	59	0
15	CO	714	0	737	58	0
16	AP	649	0	666	62	0
17	AQ	649	0	691	81	0
17	CQ	649	0	691	70	0
18	AR	456	0	478	31	0
18	CR	456	0	478	47	0
19	AS	638	0	665	47	0
19	CS	638	0	665	64	0
20	AT	665	0	714	65	0
20	CT	665	0	714	61	0
21	AU	426	0	449	79	0
21	CU	426	0	449	80	0
22	BA	61274	0	30819	2356	0
23	BB	2529	0	1281	83	0
24	BC	2083	0	2157	223	0
24	DC	2083	0	2157	262	0
25	BD	1565	0	1616	223	0
25	DD	1565	0	1616	197	0
26	BE	1552	0	1619	152	0
26	DE	1552	0	1619	179	0
27	BF	1411	0	1447	140	0
28	BG	1323	0	1374	147	0
28	DG	1323	0	1374	131	0
29	BH	1111	0	1148	107	0
29	DH	1111	0	1148	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	BI	1032	0	1088	109	0
30	DI	1032	0	1088	76	0
31	BJ	1129	0	1162	171	0
31	DJ	1129	0	1162	133	0
32	BK	939	0	1012	113	0
32	DK	939	0	1012	128	0
33	BL	1045	0	1117	122	0
33	DL	1045	0	1117	117	0
34	BM	1074	0	1157	99	0
34	DM	1074	0	1157	107	0
35	BN	961	0	1000	96	0
35	DN	961	0	1000	134	0
36	BO	892	0	923	75	0
36	DO	892	0	923	71	0
37	BP	917	0	965	139	0
37	DP	917	0	965	130	0
38	BQ	947	0	1022	153	0
38	DQ	947	0	1022	124	0
39	BR	816	0	839	116	0
39	DR	816	0	839	87	0
40	BS	857	0	922	81	0
40	DS	857	0	922	78	0
41	BT	739	0	807	112	0
41	DT	739	0	807	108	0
42	BU	780	0	834	52	0
42	DU	780	0	834	92	0
43	BV	753	0	780	70	0
43	DV	753	0	780	71	0
44	BW	596	0	610	201	0
44	DW	596	0	610	117	0
45	BX	625	0	655	67	0
45	DX	625	0	655	85	0
46	BY	509	0	543	44	0
46	DY	509	0	543	63	0
47	BZ	449	0	491	39	0
47	DZ	449	0	491	42	0
48	B0	444	0	461	33	0
48	D0	444	0	461	64	0
49	B1	410	0	440	38	0
49	D1	410	0	440	38	0
50	B2	377	0	418	37	0
50	D2	377	0	418	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	B3	504	0	574	46	0
51	D3	504	0	574	56	0
52	B4	302	0	340	39	0
52	D4	302	0	343	36	0
53	CA	32831	0	16521	1811	0
54	CG	1175	0	1230	125	0
55	CM	877	0	937	97	0
56	CP	639	0	656	71	0
57	DA	60995	0	30679	3815	0
58	DB	2507	0	1270	168	0
59	DF	1420	0	1460	194	0
60	AA	42	0	0	0	0
60	AN	1	0	0	0	0
60	BA	135	0	0	0	0
60	BB	4	0	0	0	0
60	BL	1	0	0	0	0
60	CA	42	0	0	0	0
60	DA	133	0	0	0	0
60	DB	1	0	0	0	0
60	DC	1	0	0	0	0
60	DE	1	0	0	0	0
60	DJ	1	0	0	0	0
61	BA	20	0	11	1	0
62	B4	1	0	0	0	0
62	D4	1	0	0	0	0
63	AA	197	0	0	11	0
63	AL	2	0	0	0	0
63	AN	6	0	0	1	0
63	AT	2	0	0	0	0
63	AU	1	0	0	0	0
63	B2	2	0	0	0	0
63	B3	2	0	0	0	0
63	B4	2	0	0	0	0
63	BA	608	0	0	43	0
63	BB	19	0	0	0	0
63	BC	8	0	0	0	0
63	BD	2	0	0	3	0
63	BE	1	0	0	0	0
63	BL	4	0	0	1	0
63	BN	2	0	0	0	0
63	BQ	1	0	0	0	0
63	BT	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	BV	1	0	0	1	0
63	CA	195	0	0	7	0
63	CE	3	0	0	1	0
63	CI	1	0	0	0	0
63	CL	1	0	0	0	0
63	CN	3	0	0	0	0
63	CT	2	0	0	0	0
63	CU	2	0	0	0	0
63	D2	1	0	0	1	0
63	D3	1	0	0	0	0
63	D4	4	0	0	0	0
63	DA	603	0	0	19	0
63	DB	4	0	0	0	0
63	DC	10	0	0	0	0
63	DD	1	0	0	0	0
63	DE	3	0	0	0	0
63	DJ	4	0	0	0	0
63	DL	5	0	0	0	0
63	DN	2	0	0	0	0
63	DT	2	0	0	0	0
63	DU	2	0	0	0	0
63	DV	1	0	0	0	0
All	All	284499	0	190851	17927	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

The worst 5 of 17927 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
57:DA:2092:U:H1'	57:DA:2093:G:C8	1.52	1.43
38:BQ:63:ARG:NH1	38:BQ:96:ASP:HA	1.44	1.29
57:DA:2092:U:O2'	57:DA:2093:G:H5''	1.08	1.24
38:BQ:63:ARG:HH12	38:BQ:96:ASP:CA	1.55	1.20
28:BG:83:THR:HA	28:BG:84:LYS:NZ	1.57	1.19

