



wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2014 – 08:03 PM BST

PDB ID : 4V8J
Title : Crystal structure of the bacterial ribosome ram mutation G347U.
Authors : Fagan, C.E.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2011-12-20
Resolution : 3.90 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

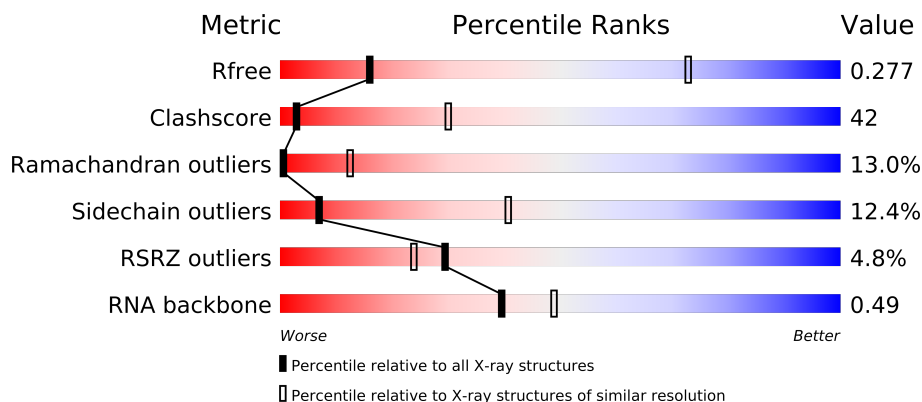
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1022 (4.38-3.42)
Clashscore	79885	1173 (4.30-3.50)
Ramachandran outliers	78287	1118 (4.30-3.50)
Sidechain outliers	78261	1107 (4.30-3.50)
RSRZ outliers	66119	1000 (4.36-3.44)
RNA backbone	1838	1018 (5.00-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1522	
1	CA	1522	
2	AB	256	
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	

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Mol	Chain	Length	Quality of chain
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AW	76	
22	AY	76	
22	CW	76	
22	CY	76	
23	AV	77	
23	CV	77	
24	AX	24	
24	CX	24	
25	BA	2916	
25	DA	2916	
26	BB	122	
26	DB	122	

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Mol	Chain	Length	Quality of chain
27	BC	229	
27	DC	229	
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	
39	DS	112	
40	BT	146	
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	

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Mol	Chain	Length	Quality of chain
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	71	
51	D4	71	
52	B5	60	
52	D5	60	
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	
56	B9	37	
56	D9	37	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 292667 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	1504	Total	C	N	O	P	0	0	0
			32326	14389	5989	10445	1503			
1	CA	1503	Total	C	N	O	P	0	0	0
			32304	14379	5984	10439	1502			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	342	U	G	ENGINEERED MUTATION	GB AP008226.1
CA	342	U	G	ENGINEERED MUTATION	GB AP008226.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1010	639	197	174			
9	CI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- 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
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- 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	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	AY	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
22	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CY	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			

- Molecule 23 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
23	CV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 24 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	8	Total	C	N	O	P	0	0	0
			169	76	29	56	8			
24	CX	10	Total	C	N	O	P	0	0	0
			210	96	39	66	9			

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2803	Total 60378	C 26870	N 11297	O 19409	P 2802	0	0	0
25	DA	2803	Total 60378	C 26870	N 11297	O 19409	P 2802	0	0	0

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	119	Total 2551	C 1136	N 471	O 826	P 118	0	0	0
26	DB	119	Total 2551	C 1136	N 471	O 826	P 118	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	BC	191	Total 1142	C 691	N 221	O 230	0	0	1
27	DC	191	Total 1142	C 691	N 221	O 230	0	0	1

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	272	Total 2105	C 1329	N 417	O 356	S 3	0	0	1
28	DD	272	Total 2105	C 1329	N 417	O 356	S 3	0	0	1

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	205	Total 1564	C 988	N 300	O 270	S 6	0	0	1
29	DE	205	Total 1564	C 988	N 300	O 270	S 6	0	0	1

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	208	Total 1624	C 1035	N 304	O 282	S 3	0	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
31	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
32	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
33	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
34	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
35	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
36	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
37	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
38	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BS	99	Total	C	N	O	0	0	1
			771	486	155	130			
39	DS	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
40	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
41	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
42	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
43	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BX	93	Total	C	N	O		0	0	1
			726	471	132	123				
44	DX	93	Total	C	N	O		0	0	1
			726	471	132	123				

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
45	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
47	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
48	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
49	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
50	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
51	D4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
52	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			
53	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
54	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
55	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

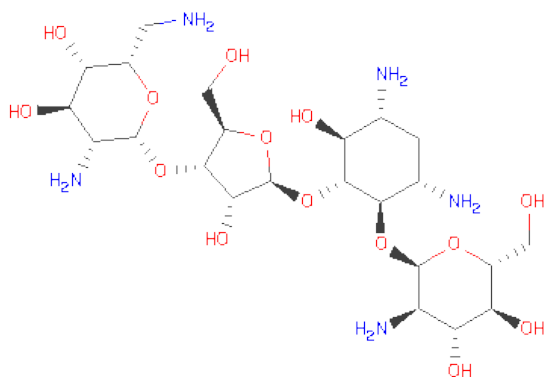
- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
56	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	BU	1	Total 1 Mg 1	0	0
57	BB	4	Total 4 Mg 4	0	0
57	BO	1	Total 1 Mg 1	0	0
57	BA	261	Total 261 Mg 261	0	0
57	CA	94	Total 94 Mg 94	0	0
57	D0	1	Total 1 Mg 1	0	0
57	CV	2	Total 2 Mg 2	0	0
57	BF	2	Total 2 Mg 2	0	0
57	B3	1	Total 1 Mg 1	0	0
57	B5	2	Total 2 Mg 2	0	0
57	BE	1	Total 1 Mg 1	0	0
57	D5	2	Total 2 Mg 2	0	0
57	AA	93	Total 93 Mg 93	0	0
57	B1	1	Total 1 Mg 1	0	0
57	DE	1	Total 1 Mg 1	0	0
57	DA	268	Total 268 Mg 268	0	0
57	AX	2	Total 2 Mg 2	0	0
57	DD	1	Total 1 Mg 1	0	0
57	DB	2	Total 2 Mg 2	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

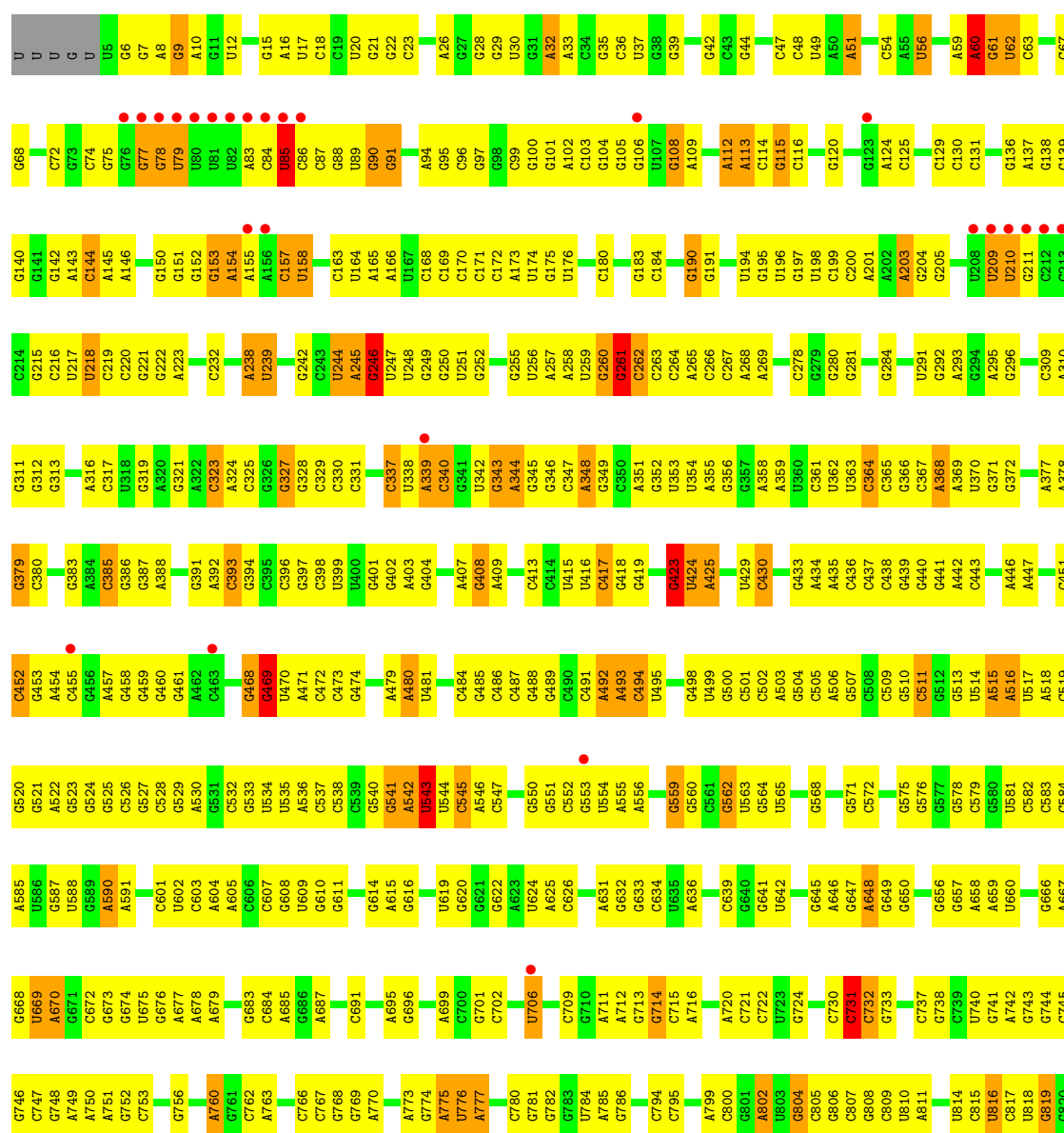
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CN	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		