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	132 (61%)	55 (26%)	29 (13%)	0	2
2	CB	216/218 (99%)	149 (69%)	49 (23%)	18 (8%)	1	9
3	AC	204/206 (99%)	153 (75%)	34 (17%)	17 (8%)	1	9
3	CC	204/206 (99%)	145 (71%)	39 (19%)	20 (10%)	1	7
4	AD	203/205 (99%)	133 (66%)	43 (21%)	27 (13%)	0	2
4	CD	203/205 (99%)	138 (68%)	42 (21%)	23 (11%)	1	4
5	AE	148/150 (99%)	103 (70%)	28 (19%)	17 (12%)	1	4
5	CE	148/150 (99%)	106 (72%)	24 (16%)	18 (12%)	1	3
6	AF	98/100 (98%)	71 (72%)	20 (20%)	7 (7%)	2	13
6	CF	98/100 (98%)	68 (69%)	19 (19%)	11 (11%)	1	4
7	AG	149/151 (99%)	108 (72%)	35 (24%)	6 (4%)	5	32
8	AH	127/129 (98%)	94 (74%)	27 (21%)	6 (5%)	4	27
8	CH	127/129 (98%)	89 (70%)	29 (23%)	9 (7%)	2	13
9	AI	125/127 (98%)	84 (67%)	30 (24%)	11 (9%)	1	8
9	CI	125/127 (98%)	90 (72%)	23 (18%)	12 (10%)	1	7
10	AJ	96/98 (98%)	70 (73%)	16 (17%)	10 (10%)	1	5
10	CJ	96/98 (98%)	55 (57%)	26 (27%)	15 (16%)	0	1
11	AK	115/117 (98%)	86 (75%)	20 (17%)	9 (8%)	1	11
11	CK	115/117 (98%)	86 (75%)	20 (17%)	9 (8%)	1	11
12	AL	121/123 (98%)	88 (73%)	16 (13%)	17 (14%)	0	2
12	CL	121/123 (98%)	83 (69%)	30 (25%)	8 (7%)	2	16
13	AM	112/114 (98%)	84 (75%)	19 (17%)	9 (8%)	1	10
14	AN	92/100 (92%)	58 (63%)	22 (24%)	12 (13%)	0	3
14	CN	91/100 (91%)	60 (66%)	26 (29%)	5 (6%)	3	23
15	AO	86/88 (98%)	62 (72%)	13 (15%)	11 (13%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	6	37
16	AP	80/82 (98%)	56 (70%)	15 (19%)	9 (11%)	1	4
17	AQ	78/80 (98%)	55 (70%)	11 (14%)	12 (15%)	0	1
17	CQ	78/80 (98%)	61 (78%)	8 (10%)	9 (12%)	1	4
18	AR	53/55 (96%)	41 (77%)	10 (19%)	2 (4%)	5	34
18	CR	53/55 (96%)	42 (79%)	10 (19%)	1 (2%)	12	59
19	AS	77/79 (98%)	59 (77%)	12 (16%)	6 (8%)	1	11
19	CS	77/79 (98%)	46 (60%)	24 (31%)	7 (9%)	1	8
20	AT	83/85 (98%)	65 (78%)	10 (12%)	8 (10%)	1	7
20	CT	83/85 (98%)	61 (74%)	13 (16%)	9 (11%)	1	5
21	AU	49/51 (96%)	26 (53%)	15 (31%)	8 (16%)	0	1
21	CU	49/51 (96%)	21 (43%)	12 (24%)	16 (33%)	0	0
24	BC	269/271 (99%)	180 (67%)	61 (23%)	28 (10%)	1	5
24	DC	269/271 (99%)	164 (61%)	72 (27%)	33 (12%)	1	3
25	BD	207/209 (99%)	141 (68%)	37 (18%)	29 (14%)	0	2
25	DD	207/209 (99%)	134 (65%)	41 (20%)	32 (16%)	0	1
26	BE	199/201 (99%)	148 (74%)	31 (16%)	20 (10%)	1	6
26	DE	199/201 (99%)	120 (60%)	54 (27%)	25 (13%)	0	3
27	BF	175/177 (99%)	127 (73%)	29 (17%)	19 (11%)	1	5
28	BG	174/176 (99%)	116 (67%)	34 (20%)	24 (14%)	0	2
28	DG	174/176 (99%)	104 (60%)	39 (22%)	31 (18%)	0	1
29	BH	147/149 (99%)	63 (43%)	52 (35%)	32 (22%)	0	0
29	DH	147/149 (99%)	73 (50%)	53 (36%)	21 (14%)	0	2
30	BI	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	1	6
30	DI	139/141 (99%)	83 (60%)	38 (27%)	18 (13%)	0	3
31	BJ	140/142 (99%)	106 (76%)	20 (14%)	14 (10%)	1	6
31	DJ	140/142 (99%)	92 (66%)	30 (21%)	18 (13%)	0	3
32	BK	120/122 (98%)	83 (69%)	20 (17%)	17 (14%)	0	2
32	DK	120/122 (98%)	77 (64%)	21 (18%)	22 (18%)	0	1
33	BL	141/143 (99%)	95 (67%)	30 (21%)	16 (11%)	1	4
33	DL	141/143 (99%)	78 (55%)	42 (30%)	21 (15%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BM	134/136 (98%)	96 (72%)	24 (18%)	14 (10%)	1	5
34	DM	134/136 (98%)	94 (70%)	25 (19%)	15 (11%)	1	4
35	BN	118/120 (98%)	88 (75%)	20 (17%)	10 (8%)	1	9
35	DN	118/120 (98%)	67 (57%)	35 (30%)	16 (14%)	0	2
36	BO	114/116 (98%)	88 (77%)	17 (15%)	9 (8%)	1	11
36	DO	114/116 (98%)	79 (69%)	27 (24%)	8 (7%)	2	13
37	BP	112/114 (98%)	74 (66%)	23 (20%)	15 (13%)	0	2
37	DP	112/114 (98%)	66 (59%)	28 (25%)	18 (16%)	0	1
38	BQ	115/117 (98%)	99 (86%)	9 (8%)	7 (6%)	2	19
38	DQ	115/117 (98%)	78 (68%)	24 (21%)	13 (11%)	1	4
39	BR	101/103 (98%)	82 (81%)	11 (11%)	8 (8%)	1	11
39	DR	101/103 (98%)	70 (69%)	21 (21%)	10 (10%)	1	7
40	BS	108/110 (98%)	83 (77%)	16 (15%)	9 (8%)	1	9
40	DS	108/110 (98%)	76 (70%)	24 (22%)	8 (7%)	2	12
41	BT	91/93 (98%)	58 (64%)	20 (22%)	13 (14%)	0	2
41	DT	91/93 (98%)	49 (54%)	26 (29%)	16 (18%)	0	1
42	BU	100/102 (98%)	70 (70%)	16 (16%)	14 (14%)	0	2
42	DU	100/102 (98%)	51 (51%)	27 (27%)	22 (22%)	0	0
43	BV	92/94 (98%)	77 (84%)	14 (15%)	1 (1%)	21	72
43	DV	92/94 (98%)	65 (71%)	22 (24%)	5 (5%)	3	24
44	BW	77/79 (98%)	31 (40%)	18 (23%)	28 (36%)	0	0
44	DW	77/79 (98%)	32 (42%)	26 (34%)	19 (25%)	0	0
45	BX	75/77 (97%)	58 (77%)	13 (17%)	4 (5%)	3	24
45	DX	75/77 (97%)	48 (64%)	19 (25%)	8 (11%)	1	5
46	BY	61/63 (97%)	40 (66%)	13 (21%)	8 (13%)	0	2
46	DY	61/63 (97%)	43 (70%)	13 (21%)	5 (8%)	1	10
47	BZ	56/58 (97%)	43 (77%)	10 (18%)	3 (5%)	3	24
47	DZ	56/58 (97%)	34 (61%)	16 (29%)	6 (11%)	1	5
48	B0	54/56 (96%)	42 (78%)	7 (13%)	5 (9%)	1	8
48	D0	54/56 (96%)	40 (74%)	7 (13%)	7 (13%)	0	3
49	B1	48/50 (96%)	35 (73%)	10 (21%)	3 (6%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	D1	48/50 (96%)	37 (77%)	6 (12%)	5 (10%)	1	5
50	B2	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	10	52
50	D2	44/46 (96%)	30 (68%)	7 (16%)	7 (16%)	0	1
51	B3	62/64 (97%)	51 (82%)	8 (13%)	3 (5%)	4	27
51	D3	62/64 (97%)	40 (64%)	17 (27%)	5 (8%)	1	10
52	B4	36/38 (95%)	27 (75%)	6 (17%)	3 (8%)	1	9
52	D4	36/38 (95%)	22 (61%)	9 (25%)	5 (14%)	0	2
54	CG	148/150 (99%)	98 (66%)	42 (28%)	8 (5%)	3	24
55	CM	111/113 (98%)	63 (57%)	36 (32%)	12 (11%)	1	5
56	CP	78/80 (98%)	49 (63%)	19 (24%)	10 (13%)	0	3
59	DF	176/178 (99%)	98 (56%)	44 (25%)	34 (19%)	0	0
All	All	11238/11447 (98%)	7571 (67%)	2387 (21%)	1280 (11%)	1	4

5 of 1280 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	20	ARG
2	AB	40	ILE
2	AB	72	LYS
2	AB	75	ALA
2	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	
2	AB	180/180 (100%)	142 (79%)	38 (21%)	1	8
2	CB	180/180 (100%)	156 (87%)	24 (13%)	6	27
3	AC	170/170 (100%)	142 (84%)	28 (16%)	3	14
3	CC	170/170 (100%)	152 (89%)	18 (11%)	10	38
4	AD	172/172 (100%)	146 (85%)	26 (15%)	4	19
4	CD	172/172 (100%)	140 (81%)	32 (19%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	113/113 (100%)	90 (80%)	23 (20%)	2	8
5	CE	113/113 (100%)	94 (83%)	19 (17%)	3	14
6	AF	87/87 (100%)	75 (86%)	12 (14%)	5	24
6	CF	87/87 (100%)	75 (86%)	12 (14%)	5	24
7	AG	124/124 (100%)	108 (87%)	16 (13%)	6	28
8	AH	104/104 (100%)	87 (84%)	17 (16%)	3	15
8	CH	104/104 (100%)	87 (84%)	17 (16%)	3	15
9	AI	105/105 (100%)	84 (80%)	21 (20%)	2	9
9	CI	105/105 (100%)	89 (85%)	16 (15%)	4	19
10	AJ	86/86 (100%)	72 (84%)	14 (16%)	3	15
10	CJ	86/86 (100%)	77 (90%)	9 (10%)	10	39
11	AK	90/90 (100%)	73 (81%)	17 (19%)	2	11
11	CK	90/90 (100%)	77 (86%)	13 (14%)	5	22
12	AL	103/103 (100%)	82 (80%)	21 (20%)	2	8
12	CL	103/103 (100%)	86 (84%)	17 (16%)	3	14
13	AM	92/92 (100%)	87 (95%)	5 (5%)	31	75
14	AN	79/83 (95%)	72 (91%)	7 (9%)	14	49
14	CN	79/83 (95%)	67 (85%)	12 (15%)	4	19
15	AO	76/76 (100%)	67 (88%)	9 (12%)	8	33
15	CO	76/76 (100%)	69 (91%)	7 (9%)	13	47
16	AP	65/65 (100%)	57 (88%)	8 (12%)	7	31
17	AQ	74/74 (100%)	58 (78%)	16 (22%)	1	7
17	CQ	74/74 (100%)	61 (82%)	13 (18%)	3	13
18	AR	48/48 (100%)	46 (96%)	2 (4%)	40	82
18	CR	48/48 (100%)	44 (92%)	4 (8%)	16	55
19	AS	70/70 (100%)	61 (87%)	9 (13%)	6	28
19	CS	70/70 (100%)	62 (89%)	8 (11%)	8	35
20	AT	65/65 (100%)	49 (75%)	16 (25%)	1	3
20	CT	65/65 (100%)	53 (82%)	12 (18%)	2	11
21	AU	44/44 (100%)	33 (75%)	11 (25%)	1	3
21	CU	44/44 (100%)	33 (75%)	11 (25%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	BC	216/216 (100%)	169 (78%)	47 (22%)	1	7
24	DC	216/216 (100%)	189 (88%)	27 (12%)	7	30
25	BD	164/164 (100%)	131 (80%)	33 (20%)	2	9
25	DD	164/164 (100%)	141 (86%)	23 (14%)	5	23
26	BE	165/165 (100%)	123 (74%)	42 (26%)	1	3
26	DE	165/165 (100%)	147 (89%)	18 (11%)	9	37
27	BF	148/148 (100%)	127 (86%)	21 (14%)	5	22
28	BG	137/137 (100%)	108 (79%)	29 (21%)	1	8
28	DG	137/137 (100%)	118 (86%)	19 (14%)	5	24
29	BH	114/114 (100%)	96 (84%)	18 (16%)	4	16
29	DH	114/114 (100%)	94 (82%)	20 (18%)	3	13
30	BI	109/109 (100%)	91 (84%)	18 (16%)	3	14
30	DI	109/109 (100%)	102 (94%)	7 (6%)	25	69
31	BJ	116/116 (100%)	87 (75%)	29 (25%)	1	3
31	DJ	116/116 (100%)	102 (88%)	14 (12%)	7	32
32	BK	103/103 (100%)	86 (84%)	17 (16%)	3	14
32	DK	103/103 (100%)	81 (79%)	22 (21%)	1	7
33	BL	102/102 (100%)	77 (76%)	25 (24%)	1	3
33	DL	102/102 (100%)	87 (85%)	15 (15%)	4	21
34	BM	109/109 (100%)	85 (78%)	24 (22%)	1	7
34	DM	109/109 (100%)	97 (89%)	12 (11%)	9	36
35	BN	100/100 (100%)	77 (77%)	23 (23%)	1	5
35	DN	100/100 (100%)	82 (82%)	18 (18%)	2	12
36	BO	86/86 (100%)	69 (80%)	17 (20%)	2	9
36	DO	86/86 (100%)	79 (92%)	7 (8%)	17	56
37	BP	99/99 (100%)	69 (70%)	30 (30%)	0	1
37	DP	99/99 (100%)	88 (89%)	11 (11%)	9	36
38	BQ	89/89 (100%)	75 (84%)	14 (16%)	4	17
38	DQ	89/89 (100%)	75 (84%)	14 (16%)	4	17
39	BR	84/84 (100%)	68 (81%)	16 (19%)	2	11
39	DR	84/84 (100%)	71 (84%)	13 (16%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	BS	93/93 (100%)	71 (76%)	22 (24%)	1	4
40	DS	93/93 (100%)	77 (83%)	16 (17%)	3	14
41	BT	80/80 (100%)	59 (74%)	21 (26%)	1	2
41	DT	80/80 (100%)	74 (92%)	6 (8%)	19	61
42	BU	83/83 (100%)	66 (80%)	17 (20%)	2	8
42	DU	83/83 (100%)	72 (87%)	11 (13%)	6	27
43	BV	78/78 (100%)	59 (76%)	19 (24%)	1	3
43	DV	78/78 (100%)	67 (86%)	11 (14%)	5	23
44	BW	59/59 (100%)	42 (71%)	17 (29%)	0	1
44	DW	59/59 (100%)	46 (78%)	13 (22%)	1	7
45	BX	67/67 (100%)	51 (76%)	16 (24%)	1	4
45	DX	67/67 (100%)	58 (87%)	9 (13%)	6	26
46	BY	55/55 (100%)	42 (76%)	13 (24%)	1	4
46	DY	55/55 (100%)	52 (94%)	3 (6%)	30	75
47	BZ	48/48 (100%)	34 (71%)	14 (29%)	0	1
47	DZ	48/48 (100%)	40 (83%)	8 (17%)	3	14
48	B0	47/47 (100%)	38 (81%)	9 (19%)	2	11
48	D0	47/47 (100%)	40 (85%)	7 (15%)	4	20
49	B1	45/45 (100%)	36 (80%)	9 (20%)	2	9
49	D1	45/45 (100%)	41 (91%)	4 (9%)	14	49
50	B2	38/38 (100%)	31 (82%)	7 (18%)	2	11
50	D2	38/38 (100%)	34 (90%)	4 (10%)	10	39
51	B3	51/51 (100%)	44 (86%)	7 (14%)	5	25
51	D3	51/51 (100%)	42 (82%)	9 (18%)	3	13
52	B4	34/34 (100%)	29 (85%)	5 (15%)	4	21
52	D4	34/34 (100%)	27 (79%)	7 (21%)	2	8
54	CG	123/123 (100%)	101 (82%)	22 (18%)	2	12
55	CM	91/91 (100%)	80 (88%)	11 (12%)	7	32
56	CP	65/65 (100%)	52 (80%)	13 (20%)	2	9
59	DF	149/149 (100%)	123 (83%)	26 (17%)	3	13
All	All	9331/9339 (100%)	7772 (83%)	1559 (17%)	3	14

5 of 1559 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	BR	25	LEU
49	B1	35	LEU
39	DR	13	ARG
40	BS	33	LEU
43	BV	43	ASP

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

Mol	Chain	Res	Type
41	BT	72	GLN
3	CC	7	ASN
41	DT	48	GLN
43	BV	5	ASN
50	B2	6	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	478 (31%)	237 (15%)
22	BA	2850/2903 (98%)	829 (29%)	411 (14%)
23	BB	117/118 (99%)	31 (26%)	17 (14%)
53	CA	1529/1530 (99%)	540 (35%)	242 (15%)
57	DA	2838/2904 (97%)	1042 (36%)	504 (17%)
58	DB	116/117 (99%)	37 (31%)	17 (14%)
All	All	8982/9105 (98%)	2957 (32%)	1428 (15%)

5 of 2957 RNA backbone outliers are listed below:

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

5 of 1428 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2880	C

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Mol	Chain	Res	Type
53	CA	816	A
57	DA	2289	G
23	BB	109	A
53	CA	331	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 365 ligands modelled in this entry, 364 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	CLM	BA	3136	-	20,20,20	2.58	5 (25%)	27,27,27	2.12	10 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	CLM	BA	3136	-	-	0/22/22/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BA	3136	CLM	O9B-N9	6.43	1.35	1.22
61	BA	3136	CLM	O9A-N9	5.51	1.35	1.25
61	BA	3136	CLM	C11-C6	5.34	1.47	1.39
61	BA	3136	CLM	C2-N2	3.83	1.42	1.34
61	BA	3136	CLM	C8-C9	2.40	1.43	1.38

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	BA	3136	CLM	C3-N2-C2	-4.91	114.11	123.24
61	BA	3136	CLM	O9B-N9-C9	4.73	122.08	118.62
61	BA	3136	CLM	C6-C5-C3	4.26	119.68	111.62
61	BA	3136	CLM	O4-C4-C3	2.81	118.37	111.17
61	BA	3136	CLM	C4-C3-N2	2.69	114.10	109.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	AA	1533/1533 (100%)	-0.70	15 (0%) 79 29	28, 82, 201, 415	0
2	AB	218/218 (100%)	0.88	24 (11%) 6 2	117, 160, 233, 278	0
2	CB	218/218 (100%)	0.62	9 (4%) 35 7	121, 173, 237, 292	0
3	AC	206/206 (100%)	0.16	3 (1%) 70 21	64, 107, 164, 196	0
3	CC	206/206 (100%)	0.57	14 (6%) 17 4	79, 158, 229, 303	0
4	AD	205/205 (100%)	-0.12	2 (0%) 79 29	45, 89, 164, 275	0
4	CD	205/205 (100%)	-0.23	0 100 100	39, 61, 122, 254	0
5	AE	150/150 (100%)	-0.13	0 100 100	57, 81, 142, 210	0
5	CE	150/150 (100%)	0.13	0 100 100	67, 99, 157, 252	0
6	AF	100/100 (100%)	-0.00	0 100 100	55, 103, 161, 189	0
6	CF	100/100 (100%)	-0.09	0 100 100	72, 116, 176, 217	0
7	AG	151/151 (100%)	0.24	2 (1%) 74 24	88, 150, 218, 247	0
8	AH	129/129 (100%)	-0.01	0 100 100	44, 82, 127, 184	0
8	CH	129/129 (100%)	0.31	1 (0%) 83 35	68, 113, 170, 246	0
9	AI	127/127 (100%)	0.63	9 (7%) 16 4	72, 154, 248, 287	0
9	CI	127/127 (100%)	1.12	26 (20%) 1 1	116, 201, 289, 319	0
10	AJ	98/98 (100%)	0.40	4 (4%) 35 7	78, 127, 203, 244	0
10	CJ	98/98 (100%)	1.43	26 (26%) 1 1	114, 204, 278, 301	0
11	AK	117/117 (100%)	0.37	2 (1%) 67 19	47, 117, 196, 238	0
11	CK	117/117 (100%)	0.10	1 (0%) 81 32	68, 117, 175, 239	0
12	AL	123/123 (100%)	-0.16	1 (0%) 83 35	24, 57, 121, 180	0
12	CL	123/123 (100%)	0.22	2 (1%) 68 20	44, 89, 144, 226	0
13	AM	114/114 (100%)	0.28	3 (2%) 53 11	90, 158, 240, 281	0
14	AN	96/100 (96%)	0.39	5 (5%) 26 5	76, 122, 214, 271	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	CN	95/100 (95%)	1.51	24 (25%) 1 1	123, 239, 369, 399	0
15	AO	88/88 (100%)	-0.26	0 100 100	40, 81, 123, 187	0
15	CO	88/88 (100%)	-0.07	0 100 100	76, 122, 190, 265	0
16	AP	82/82 (100%)	0.19	3 (3%) 39 8	46, 79, 155, 228	0
17	AQ	80/80 (100%)	0.16	3 (3%) 38 7	36, 79, 146, 244	0
17	CQ	80/80 (100%)	0.51	5 (6%) 19 4	61, 112, 163, 194	0
18	AR	55/55 (100%)	0.01	2 (3%) 41 8	60, 92, 174, 242	0
18	CR	55/55 (100%)	-0.05	0 100 100	48, 91, 159, 236	0
19	AS	79/79 (100%)	0.63	5 (6%) 19 4	95, 156, 236, 256	0
19	CS	79/79 (100%)	1.62	29 (36%) 1 0	206, 416, 490, 515	0
20	AT	85/85 (100%)	-0.15	0 100 100	46, 83, 124, 174	0
20	CT	85/85 (100%)	0.75	4 (4%) 30 6	76, 142, 200, 234	0
21	AU	51/51 (100%)	1.14	11 (21%) 1 1	91, 152, 216, 243	0
21	CU	51/51 (100%)	0.42	3 (5%) 22 5	82, 115, 208, 290	0
22	BA	2854/2903 (98%)	-0.63	35 (1%) 75 26	7, 31, 162, 401	0
23	BB	118/118 (100%)	-0.76	0 100 100	20, 45, 78, 115	0
24	BC	271/271 (100%)	-0.28	0 100 100	13, 41, 96, 201	0
24	DC	271/271 (100%)	0.36	12 (4%) 33 7	45, 101, 160, 200	0
25	BD	209/209 (100%)	-0.34	0 100 100	7, 29, 80, 144	0
25	DD	209/209 (100%)	0.52	11 (5%) 25 5	60, 123, 193, 270	0
26	BE	201/201 (100%)	-0.27	0 100 100	7, 42, 105, 189	0
26	DE	201/201 (100%)	1.05	45 (22%) 1 1	68, 254, 429, 475	0
27	BF	177/177 (100%)	-0.03	3 (1%) 67 19	33, 78, 142, 205	0
28	BG	176/176 (100%)	-0.17	0 100 100	23, 62, 124, 215	0
28	DG	176/176 (100%)	1.14	31 (17%) 2 1	79, 207, 297, 363	0
29	BH	149/149 (100%)	1.46	44 (29%) 1 1	41, 178, 274, 301	0
29	DH	149/149 (100%)	1.51	39 (26%) 1 1	93, 182, 270, 305	0
30	BI	141/141 (100%)	1.40	26 (18%) 2 1	171, 257, 316, 355	0
30	DI	141/141 (100%)	2.17	62 (43%) 1 0	227, 344, 382, 400	0
31	BJ	142/142 (100%)	-0.38	0 100 100	9, 23, 68, 127	0
31	DJ	142/142 (100%)	0.34	6 (4%) 35 7	63, 122, 184, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
32	BK	122/122 (100%)	-0.38	0 100 100	14, 31, 84, 254	0
32	DK	122/122 (100%)	0.47	4 (3%) 44 9	57, 106, 172, 204	0
33	BL	143/143 (100%)	-0.37	0 100 100	9, 37, 80, 126	0
33	DL	143/143 (100%)	0.86	18 (12%) 4 1	68, 176, 296, 329	0
34	BM	136/136 (100%)	-0.41	0 100 100	9, 29, 71, 133	0
34	DM	136/136 (100%)	0.47	7 (5%) 27 5	47, 126, 187, 223	0
35	BN	120/120 (100%)	-0.38	0 100 100	10, 25, 48, 123	0
35	DN	120/120 (100%)	0.98	19 (15%) 3 1	90, 149, 231, 305	0
36	BO	116/116 (100%)	-0.26	0 100 100	28, 49, 93, 126	0
36	DO	116/116 (100%)	0.87	12 (10%) 7 2	132, 176, 238, 280	0
37	BP	114/114 (100%)	-0.26	0 100 100	17, 39, 95, 184	0
37	DP	114/114 (100%)	0.58	8 (7%) 16 4	63, 122, 187, 204	0
38	BQ	117/117 (100%)	-0.45	0 100 100	7, 20, 46, 100	0
38	DQ	117/117 (100%)	0.66	8 (6%) 17 4	78, 127, 221, 298	0
39	BR	103/103 (100%)	-0.39	0 100 100	7, 34, 78, 139	0
39	DR	103/103 (100%)	1.22	25 (24%) 1 1	80, 157, 275, 306	0
40	BS	110/110 (100%)	-0.41	0 100 100	8, 23, 56, 172	0
40	DS	110/110 (100%)	1.11	18 (16%) 2 1	69, 142, 254, 323	0
41	BT	93/93 (100%)	-0.09	1 (1%) 77 27	22, 53, 135, 194	0
41	DT	93/93 (100%)	1.36	21 (22%) 1 1	125, 241, 359, 398	0
42	BU	102/102 (100%)	-0.04	0 100 100	22, 54, 111, 237	0
42	DU	102/102 (100%)	2.16	43 (42%) 1 0	135, 334, 460, 561	0
43	BV	94/94 (100%)	-0.27	0 100 100	18, 47, 89, 149	0
43	DV	94/94 (100%)	0.55	3 (3%) 45 9	109, 156, 208, 233	0
44	BW	79/79 (100%)	-0.15	0 100 100	13, 36, 90, 194	0
44	DW	79/79 (100%)	1.24	15 (18%) 2 1	99, 166, 250, 315	0
45	BX	77/77 (100%)	-0.27	0 100 100	17, 42, 87, 113	0
45	DX	77/77 (100%)	0.53	4 (5%) 26 5	72, 122, 190, 222	0
46	BY	63/63 (100%)	-0.14	0 100 100	34, 73, 121, 155	0
46	DY	63/63 (100%)	0.95	12 (19%) 2 1	159, 374, 464, 494	0
47	BZ	58/58 (100%)	-0.37	0 100 100	7, 26, 61, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	DZ	58/58 (100%)	0.26	1 (1%) 67 19	80, 142, 228, 257	0
48	B0	56/56 (100%)	-0.50	0 100 100	6, 26, 80, 127	0
48	D0	56/56 (100%)	0.81	5 (8%) 10 2	75, 148, 244, 284	0
49	B1	50/50 (100%)	0.34	1 (2%) 62 17	42, 66, 121, 173	0
49	D1	50/50 (100%)	1.38	12 (24%) 1 1	114, 179, 216, 264	0
50	B2	46/46 (100%)	-0.42	0 100 100	11, 27, 56, 164	0
50	D2	46/46 (100%)	0.72	4 (8%) 10 3	79, 130, 179, 205	0
51	B3	64/64 (100%)	-0.43	0 100 100	11, 29, 53, 81	0
51	D3	64/64 (100%)	1.17	13 (20%) 1 1	85, 145, 232, 281	0
52	B4	38/38 (100%)	0.17	0 100 100	29, 53, 95, 103	0
52	D4	38/38 (100%)	1.94	18 (47%) 1 0	87, 165, 229, 248	0
53	CA	1530/1530 (100%)	-0.19	32 (2%) 60 15	43, 110, 301, 420	0
54	CG	150/150 (100%)	1.31	42 (28%) 1 1	101, 233, 303, 344	0
55	CM	113/113 (100%)	1.83	41 (36%) 1 0	226, 447, 522, 562	0
56	CP	80/80 (100%)	0.53	3 (3%) 38 7	49, 105, 165, 226	0
57	DA	2841/2904 (97%)	0.06	62 (2%) 59 14	51, 132, 279, 491	0
58	DB	117/117 (100%)	-0.31	0 100 100	107, 180, 240, 264	0
59	DF	178/178 (100%)	1.32	38 (21%) 1 1	175, 239, 286, 345	0
All	All	20431/20552 (99%)	0.08	1042 (5%) 27 5	6, 103, 285, 562	0

The worst 5 of 1042 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	DH	92	GLY	13.6
30	DI	51	GLY	11.8
30	DI	50	LYS	11.7
55	CM	93	GLY	11.4
29	DH	124	THR	10.9

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	MG	DA	3062	1/1	2.41	296.60	262,262,262,262	0
60	MG	DA	3108	1/1	0.31	247.00	123,123,123,123	0
60	MG	DA	3019	1/1	0.83	223.67	252,252,252,252	0
60	MG	DA	3127	1/1	1.82	131.55	274,274,274,274	0
60	MG	AA	1618	1/1	0.68	66.75	217,217,217,217	0
60	MG	BA	3118	1/1	0.27	43.74	136,136,136,136	0
60	MG	DA	3073	1/1	1.05	40.71	276,276,276,276	0
60	MG	BA	3097	1/1	0.19	39.00	182,182,182,182	0
60	MG	AA	1614	1/1	0.62	35.24	201,201,201,201	0
60	MG	BA	3043	1/1	0.24	34.67	19,19,19,19	0
60	MG	DA	3063	1/1	0.97	33.13	305,305,305,305	0
60	MG	BA	3024	1/1	0.33	31.67	206,206,206,206	0
60	MG	BA	3055	1/1	0.39	31.53	240,240,240,240	0
60	MG	DA	3077	1/1	0.74	29.46	259,259,259,259	0
60	MG	DJ	201	1/1	1.51	27.81	331,331,331,331	0
60	MG	BA	3054	1/1	0.25	27.01	214,214,214,214	0
60	MG	BA	3086	1/1	0.21	26.87	144,144,144,144	0
60	MG	CA	1614	1/1	0.90	25.70	271,271,271,271	0
60	MG	AA	1626	1/1	0.21	22.50	185,185,185,185	0
60	MG	BB	201	1/1	0.15	22.50	246,246,246,246	0
60	MG	DA	3059	1/1	0.54	22.35	241,241,241,241	0
60	MG	DA	3005	1/1	0.34	20.36	280,280,280,280	0
60	MG	DA	3025	1/1	1.75	16.89	253,253,253,253	0
60	MG	BA	3130	1/1	0.43	16.53	257,257,257,257	0
60	MG	DA	3107	1/1	0.71	16.03	201,201,201,201	0
60	MG	CA	1640	1/1	0.34	14.87	171,171,171,171	0
60	MG	DA	3003	1/1	0.99	14.52	253,253,253,253	0
60	MG	BA	3075	1/1	0.17	14.50	74,74,74,74	0
60	MG	DA	3061	1/1	0.61	14.44	210,210,210,210	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	MG	DA	3010	1/1	0.68	13.66	261,261,261,261	0
60	MG	DA	3075	1/1	0.47	13.40	229,229,229,229	0
60	MG	AA	1640	1/1	0.28	13.18	189,189,189,189	0
60	MG	CA	1627	1/1	0.32	12.56	220,220,220,220	0
60	MG	CA	1615	1/1	0.18	12.40	243,243,243,243	0
60	MG	BA	3123	1/1	0.55	10.33	112,112,112,112	0
60	MG	DA	3057	1/1	0.37	9.98	257,257,257,257	0
60	MG	BA	3132	1/1	0.46	8.39	145,145,145,145	0
60	MG	CA	1626	1/1	0.24	8.13	27,27,27,27	0
60	MG	DA	3014	1/1	0.39	7.47	177,177,177,177	0
60	MG	AA	1625	1/1	0.21	7.22	31,31,31,31	0
60	MG	BA	3060	1/1	0.28	6.84	257,257,257,257	0
60	MG	BA	3135	1/1	0.34	6.81	204,204,204,204	0
60	MG	BA	3018	1/1	0.30	6.76	10,10,10,10	0
60	MG	DE	301	1/1	0.32	5.79	191,191,191,191	0
60	MG	BA	3035	1/1	0.19	5.67	241,241,241,241	0
60	MG	BA	3107	1/1	0.20	5.39	8,8,8,8	0
60	MG	DA	3027	1/1	0.70	5.11	277,277,277,277	0
60	MG	BA	3038	1/1	0.17	4.94	21,21,21,21	0
60	MG	DA	3130	1/1	1.27	4.57	305,305,305,305	0
60	MG	DA	3093	1/1	0.33	4.41	166,166,166,166	0
60	MG	BA	3029	1/1	0.20	4.37	10,10,10,10	0
60	MG	DA	3035	1/1	0.28	4.26	228,228,228,228	0
60	MG	BA	3033	1/1	0.16	4.03	89,89,89,89	0
60	MG	BA	3056	1/1	0.14	4.02	86,86,86,86	0
60	MG	BA	3039	1/1	0.20	3.98	9,9,9,9	0
60	MG	BA	3115	1/1	0.18	3.82	8,8,8,8	0
60	MG	DA	3124	1/1	0.57	3.70	211,211,211,211	0
60	MG	BA	3096	1/1	0.18	3.59	59,59,59,59	0
60	MG	BA	3124	1/1	0.16	3.58	22,22,22,22	0
60	MG	DA	3074	1/1	0.33	3.47	239,239,239,239	0
60	MG	DA	3105	1/1	0.30	3.45	305,305,305,305	0
60	MG	BA	3082	1/1	0.15	3.33	98,98,98,98	0
60	MG	DA	3002	1/1	0.37	3.30	229,229,229,229	0
60	MG	DA	3013	1/1	0.36	3.25	209,209,209,209	0
60	MG	BA	3104	1/1	0.17	3.12	27,27,27,27	0
60	MG	BA	3103	1/1	0.19	3.06	8,8,8,8	0
60	MG	DA	3034	1/1	0.33	2.99	156,156,156,156	0
60	MG	AA	1621	1/1	0.17	2.91	35,35,35,35	0
60	MG	BA	3014	1/1	0.17	2.83	75,75,75,75	0
60	MG	DA	3114	1/1	0.25	2.62	166,166,166,166	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	MG	CA	1612	1/1	0.26	2.60	133,133,133,133	0
60	MG	DA	3007	1/1	0.33	2.56	188,188,188,188	0
60	MG	BA	3069	1/1	0.18	2.52	223,223,223,223	0
60	MG	CA	1620	1/1	0.20	2.49	209,209,209,209	0
60	MG	DA	3096	1/1	0.28	2.44	180,180,180,180	0
60	MG	BA	3074	1/1	0.17	2.42	15,15,15,15	0
60	MG	DA	3052	1/1	0.17	2.40	105,105,105,105	0
60	MG	AA	1627	1/1	0.19	2.29	165,165,165,165	0
60	MG	BA	3090	1/1	0.11	2.13	93,93,93,93	0
60	MG	DA	3008	1/1	0.26	2.07	153,153,153,153	0
60	MG	DA	3046	1/1	0.18	2.02	152,152,152,152	0
60	MG	CA	1603	1/1	0.15	2.00	140,140,140,140	0
60	MG	DA	3011	1/1	0.27	1.92	215,215,215,215	0
60	MG	AA	1630	1/1	0.15	1.92	209,209,209,209	0
60	MG	BA	3026	1/1	0.17	1.90	122,122,122,122	0
60	MG	DA	3028	1/1	0.38	1.84	195,195,195,195	0
60	MG	AA	1635	1/1	0.15	1.83	198,198,198,198	0
60	MG	BA	3036	1/1	0.16	1.78	30,30,30,30	0
60	MG	BA	3013	1/1	0.17	1.65	6,6,6,6	0
60	MG	DA	3030	1/1	0.21	1.63	66,66,66,66	0
60	MG	BA	3058	1/1	0.18	1.60	106,106,106,106	0
60	MG	DA	3129	1/1	0.70	1.57	271,271,271,271	0
60	MG	CA	1608	1/1	0.21	1.50	82,82,82,82	0
60	MG	CA	1607	1/1	0.21	1.37	222,222,222,222	0
60	MG	CA	1628	1/1	0.28	1.36	259,259,259,259	0
60	MG	DA	3100	1/1	0.26	1.31	149,149,149,149	0
60	MG	DA	3081	1/1	0.22	1.30	143,143,143,143	0
60	MG	BA	3108	1/1	0.17	1.29	6,6,6,6	0
60	MG	BA	3077	1/1	0.13	1.21	151,151,151,151	0
60	MG	BA	3100	1/1	0.16	1.08	26,26,26,26	0
60	MG	DA	3070	1/1	0.21	1.07	61,61,61,61	0
60	MG	DA	3043	1/1	0.22	1.03	112,112,112,112	0
60	MG	BA	3065	1/1	0.14	1.01	27,27,27,27	0
60	MG	AA	1604	1/1	0.11	0.95	112,112,112,112	0
60	MG	DA	3080	1/1	0.22	0.88	70,70,70,70	0
60	MG	DA	3119	1/1	0.23	0.87	84,84,84,84	0
60	MG	CA	1619	1/1	0.18	0.85	243,243,243,243	0
60	MG	DA	3015	1/1	0.26	0.83	277,277,277,277	0
60	MG	BA	3091	1/1	0.12	0.83	131,131,131,131	0
60	MG	DA	3056	1/1	0.42	0.74	243,243,243,243	0
60	MG	DA	3026	1/1	0.23	0.72	139,139,139,139	0
60	MG	DA	3098	1/1	0.18	0.68	218,218,218,218	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3020	1/1	0.20	0.64	36,36,36,36	0
60	MG	DA	3084	1/1	0.25	0.63	157,157,157,157	0
61	CLM	BA	3136	20/20	0.20	0.62	2,26,77,92	0
60	MG	BA	3044	1/1	0.16	0.59	56,56,56,56	0
60	MG	DA	3068	1/1	0.27	0.58	225,225,225,225	0
60	MG	CA	1616	1/1	0.32	0.55	279,279,279,279	0
60	MG	DA	3090	1/1	0.24	0.50	209,209,209,209	0
60	MG	AA	1641	1/1	0.15	0.50	27,27,27,27	0
60	MG	DA	3085	1/1	0.18	0.42	127,127,127,127	0
60	MG	BA	3048	1/1	0.15	0.39	18,18,18,18	0
60	MG	DA	3004	1/1	0.17	0.38	86,86,86,86	0
60	MG	CA	1624	1/1	0.22	0.37	123,123,123,123	0
60	MG	DA	3087	1/1	0.18	0.36	178,178,178,178	0
60	MG	AN	201	1/1	0.23	0.34	219,219,219,219	0
60	MG	DA	3132	1/1	0.27	0.33	225,225,225,225	0
60	MG	BA	3037	1/1	0.15	0.33	7,7,7,7	0
60	MG	CA	1605	1/1	0.15	0.32	47,47,47,47	0
60	MG	DA	3022	1/1	0.21	0.32	118,118,118,118	0
60	MG	BA	3019	1/1	0.14	0.32	50,50,50,50	0
60	MG	CA	1602	1/1	0.17	0.25	131,131,131,131	0
60	MG	BA	3008	1/1	0.15	0.23	29,29,29,29	0
60	MG	CA	1631	1/1	0.21	0.20	111,111,111,111	0
60	MG	DA	3018	1/1	0.21	0.18	225,225,225,225	0
60	MG	DA	3037	1/1	0.18	0.10	203,203,203,203	0
60	MG	DA	3097	1/1	0.20	0.10	143,143,143,143	0
60	MG	CA	1641	1/1	0.16	0.10	73,73,73,73	0
60	MG	DA	3133	1/1	0.22	0.09	241,241,241,241	0
60	MG	DA	3110	1/1	0.24	0.08	174,174,174,174	0
60	MG	CA	1621	1/1	0.17	0.03	60,60,60,60	0
60	MG	BA	3041	1/1	0.14	0.01	12,12,12,12	0
60	MG	BA	3072	1/1	0.15	-0.01	81,81,81,81	0
60	MG	BA	3112	1/1	0.15	-0.05	33,33,33,33	0
60	MG	DA	3041	1/1	0.21	-0.06	133,133,133,133	0
60	MG	DA	3088	1/1	0.22	-0.06	102,102,102,102	0
60	MG	CA	1606	1/1	0.15	-0.06	77,77,77,77	0
60	MG	AA	1601	1/1	0.10	-0.09	93,93,93,93	0
60	MG	DA	3121	1/1	0.16	-0.11	114,114,114,114	0
60	MG	AA	1605	1/1	0.12	-0.13	30,30,30,30	0
60	MG	CA	1629	1/1	0.20	-0.13	214,214,214,214	0
60	MG	BA	3106	1/1	0.15	-0.14	13,13,13,13	0
60	MG	DA	3128	1/1	0.31	-0.14	138,138,138,138	0
60	MG	BA	3126	1/1	0.13	-0.17	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3062	1/1	0.14	-0.20	9,9,9,9	0
60	MG	CA	1637	1/1	0.18	-0.23	140,140,140,140	0
60	MG	DA	3050	1/1	0.18	-0.23	89,89,89,89	0
60	MG	DA	3115	1/1	0.19	-0.24	69,69,69,69	0
60	MG	AA	1636	1/1	0.19	-0.26	149,149,149,149	0
60	MG	BA	3059	1/1	0.14	-0.29	147,147,147,147	0
60	MG	AA	1612	1/1	0.13	-0.31	103,103,103,103	0
60	MG	BA	3129	1/1	0.14	-0.31	15,15,15,15	0
60	MG	BA	3032	1/1	0.14	-0.32	6,6,6,6	0
60	MG	AA	1608	1/1	0.14	-0.37	38,38,38,38	0
60	MG	DA	3048	1/1	0.16	-0.37	243,243,243,243	0
60	MG	DA	3017	1/1	0.20	-0.38	147,147,147,147	0
60	MG	AA	1638	1/1	0.10	-0.40	139,139,139,139	0
60	MG	DA	3109	1/1	0.24	-0.42	169,169,169,169	0
60	MG	AA	1617	1/1	0.13	-0.48	111,111,111,111	0
60	MG	CA	1632	1/1	0.20	-0.48	143,143,143,143	0
60	MG	DA	3104	1/1	0.18	-0.49	48,48,48,48	0
60	MG	BA	3114	1/1	0.14	-0.52	148,148,148,148	0
60	MG	BA	3105	1/1	0.16	-0.61	11,11,11,11	0
60	MG	BA	3040	1/1	0.12	-0.61	11,11,11,11	0
60	MG	AA	1632	1/1	0.11	-0.61	53,53,53,53	0
60	MG	BA	3003	1/1	0.13	-0.62	44,44,44,44	0
60	MG	DA	3094	1/1	0.19	-0.64	98,98,98,98	0
60	MG	CA	1625	1/1	0.18	-0.68	160,160,160,160	0
60	MG	CA	1618	1/1	0.14	-0.70	141,141,141,141	0
60	MG	DA	3079	1/1	0.14	-0.72	149,149,149,149	0
60	MG	DB	201	1/1	0.12	-0.74	109,109,109,109	0
60	MG	DA	3006	1/1	0.12	-0.76	149,149,149,149	0
60	MG	BA	3073	1/1	0.10	-0.78	116,116,116,116	0
60	MG	AA	1610	1/1	0.08	-0.80	200,200,200,200	0
60	MG	DA	3102	1/1	0.16	-0.81	105,105,105,105	0
60	MG	BA	3004	1/1	0.13	-0.81	150,150,150,150	0
60	MG	DA	3042	1/1	0.19	-0.83	166,166,166,166	0
60	MG	DA	3126	1/1	0.17	-0.83	129,129,129,129	0
60	MG	DA	3036	1/1	0.14	-0.84	111,111,111,111	0
60	MG	BA	3131	1/1	0.09	-0.85	96,96,96,96	0
60	MG	DA	3082	1/1	0.11	-0.86	214,214,214,214	0
60	MG	AA	1629	1/1	0.11	-0.87	227,227,227,227	0
60	MG	CA	1617	1/1	0.14	-0.88	205,205,205,205	0
60	MG	DA	3032	1/1	0.20	-0.89	193,193,193,193	0
60	MG	CA	1633	1/1	0.08	-0.93	82,82,82,82	0
60	MG	AA	1622	1/1	0.08	-0.93	185,185,185,185	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DC	301	1/1	0.13	-0.96	134,134,134,134	0
60	MG	CA	1636	1/1	0.10	-0.98	130,130,130,130	0
60	MG	AA	1616	1/1	0.13	-0.99	123,123,123,123	0
60	MG	BA	3120	1/1	0.06	-1.00	44,44,44,44	0
60	MG	CA	1611	1/1	0.16	-1.02	116,116,116,116	0
60	MG	BA	3119	1/1	0.14	-1.08	15,15,15,15	0
60	MG	BA	3133	1/1	0.14	-1.10	5,5,5,5	0
60	MG	DA	3103	1/1	0.17	-1.10	36,36,36,36	0
60	MG	AA	1607	1/1	0.12	-1.17	98,98,98,98	0
60	MG	BA	3068	1/1	0.10	-1.22	174,174,174,174	0
60	MG	BA	3009	1/1	0.14	-1.27	12,12,12,12	0
60	MG	DA	3047	1/1	0.14	-1.33	82,82,82,82	0
60	MG	DA	3095	1/1	0.13	-1.33	110,110,110,110	0
60	MG	BA	3011	1/1	0.10	-1.35	149,149,149,149	0
60	MG	BA	3030	1/1	0.12	-1.43	34,34,34,34	0
60	MG	AA	1634	1/1	0.07	-1.44	58,58,58,58	0
60	MG	BA	3049	1/1	0.11	-1.45	72,72,72,72	0
60	MG	CA	1638	1/1	0.10	-1.46	106,106,106,106	0
60	MG	DA	3125	1/1	0.11	-1.48	132,132,132,132	0
60	MG	DA	3001	1/1	0.11	-1.56	149,149,149,149	0
60	MG	BA	3113	1/1	0.10	-1.57	34,34,34,34	0
60	MG	DA	3083	1/1	0.10	-1.61	176,176,176,176	0
60	MG	BA	3099	1/1	0.09	-1.64	32,32,32,32	0
60	MG	DA	3024	1/1	0.13	-1.66	147,147,147,147	0
60	MG	DA	3099	1/1	0.14	-1.69	96,96,96,96	0
60	MG	DA	3029	1/1	0.15	-1.70	135,135,135,135	0
60	MG	DA	3111	1/1	0.10	-1.71	89,89,89,89	0
60	MG	DA	3023	1/1	0.16	-1.73	90,90,90,90	0
60	MG	DA	3021	1/1	0.14	-1.74	169,169,169,169	0
60	MG	CA	1634	1/1	0.15	-1.75	200,200,200,200	0
60	MG	DA	3092	1/1	0.11	-1.76	209,209,209,209	0
60	MG	AA	1639	1/1	0.07	-1.77	92,92,92,92	0
60	MG	DA	3058	1/1	0.09	-1.78	204,204,204,204	0
60	MG	BA	3007	1/1	0.09	-1.79	84,84,84,84	0
60	MG	BA	3063	1/1	0.12	-1.80	11,11,11,11	0
60	MG	DA	3045	1/1	0.16	-1.83	76,76,76,76	0
60	MG	BA	3047	1/1	0.12	-1.86	112,112,112,112	0
60	MG	BA	3046	1/1	0.11	-1.86	142,142,142,142	0
60	MG	BA	3111	1/1	0.13	-1.93	93,93,93,93	0
60	MG	AA	1603	1/1	0.08	-1.93	131,131,131,131	0
60	MG	CA	1610	1/1	0.08	-1.97	220,220,220,220	0
60	MG	DA	3040	1/1	0.19	-1.98	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	MG	BB	202	1/1	0.09	-1.99	54,54,54,54	0
60	MG	BA	3045	1/1	0.12	-2.02	13,13,13,13	0
60	MG	CA	1601	1/1	0.07	-2.02	123,123,123,123	0
60	MG	CA	1622	1/1	0.10	-2.06	196,196,196,196	0
60	MG	CA	1630	1/1	0.12	-2.09	176,176,176,176	0
60	MG	DA	3065	1/1	0.12	-2.15	40,40,40,40	0
60	MG	BA	3017	1/1	0.07	-2.17	27,27,27,27	0
60	MG	BA	3128	1/1	0.12	-2.17	6,6,6,6	0
60	MG	DA	3033	1/1	0.13	-2.21	91,91,91,91	0
60	MG	DA	3112	1/1	0.08	-2.28	114,114,114,114	0
60	MG	DA	3072	1/1	0.08	-2.29	193,193,193,193	0
60	MG	DA	3101	1/1	0.12	-2.31	73,73,73,73	0
60	MG	BA	3031	1/1	0.12	-2.32	15,15,15,15	0
60	MG	DA	3069	1/1	0.14	-2.32	93,93,93,93	0
60	MG	DA	3067	1/1	0.12	-2.34	95,95,95,95	0
60	MG	BA	3080	1/1	0.12	-2.35	25,25,25,25	0
60	MG	DA	3120	1/1	0.15	-2.36	84,84,84,84	0
60	MG	DA	3064	1/1	0.12	-2.37	65,65,65,65	0
60	MG	BA	3023	1/1	0.12	-2.39	8,8,8,8	0
60	MG	BA	3022	1/1	0.12	-2.40	20,20,20,20	0
60	MG	CA	1642	1/1	0.10	-2.43	121,121,121,121	0
60	MG	DA	3038	1/1	0.17	-2.44	163,163,163,163	0
60	MG	DA	3123	1/1	0.15	-2.57	65,65,65,65	0
60	MG	AA	1611	1/1	0.10	-2.59	81,81,81,81	0
60	MG	BA	3071	1/1	0.11	-2.59	8,8,8,8	0
60	MG	DA	3071	1/1	0.09	-2.60	136,136,136,136	0
60	MG	AA	1637	1/1	0.11	-2.65	34,34,34,34	0
60	MG	BA	3084	1/1	0.12	-2.66	9,9,9,9	0
60	MG	BA	3109	1/1	0.10	-2.69	105,105,105,105	0
60	MG	DA	3012	1/1	0.11	-2.70	57,57,57,57	0
60	MG	DA	3009	1/1	0.09	-2.71	75,75,75,75	0
60	MG	DA	3131	1/1	0.09	-2.74	104,104,104,104	0
60	MG	DA	3106	1/1	0.10	-2.75	55,55,55,55	0
60	MG	BA	3021	1/1	0.11	-2.76	15,15,15,15	0
60	MG	AA	1609	1/1	0.10	-2.78	47,47,47,47	0
60	MG	BA	3110	1/1	0.07	-2.91	65,65,65,65	0
60	MG	BA	3002	1/1	0.10	-2.91	60,60,60,60	0
60	MG	DA	3049	1/1	0.14	-2.92	150,150,150,150	0
60	MG	BA	3125	1/1	0.11	-2.92	26,26,26,26	0
60	MG	BA	3027	1/1	0.12	-2.98	34,34,34,34	0
60	MG	AA	1631	1/1	0.13	-3.00	95,95,95,95	0
60	MG	DA	3051	1/1	0.09	-3.00	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3039	1/1	0.15	-3.01	59,59,59,59	0
60	MG	BA	3085	1/1	0.12	-3.16	24,24,24,24	0
60	MG	DA	3054	1/1	0.12	-3.16	125,125,125,125	0
60	MG	DA	3089	1/1	0.06	-3.16	81,81,81,81	0
60	MG	BA	3122	1/1	0.11	-3.17	25,25,25,25	0
60	MG	AA	1619	1/1	0.07	-3.26	165,165,165,165	0
60	MG	DA	3113	1/1	0.06	-3.29	123,123,123,123	0
60	MG	BA	3066	1/1	0.11	-3.32	14,14,14,14	0
60	MG	DA	3117	1/1	0.12	-3.36	99,99,99,99	0
60	MG	CA	1623	1/1	0.13	-3.40	79,79,79,79	0
60	MG	DA	3066	1/1	0.12	-3.45	65,65,65,65	0
60	MG	BA	3095	1/1	0.11	-3.55	13,13,13,13	0
60	MG	BA	3052	1/1	0.08	-3.58	12,12,12,12	0
62	ZN	D4	101	1/1	0.11	-3.59	197,197,197,197	0
60	MG	BA	3102	1/1	0.09	-3.63	14,14,14,14	0
60	MG	DA	3044	1/1	0.13	-3.81	230,230,230,230	0
60	MG	DA	3118	1/1	0.06	-3.85	75,75,75,75	0
62	ZN	B4	101	1/1	0.06	-3.89	81,81,81,81	0
60	MG	DA	3053	1/1	0.09	-3.92	78,78,78,78	0
60	MG	BA	3042	1/1	0.11	-3.94	34,34,34,34	0
60	MG	AA	1633	1/1	0.10	-3.98	52,52,52,52	0
60	MG	BA	3087	1/1	0.11	-4.06	182,182,182,182	0
60	MG	BA	3093	1/1	0.08	-4.08	68,68,68,68	0
60	MG	BA	3083	1/1	0.09	-4.10	52,52,52,52	0
60	MG	CA	1609	1/1	0.14	-4.15	71,71,71,71	0
60	MG	CA	1639	1/1	0.06	-4.19	148,148,148,148	0
60	MG	DA	3091	1/1	0.16	-4.21	167,167,167,167	0
60	MG	BB	204	1/1	0.10	-4.24	30,30,30,30	0
60	MG	BB	203	1/1	0.10	-4.29	16,16,16,16	0
60	MG	BA	3020	1/1	0.10	-4.33	21,21,21,21	0
60	MG	AA	1628	1/1	0.07	-4.35	70,70,70,70	0
60	MG	BA	3012	1/1	0.12	-4.44	5,5,5,5	0
60	MG	AA	1613	1/1	0.08	-4.49	56,56,56,56	0
60	MG	DA	3016	1/1	0.11	-4.50	75,75,75,75	0
60	MG	BA	3028	1/1	0.10	-4.54	45,45,45,45	0
60	MG	BA	3127	1/1	0.09	-4.60	21,21,21,21	0
60	MG	BA	3121	1/1	0.13	-4.66	5,5,5,5	0
60	MG	BA	3015	1/1	0.07	-4.67	30,30,30,30	0
60	MG	CA	1604	1/1	0.04	-4.68	65,65,65,65	0
60	MG	BA	3005	1/1	0.07	-4.74	60,60,60,60	0
60	MG	BA	3134	1/1	0.10	-4.78	145,145,145,145	0
60	MG	BA	3061	1/1	0.13	-4.82	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3078	1/1	0.10	-4.88	95,95,95,95	0
60	MG	BA	3079	1/1	0.10	-4.89	20,20,20,20	0
60	MG	DA	3076	1/1	0.09	-4.97	110,110,110,110	0
60	MG	DA	3031	1/1	0.10	-4.99	121,121,121,121	0
60	MG	BL	201	1/1	0.07	-5.17	34,34,34,34	0
60	MG	BA	3078	1/1	0.07	-5.18	49,49,49,49	0
60	MG	AA	1606	1/1	0.07	-5.32	58,58,58,58	0
60	MG	BA	3067	1/1	0.10	-5.33	22,22,22,22	0
60	MG	BA	3053	1/1	0.10	-5.33	35,35,35,35	0
60	MG	DA	3060	1/1	0.07	-5.41	144,144,144,144	0
60	MG	BA	3006	1/1	0.06	-5.47	47,47,47,47	0
60	MG	DA	3116	1/1	0.10	-5.55	59,59,59,59	0
60	MG	BA	3092	1/1	0.07	-5.90	30,30,30,30	0
60	MG	AA	1623	1/1	0.07	-5.94	104,104,104,104	0
60	MG	AA	1642	1/1	0.09	-5.94	42,42,42,42	0
60	MG	AA	1620	1/1	0.08	-5.98	120,120,120,120	0
60	MG	BA	3050	1/1	0.09	-6.18	12,12,12,12	0
60	MG	BA	3016	1/1	0.08	-6.26	5,5,5,5	0
60	MG	DA	3122	1/1	0.10	-6.33	155,155,155,155	0
60	MG	BA	3064	1/1	0.08	-6.35	8,8,8,8	0
60	MG	BA	3076	1/1	0.05	-6.62	31,31,31,31	0
60	MG	AA	1602	1/1	0.09	-6.64	117,117,117,117	0
60	MG	CA	1613	1/1	0.07	-6.68	116,116,116,116	0
60	MG	BA	3094	1/1	0.08	-6.73	42,42,42,42	0
60	MG	BA	3089	1/1	0.08	-6.77	39,39,39,39	0
60	MG	AA	1615	1/1	0.04	-6.92	127,127,127,127	0
60	MG	BA	3034	1/1	0.08	-6.98	9,9,9,9	0
60	MG	AA	1624	1/1	0.06	-7.39	139,139,139,139	0
60	MG	BA	3070	1/1	0.11	-7.85	76,76,76,76	0
60	MG	BA	3088	1/1	0.09	-7.87	22,22,22,22	0
60	MG	BA	3117	1/1	0.07	-7.87	79,79,79,79	0
60	MG	BA	3025	1/1	0.10	-8.15	38,38,38,38	0
60	MG	BA	3057	1/1	0.06	-8.19	43,43,43,43	0
60	MG	BA	3081	1/1	0.04	-8.28	41,41,41,41	0
60	MG	CA	1635	1/1	0.09	-8.66	85,85,85,85	0
60	MG	BA	3098	1/1	0.12	-9.55	46,46,46,46	0
60	MG	BA	3116	1/1	0.06	-11.73	14,14,14,14	0
60	MG	BA	3001	1/1	0.08	-14.03	84,84,84,84	0
60	MG	BA	3101	1/1	0.06	-16.13	105,105,105,105	0
60	MG	BA	3010	1/1	0.09	-20.60	48,48,48,48	0
60	MG	DA	3086	1/1	0.09	-20.75	185,185,185,185	0
60	MG	BA	3051	1/1	0.09	-27.90	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3055	1/1	0.09	-38.42	121,121,121,121	0

6.5 Other polymers ⓘ

There are no such residues in this entry.