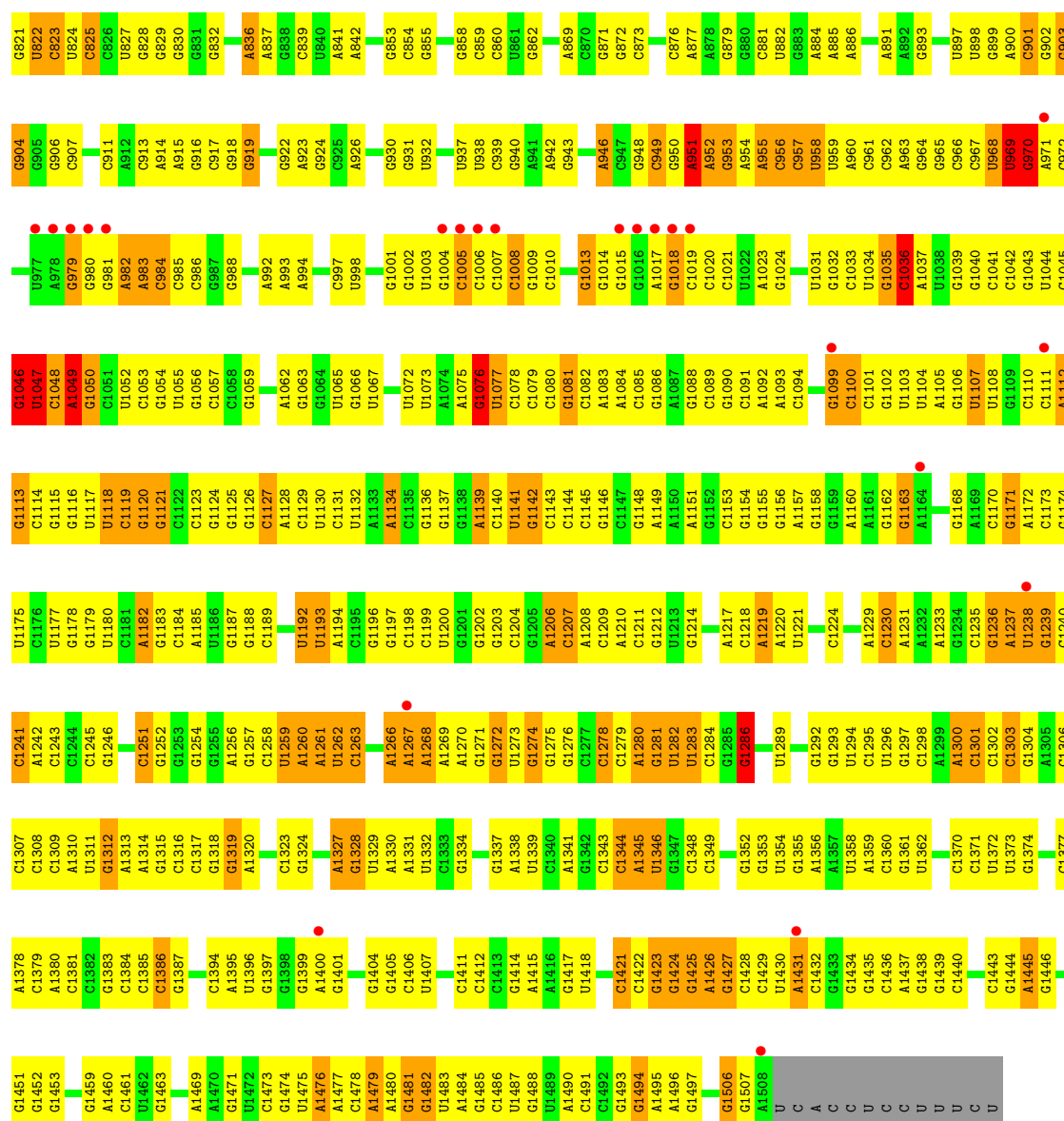
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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

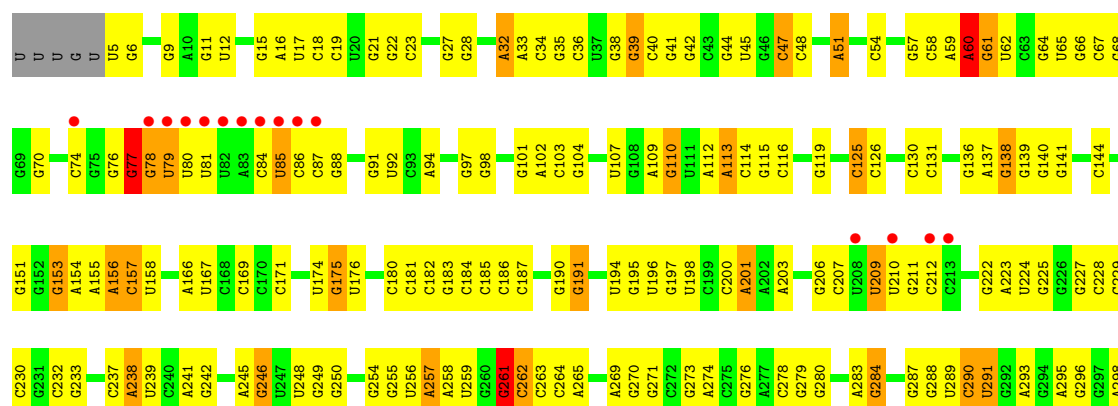
Chain AA: 

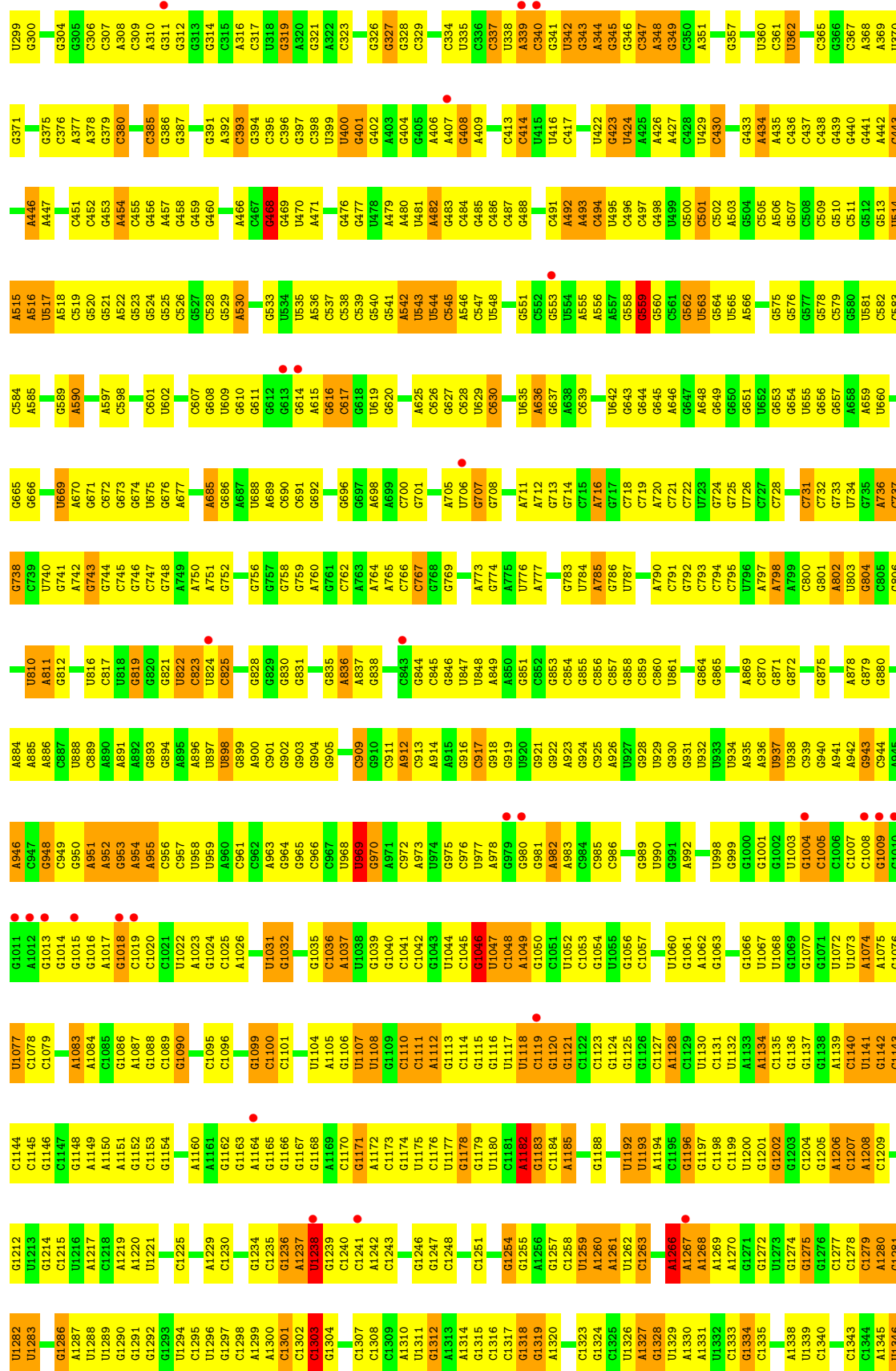


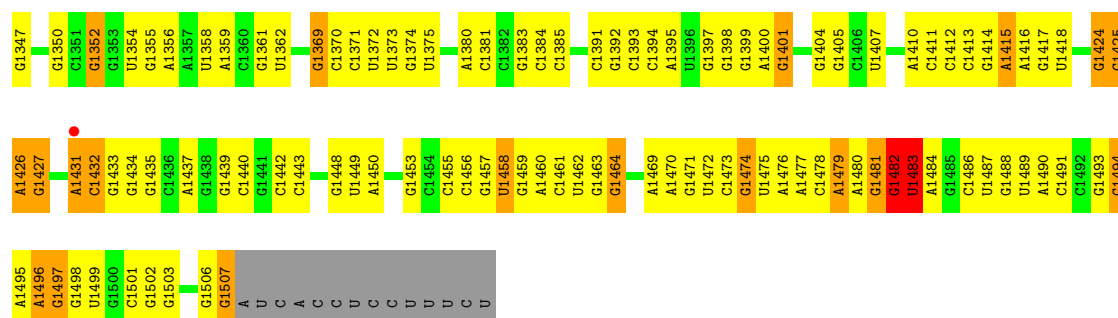


Molecule 1: 16S rRNA

Chain CA:

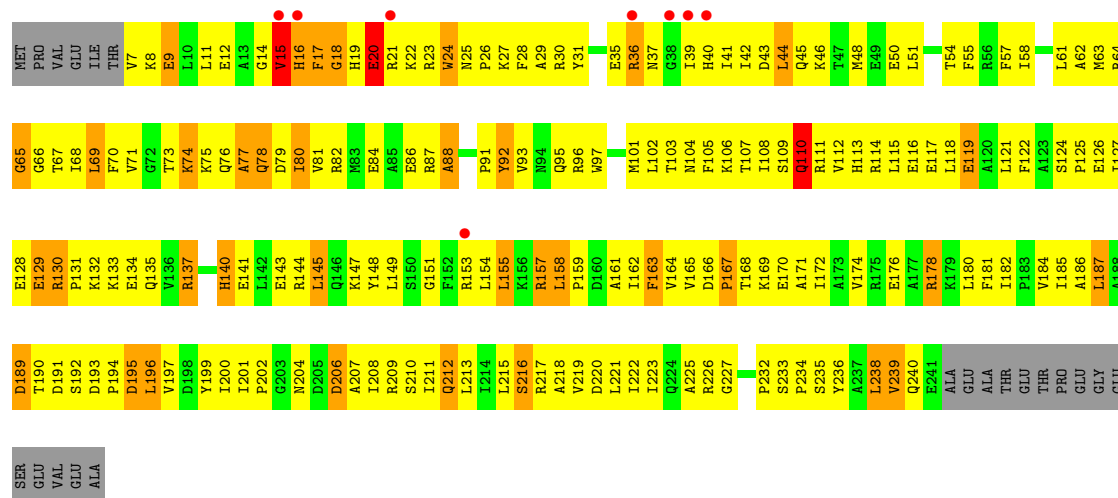






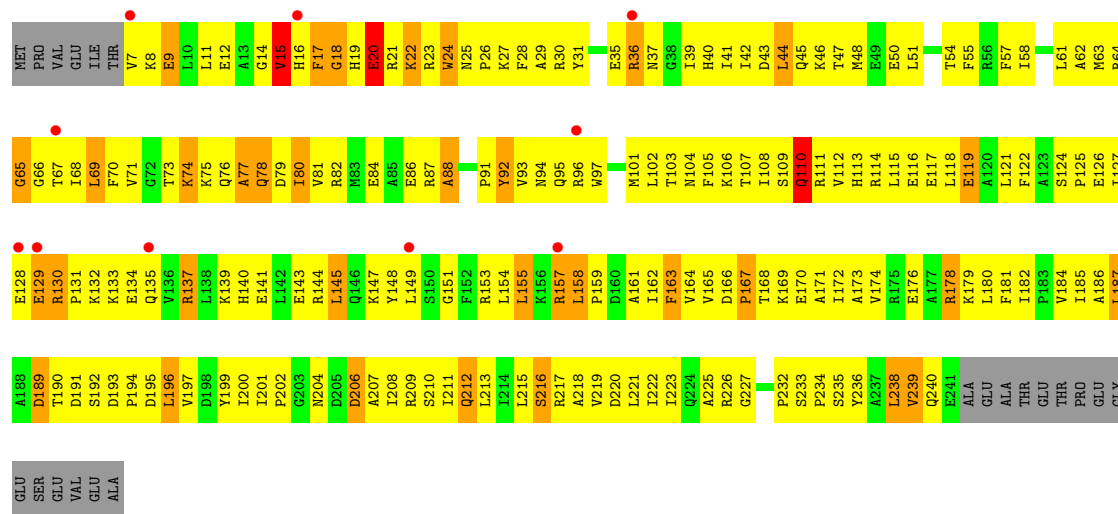
• Molecule 2: 30S ribosomal protein S2

Chain AB:



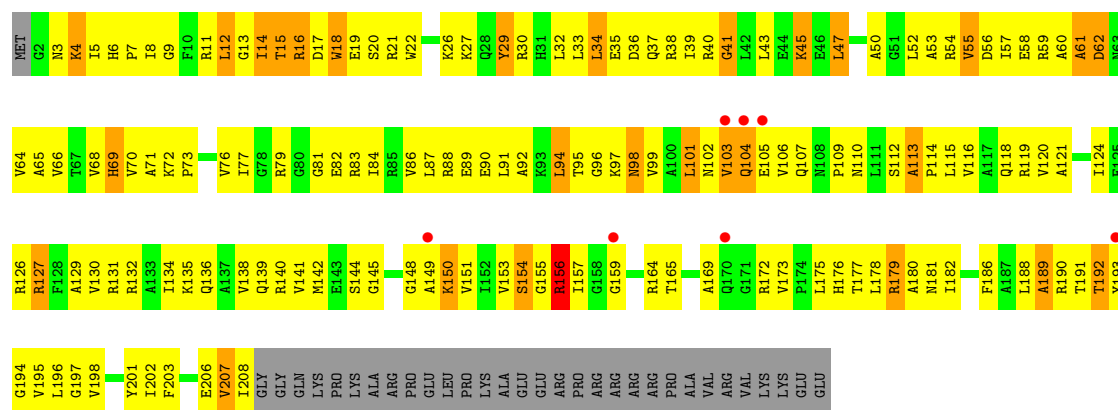
• Molecule 2: 30S ribosomal protein S2

Chain CB:



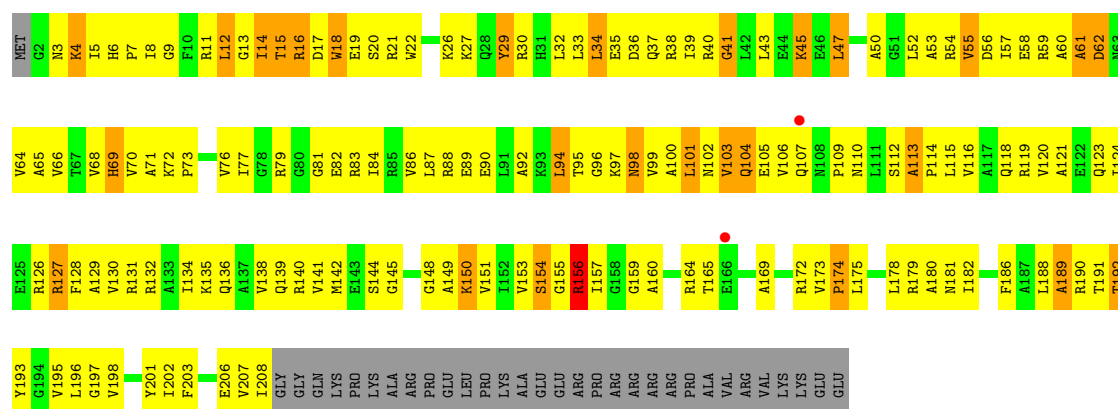
• Molecule 3: 30S ribosomal protein S3

Chain AC:



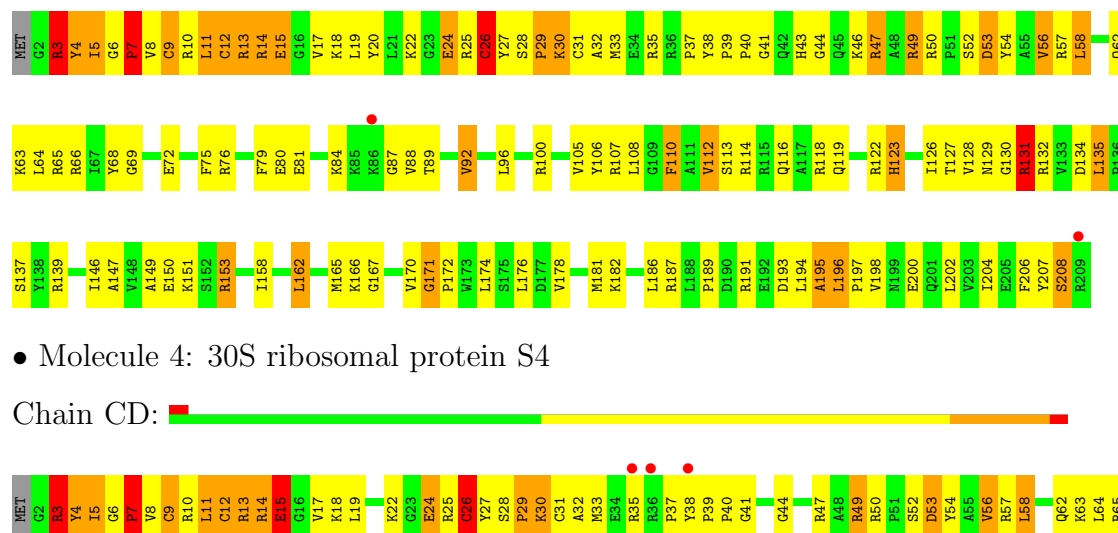
• Molecule 3: 30S ribosomal protein S3

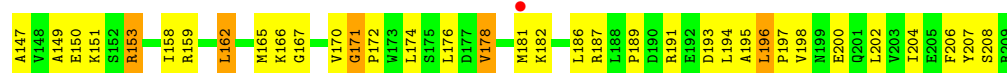
Chain CC:



• Molecule 4: 30S ribosomal protein S4

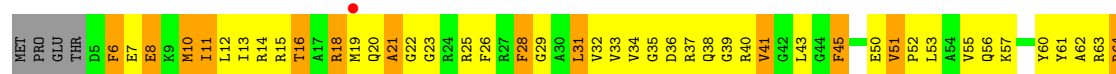
Chain AD:





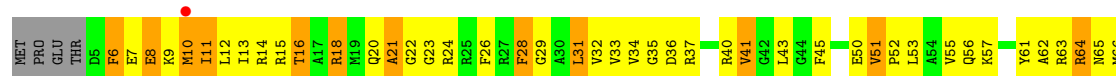
• Molecule 5: 30S ribosomal protein S5

Chain AE:



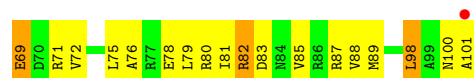
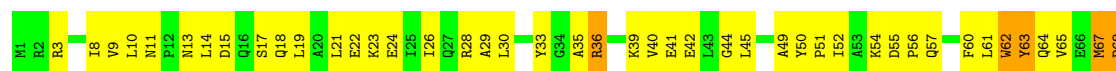
• Molecule 5: 30S ribosomal protein S5

Chain CE:



• Molecule 6: 30S ribosomal protein S6

Chain AF:



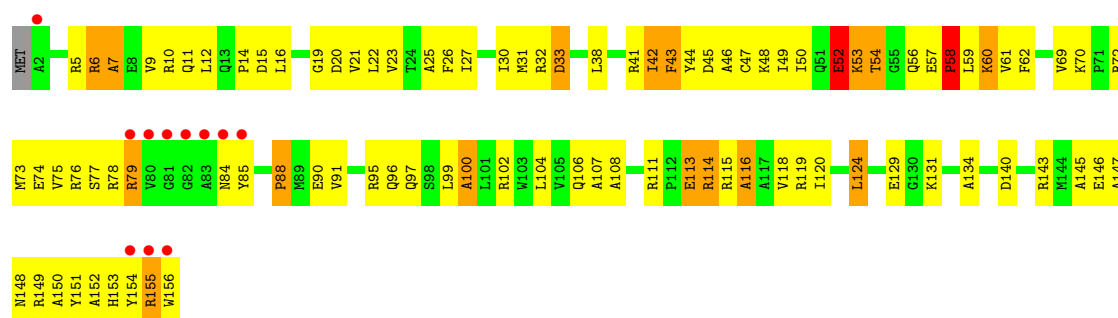
• Molecule 6: 30S ribosomal protein S6

Chain CF:



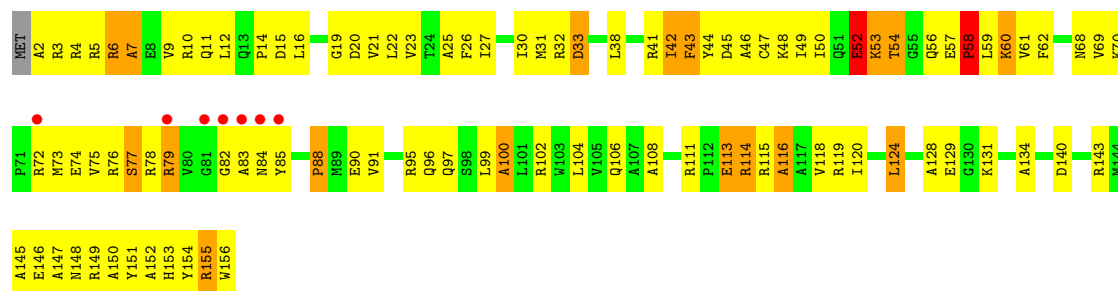
• Molecule 7: 30S ribosomal protein S7

Chain AG:



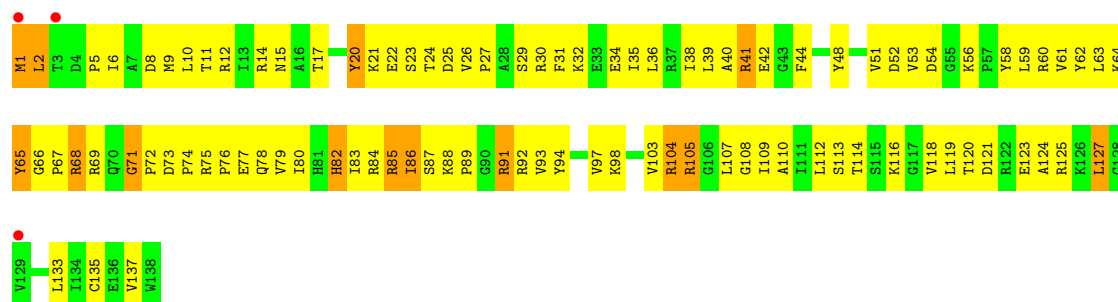
• Molecule 7: 30S ribosomal protein S7

Chain CG:



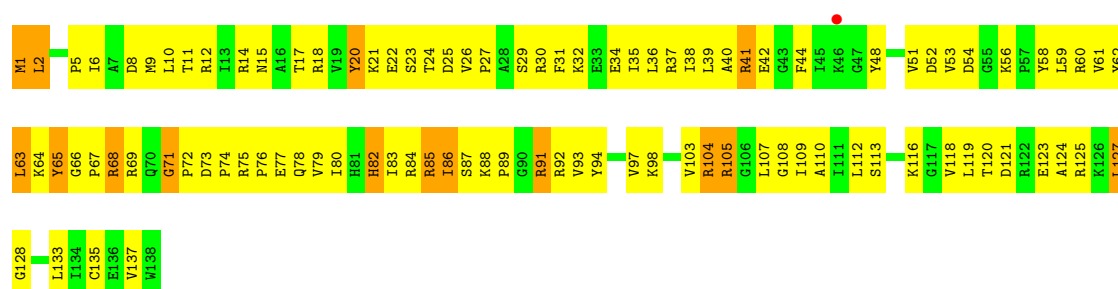
• Molecule 8: 30S ribosomal protein S8

Chain AH:



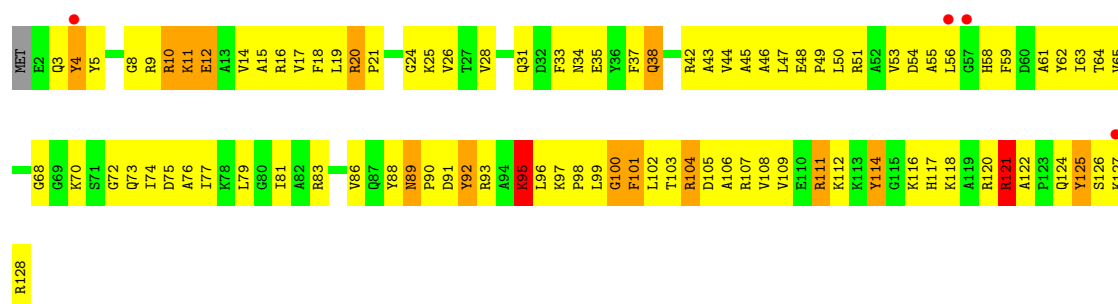
• Molecule 8: 30S ribosomal protein S8

Chain CH:



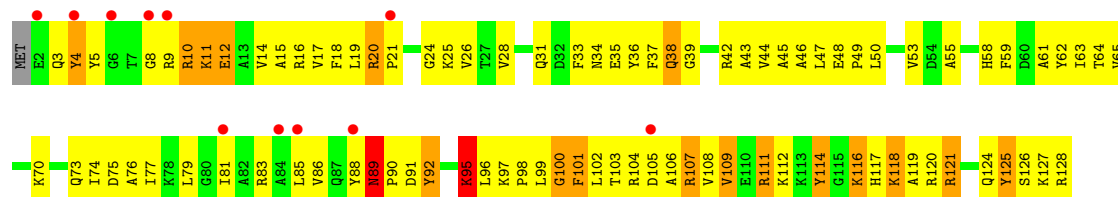
• Molecule 9: 30S ribosomal protein S9

Chain AI:



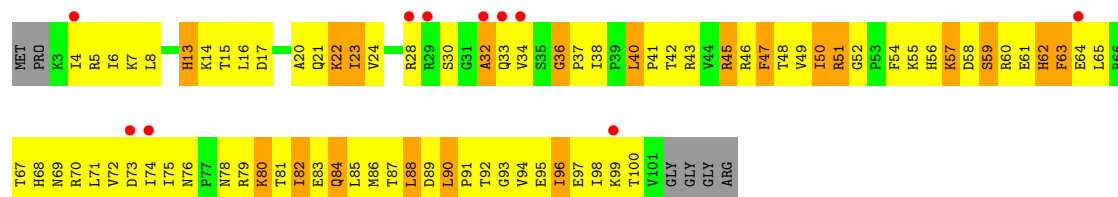
- Molecule 9: 30S ribosomal protein S9

Chain CI:



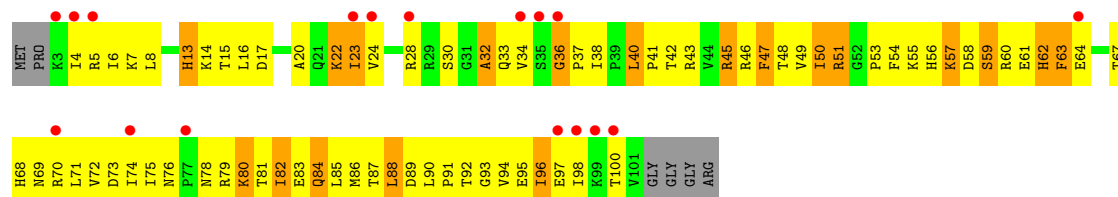
- Molecule 10: 30S ribosomal protein S10

Chain AJ:



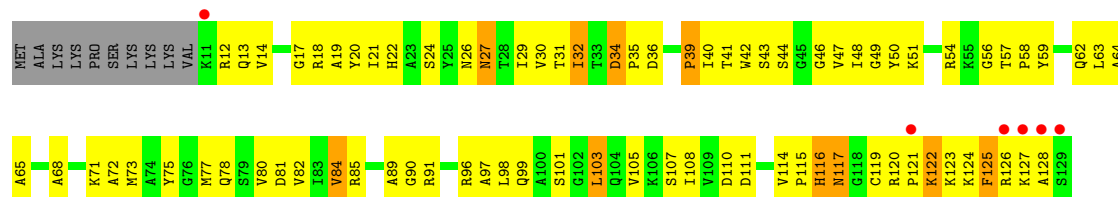
- Molecule 10: 30S ribosomal protein S10

Chain CJ:



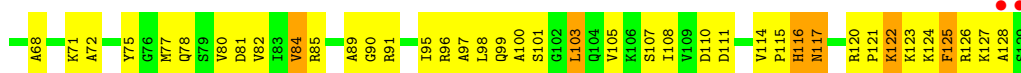
- Molecule 11: 30S ribosomal protein S11

Chain AK:



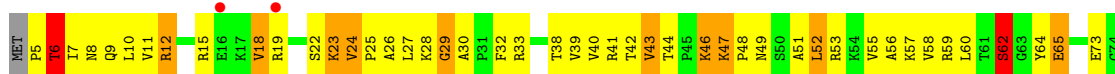
- Molecule 11: 30S ribosomal protein S11

Chain CK: 



- Molecule 12: 30S ribosomal protein S12

Chain AL: 



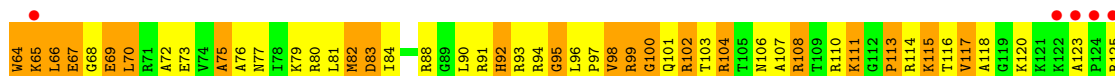
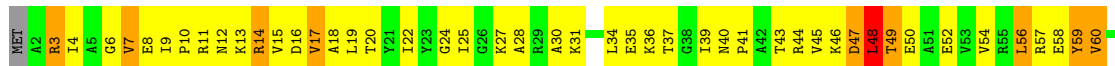
- Molecule 12: 30S ribosomal protein S12

Chain CL: 



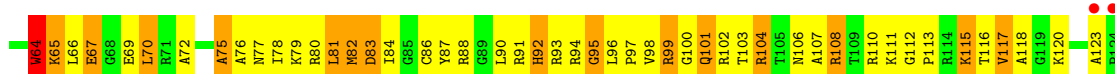
- Molecule 13: 30S ribosomal protein S13

Chain AM: 



- Molecule 13: 30S ribosomal protein S13

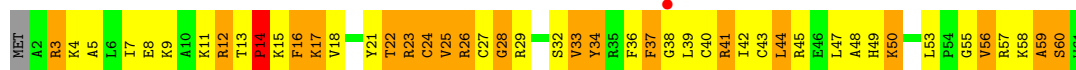
Chain CM: 





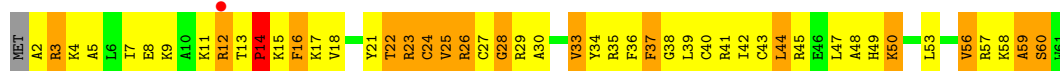
- Molecule 14: 30S ribosomal protein S14

Chain AN:



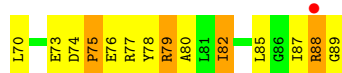
- Molecule 14: 30S ribosomal protein S14

Chain CN:



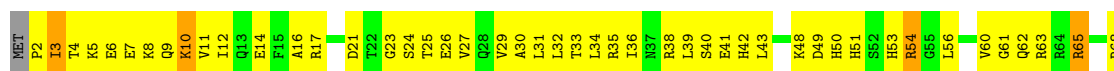
- Molecule 15: 30S ribosomal protein S15

Chain AO:



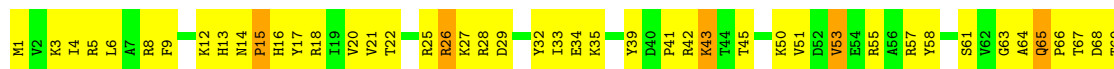
- Molecule 15: 30S ribosomal protein S15

Chain CO:



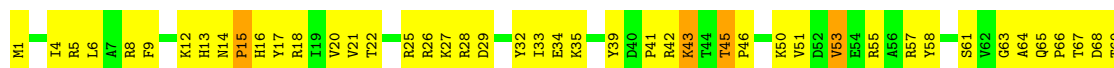
- Molecule 16: 30S ribosomal protein S16

Chain AP:



- Molecule 16: 30S ribosomal protein S16

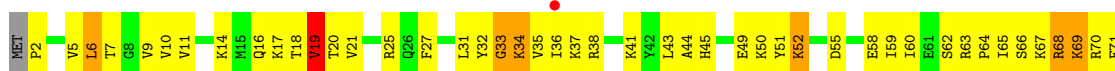
Chain CP:





- Molecule 17: 30S ribosomal protein S17

Chain AQ:



- Molecule 17: 30S ribosomal protein S17

Chain CQ:



- Molecule 18: 30S ribosomal protein S18

Chain AR:



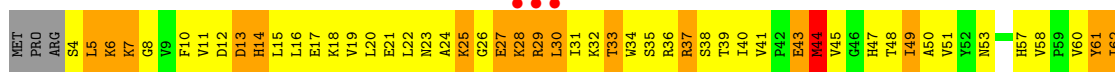
- Molecule 18: 30S ribosomal protein S18

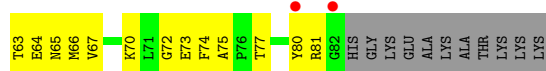
Chain CR:



- Molecule 19: 30S ribosomal protein S19

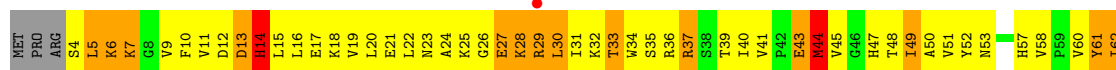
Chain AS:





- Molecule 19: 30S ribosomal protein S19

Chain CS:



- Molecule 20: 30S ribosomal protein S20

Chain AT:



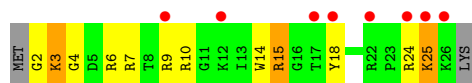
- Molecule 20: 30S ribosomal protein S20

Chain CT:



- Molecule 21: 30S ribosomal protein THX

Chain AU:



- Molecule 21: 30S ribosomal protein THX

Chain CU:



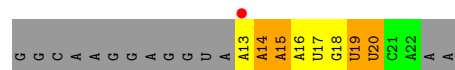
- Molecule 22: tRNA-Phe

Chain AW:

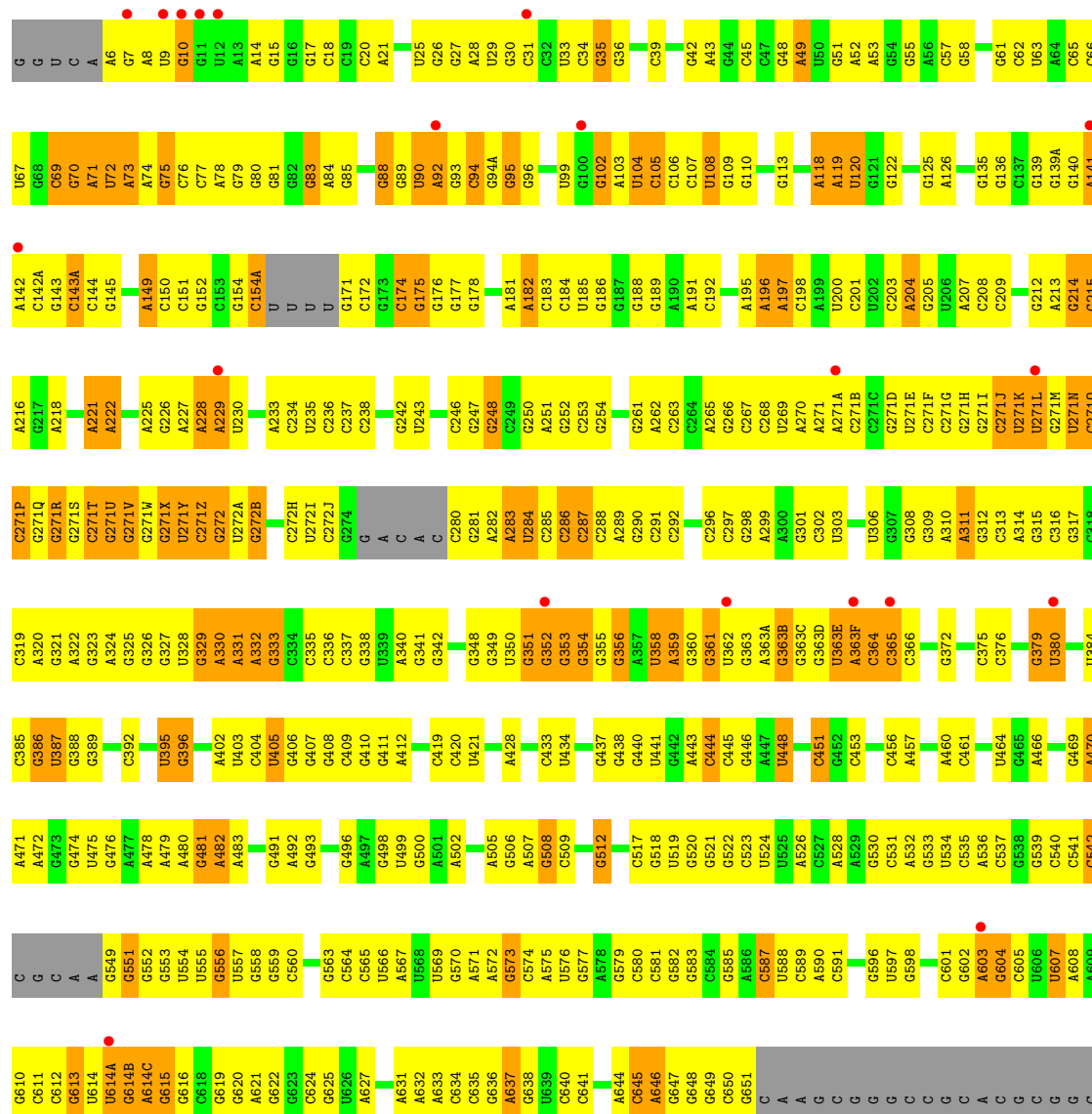
- Chain AX:



- Chain CX: 

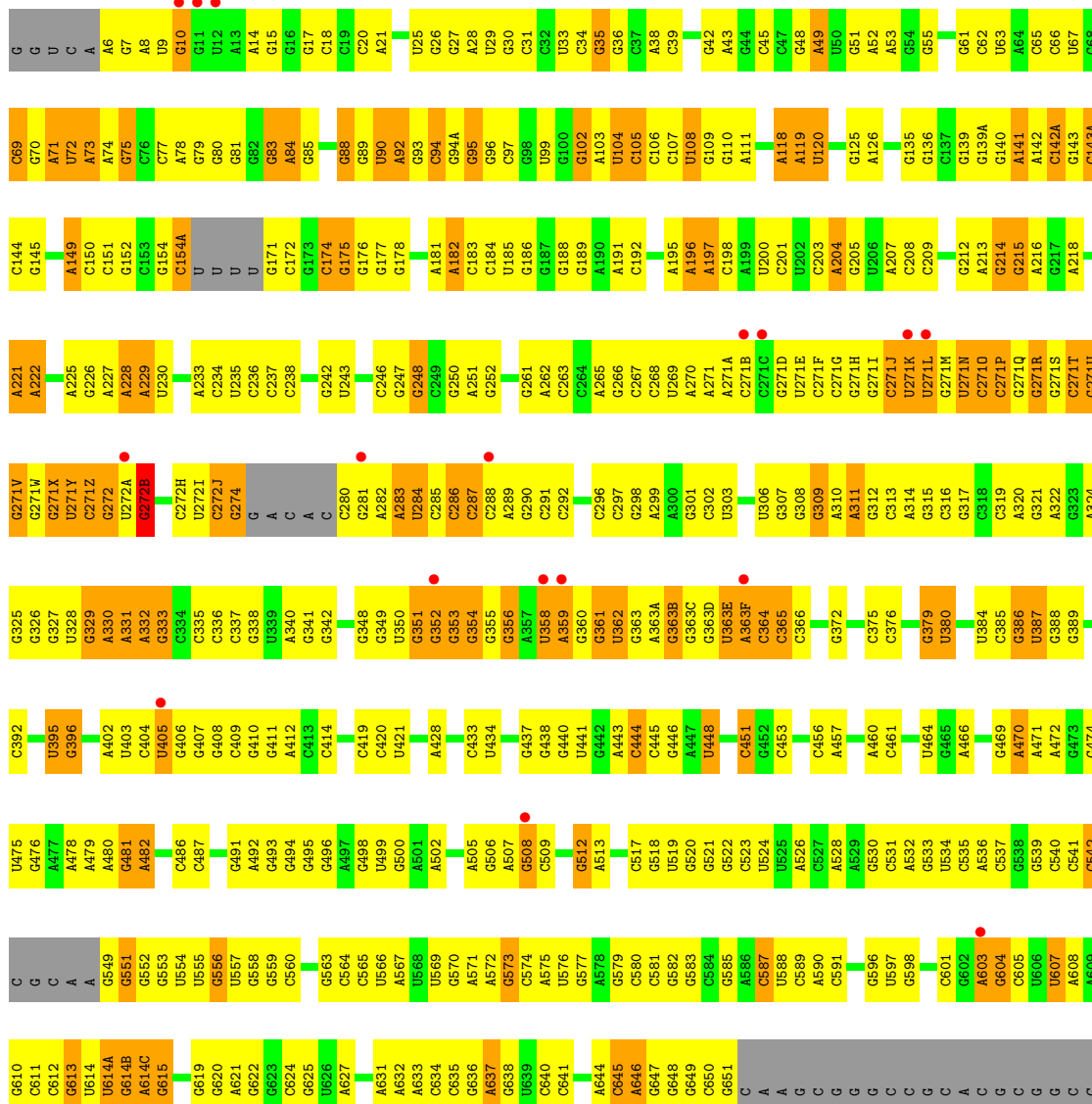


- Chain BA:



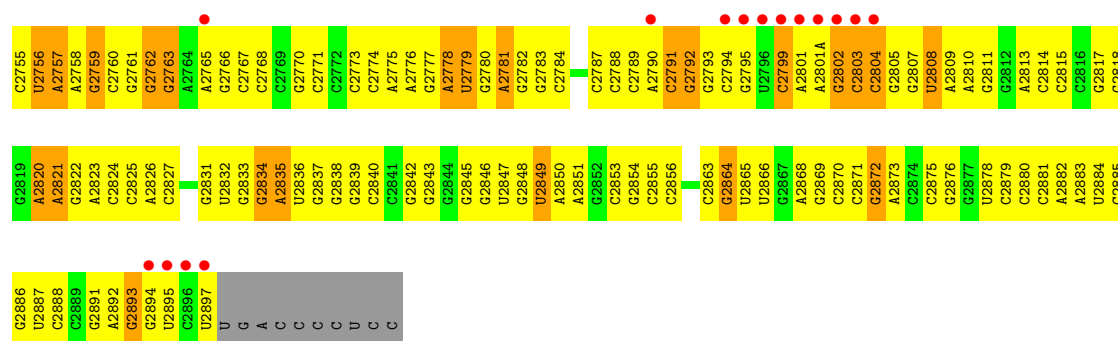
G1563	C	C812	C730	C
C1564	C	A887	C731	C
C1565	G	C888	C732	G
C1497	C	C889	G733	C
C1566	A	A890		A
A1567	A	C892	G744	A
G1500	A	C893		A
C1501		C894	U747	
C1502		U895	G748	
C1503		A896		
C1504		C897	A752	
C1505		C898	C753	
C1506		A899		
A1507		C903	C758	
A1508		C904	G759	
C1509		C905	G760	
A1509A		U906	A761	
A1509B		C907	U762	
G1510		C908	G763	
G1511		C909	A764	
C1512		C910		
U1512		C912		
C1513		C914		
C1514		C915		
G1515		C916		
U1518		C917		
C1519		C918		
G1519		C919		
C1520		C920		
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C1522		C922		
C1523		C923		
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G1527		C927		
A1528		C928		
A1528A		C929		
G1532		C930		
U		C931		
A		C932		
C		C933		
G1537		C934		
A1541		C935		
A1542		C936		
C1543		C937		
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A1554		C944		
G1555		C945		
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G1559		C949		
A1614		C950		
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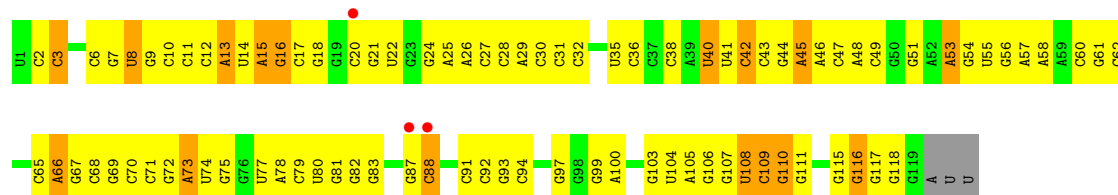
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C1648	G1568	G1500	U1438	G1369	C1224	A155	U	G962	C889	C816		A
	A1569	C1501	U1439	G1370	U1300	G1156	G	U963	A890	C817		A
G1651	A1570	C1502	G1440	A1373	G1227	A1301	C	C964	C892	C818	G747	A
A1652	A1571	U1503	G1441	G1374	A1302	G1158	U	C965	C893	A819	G748	A
G1653	A1572	C1504	G1442		C1230	U1159	U	U969	C894			G656
G1654	G1573	C1505	G1443	A1376	G1231	U1160	A	C970	U895	C825	A751	U657
A1655	C1574	C1506	G1444	A1379	G1232	G1161	A	C971	A896	U825	A752	C658
C1656		A1507	C1445	G1380	C1233	C1161	U	C972	C897	U827	C753	C659
C1657	C1577	A1508	C1446	A1384	U1234	G1162	U	C973	C898	U828		G660
A1658	U1578	C1509	G1447	G1385	G1235	G1163	A	A973	C899	A829	G758	C661
A1659	A1579	A1509B	G1448	C1386	G1236	G1164	G	C974	C903	G830	G759	C662
	G1580	G1510	A1449	C1387	A1237	U1165	C	C975	C904	G831	G760	C663
G1666	C1581	C1511	G1450	G1388	G1238	U1167	U	C976	C908	G832	A761	C664
A1667	A1583	U1512	C1450A	G1389	U1240	G1168	C	C977	C909	U833	G762	C665
A1668	C1584	C1513	G1451	A1393	A1241	G1169	A	G978	A908	C834	G763	C666
A1669	A1586	U1514	U1452	U1394	G1242	G1170	U	C979	A910	C835	A764	U667
C1670	A1587	G1515	G1453	U1395	G1243	G1171	G	A980	A911			C668
	C1588		G1455	U1396	G1244	G1173	G	U981	C912	U839	G769	C669
G1674	U1589	U1518	C1458	U1397	G1245	A1174	A	A983	U913	G843	G770	A670
C1675	C1590	G1519	G1459	U1397	A1246	U1175	A	A984	C914	C844	U773	C671
	G1591	U1520	G1460	C1398	A1247	G1176	A	A985	C915	C845	U774	C672
G1678	C1592	G1521	G1461	G1399	U1248	A1177	A	C986	C916	C846	G775	C673
	G1593	G1524	G1461	G1400	U1249	C1178	A	C987	A917	U847	G776	C674
G1681	G1594	G1525	C1462	G1401	G1250	C1179	A	A988	U918	G848	A777	A675
	G1595	G1526	C1463	C1402	C1251	U1114	A	U989	C925	C853		A676
C1685	C1598	G1527	C1464	C1403	A1253	G1115	G	C991	A926	G854	A782	C683
C1686	C1599	A1528	U1405	C1404	G1331	G1116	G	C992	C927	C855	A783	C686
G1687	G1600	A1528A	U1406	U1405	G1332	G1117	A	C993	G928	C856	G785	C691
U1688	C1601	C1532	C1407	C1407	U1335	G1118	G	C994	U930	C857	U787	C692
A1689	G1602	U	C1408	C1409	A1336	C1119	G	A996	G929	C858	A788	C696
	A1603	C	G1410	G1411	G1337	C1120	U	U999	U930	C859	G789	C697
U1692	C1607	G1537	G1412	G1413	U1340	G1121	G	A1000	C931	U858	A789	C698
U1693	A1608		G1414	G1415	U1341	G1122	G	A1001	G932	C860		
G1696	A1609	G1541	G1416	G1417	G1344	G1123	U	A1002	G933	U860	C790	U703
A1697	A1610	C1542	G1418	G1419	G1345	G1124	A	A1003	G934	A863	C791	G704
A1700	A1614	A1543	G1420	U1420	C1346	G1125	G	A1004	A941	C864	G792	C708
A1701	A1615	A1544	G1421	G1421	G1347	G1126	A	C1005	G942	C865	A793	U709
A1616	A1616	A1545	G1422	G1423	G1348	G1127	A	C1006	U943	A866		
C1617	C1617	C1546	G1424	G1424	G1349	A1129	G	C1007	G944	C869	C796	G710
A1618	A1618	C1547	G1425	G1425	A1349	U1130	C	A1010	A945	A870	C797	G711
G1619	G1619	C1547	G1426	G1426	C1350	G1131	C	U1011	G946	U871	A800	G712
G1620	G1620	C1550	G1427	G1427	C1351	A1132	G	U1012	G947	C874	G801	G715
	C1625	C1551	G1428	G1428	U1352	U1140	C	C1013	C948	G875	A802	A716
	C1626	A1554	G1429	G1429	A1353	U1141	A	G1016	G950	C876	U803	G717
	A1631A	G1555	G1430	G1430	A1354	U1142	U	G1017	C951	C877	A804	A719
	A1634	C1556	G1431	G1431	G1355	A1142A	C	C1018	G952	U877	G805	
		A1558	G1432	G1432	U1357	A1143	C	U1019	A953	C878	C806	A722
		G1559	G1433	G1433	G1358	U1144	U	A1020	G954	G879	U807	G723
			A1494	A1494	A1359	G1145	U	A1021	C955		G808	
			A1495	A1495	C1363	C1146	U	G1022	G956	G883		G729
			A1496	A1496	C1291	G1149	A	U1023	A957	C884	U811	C730
			A1497	A1497	C1292	G1149	A	U1024	U958	C885	C812	C731
					C1293	C1150	A	G1025	A959	C886	U813	C732





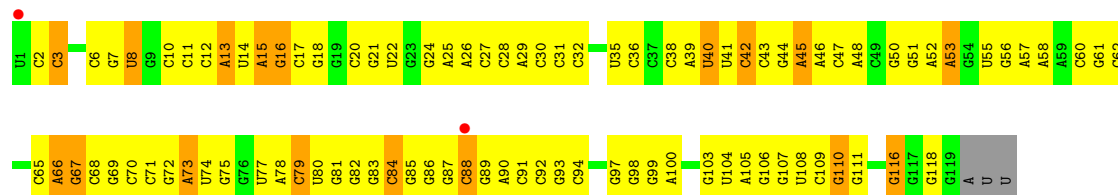
• Molecule 26: 5S rRNA

Chain BB:



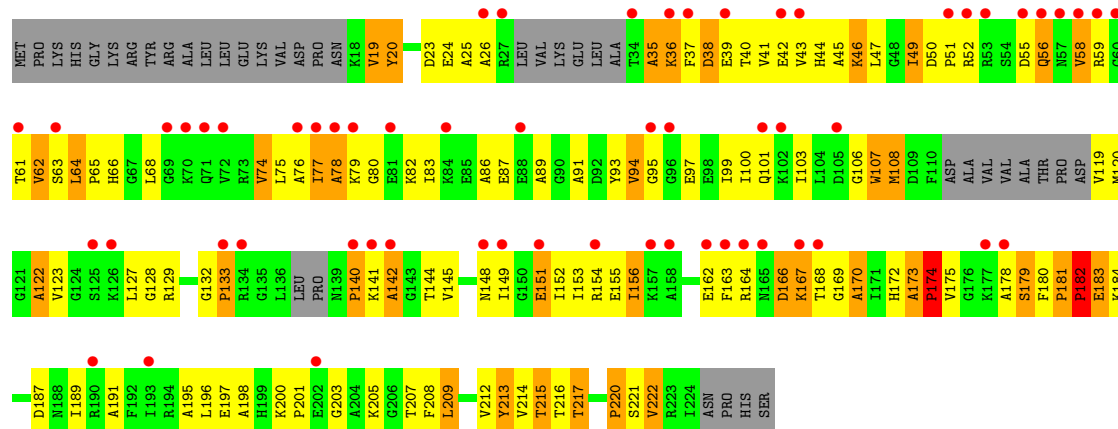
• Molecule 26: 5S rRNA

Chain DB:



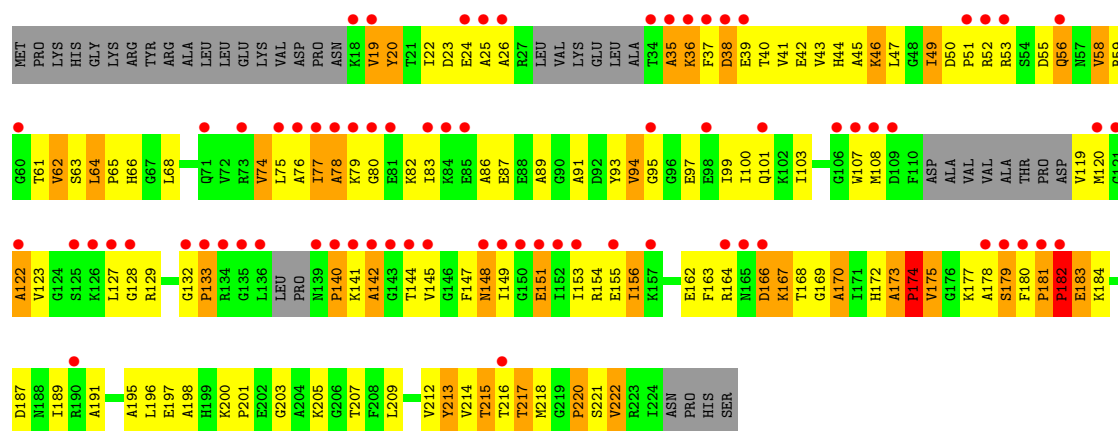
• Molecule 27: 50S ribosomal protein L1

Chain BC:



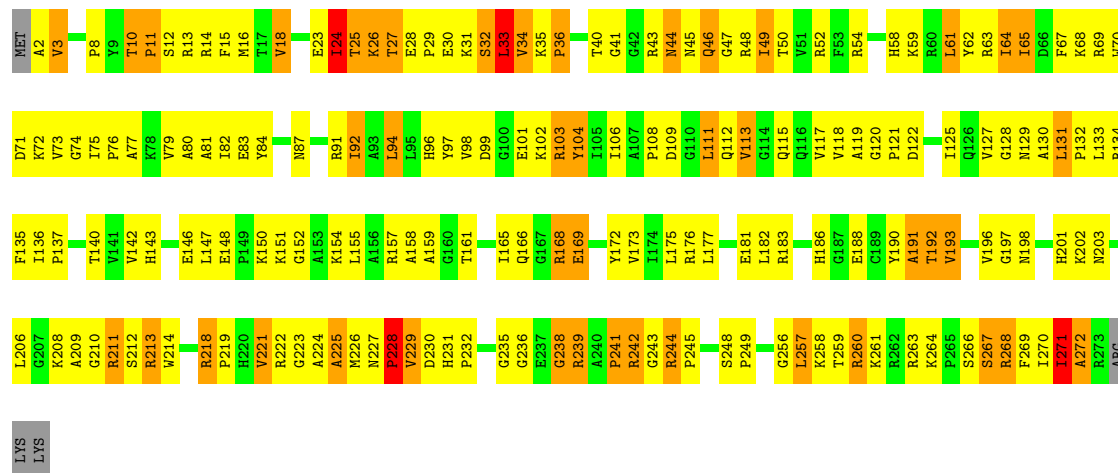
• Molecule 27: 50S ribosomal protein L1

Chain DC:



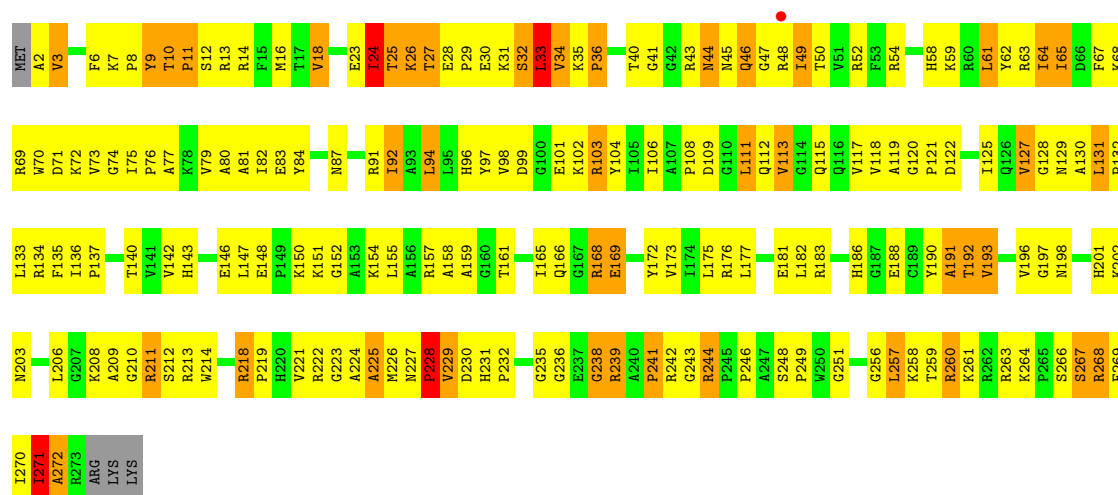
• Molecule 28: 50S ribosomal protein L2

Chain BD:



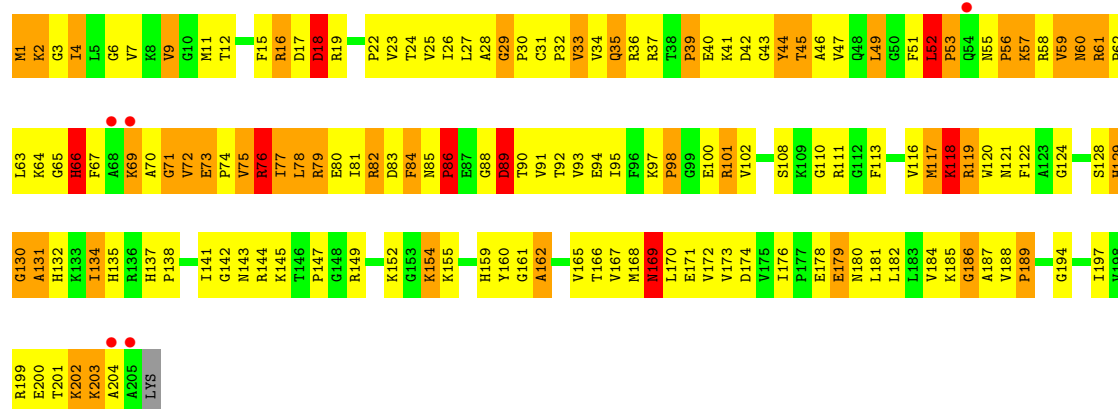
• Molecule 28: 50S ribosomal protein L2

Chain DD:



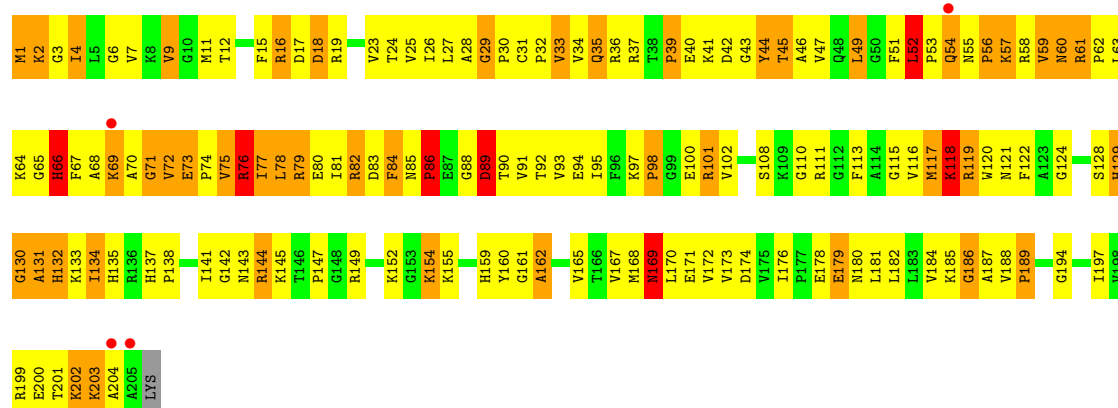
• Molecule 29: 50S ribosomal protein L3

Chain BE:



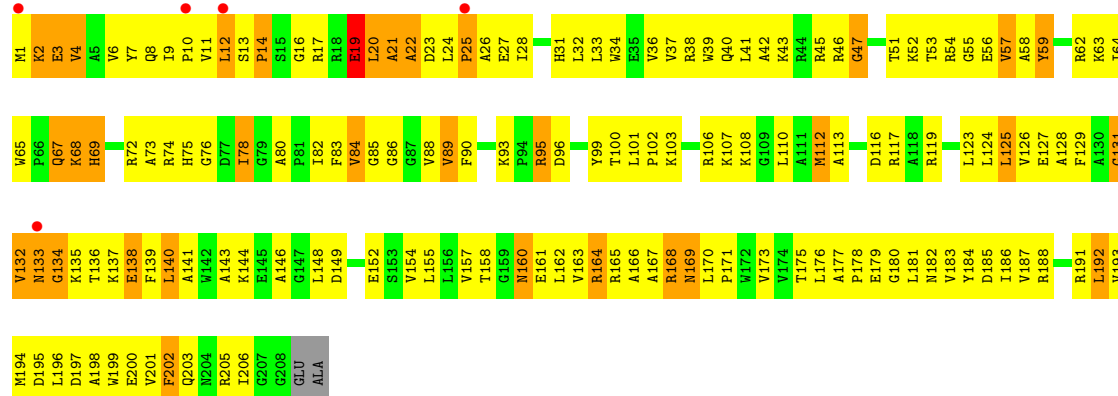
- Molecule 29: 50S ribosomal protein L3

Chain DE:



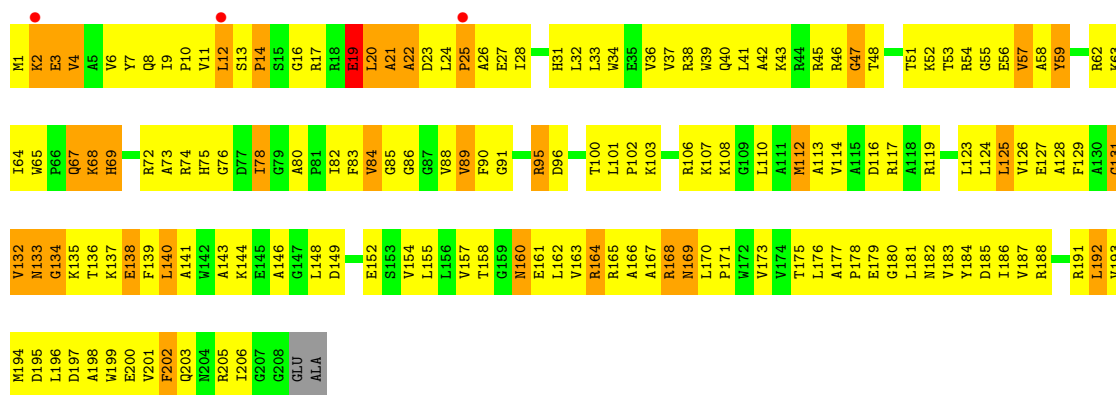
- Molecule 30: 50S ribosomal protein L4

Chain BF:



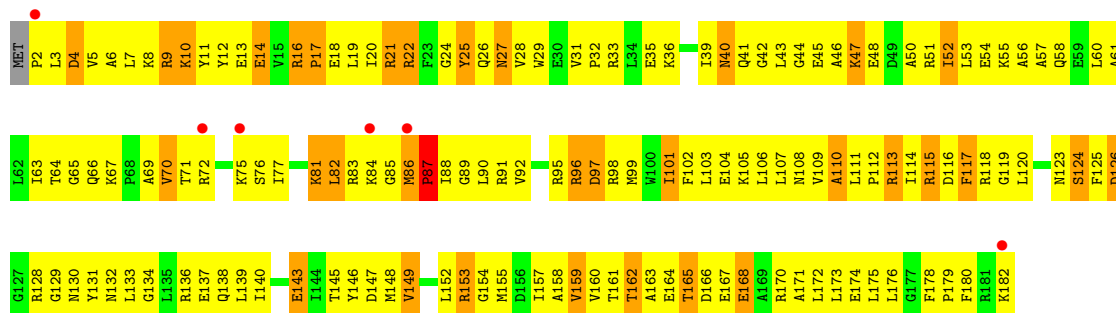
- Molecule 30: 50S ribosomal protein L4

Chain DF:



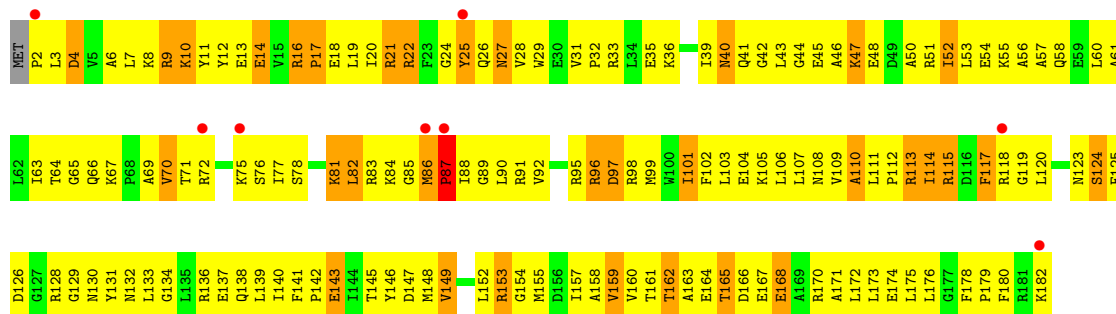
• Molecule 31: 50S ribosomal protein L5

Chain BG:



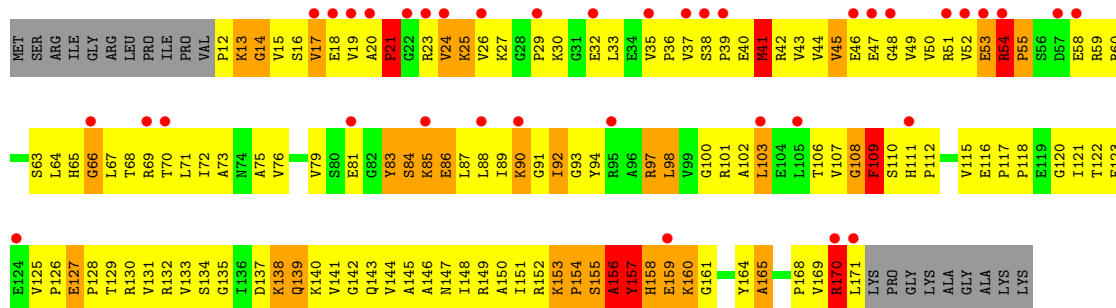
• Molecule 31: 50S ribosomal protein L5

Chain DG:

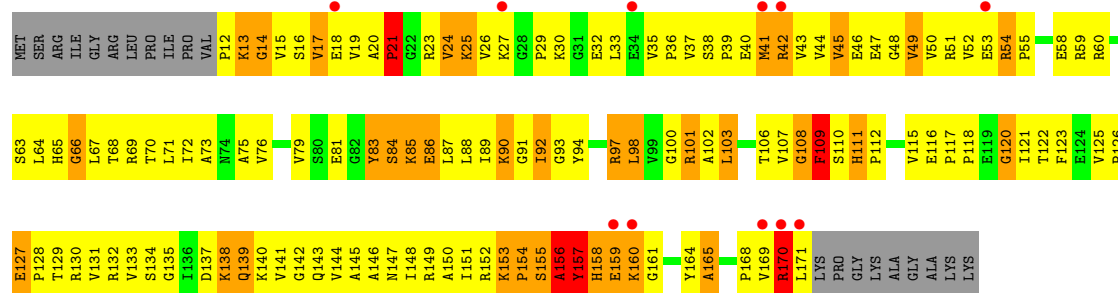


• Molecule 32: 50S ribosomal protein L6

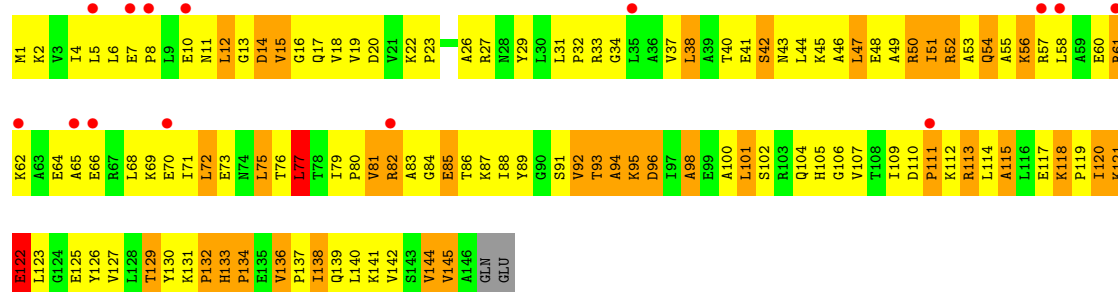
Chain BH:



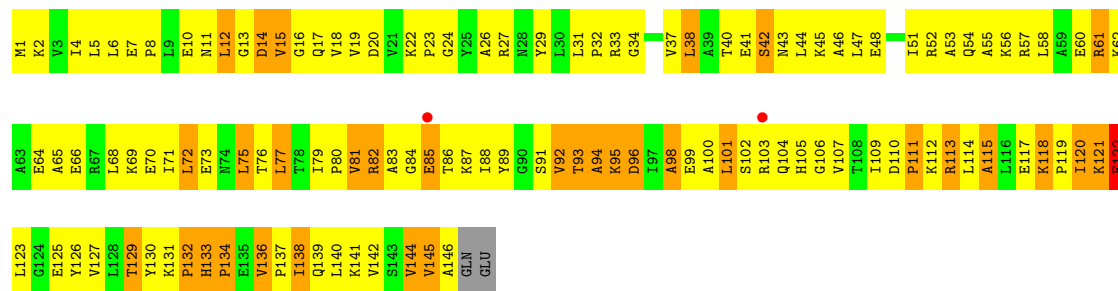
- Molecule 32: 50S ribosomal protein L6

Chain DH: 

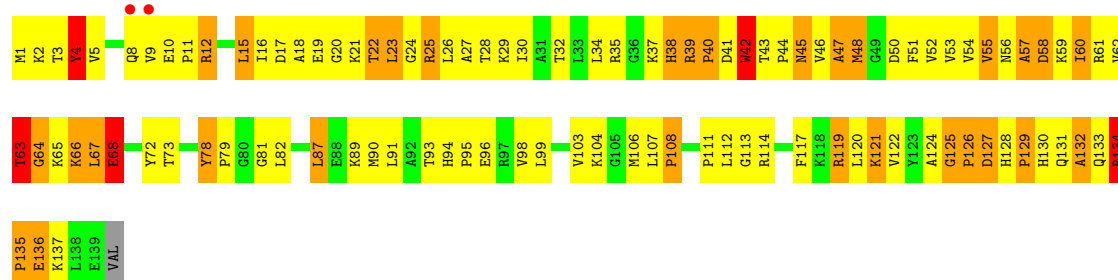
- Molecule 33: 50S ribosomal protein L9

Chain BI: 

- Molecule 33: 50S ribosomal protein L9

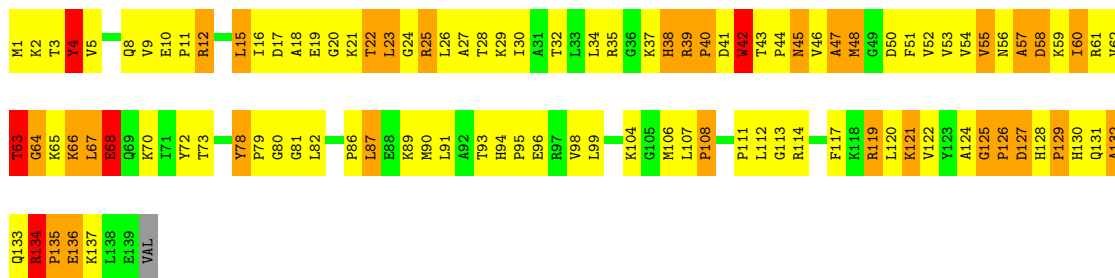
Chain DI: 

- Molecule 34: 50S ribosomal protein L13

Chain BN: 

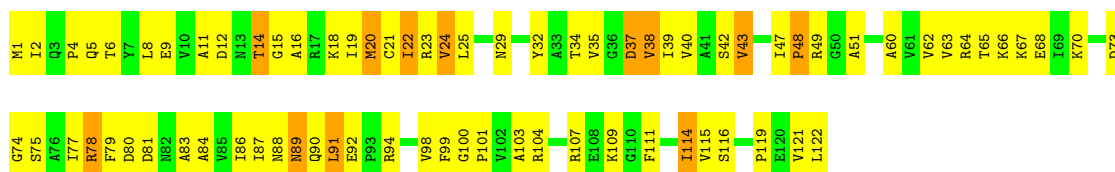
- Molecule 34: 50S ribosomal protein L13

Chain DN:



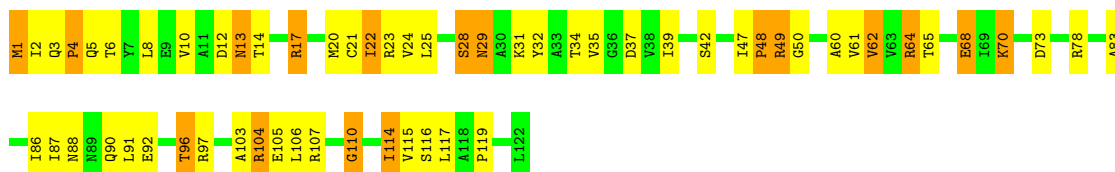
- Molecule 35: 50S ribosomal protein L14

Chain BO:



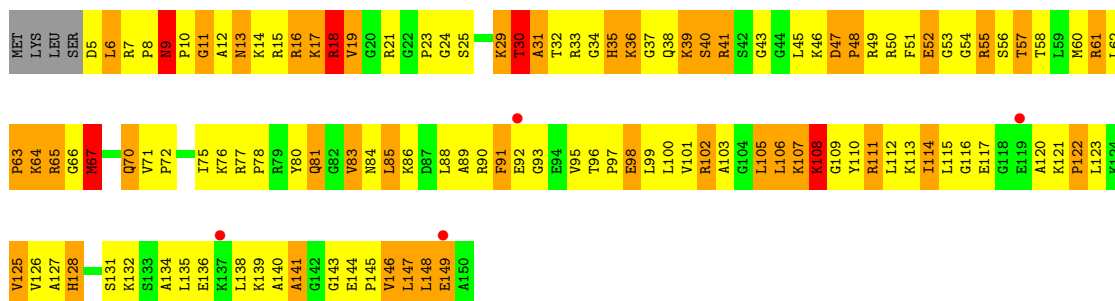
- Molecule 35: 50S ribosomal protein L14

Chain DO:



- Molecule 36: 50S ribosomal protein L15

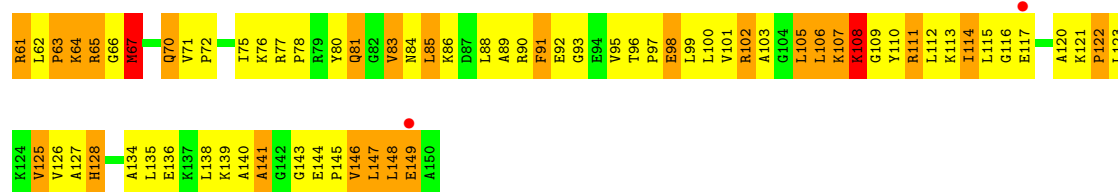
Chain BP:



- Molecule 36: 50S ribosomal protein L15

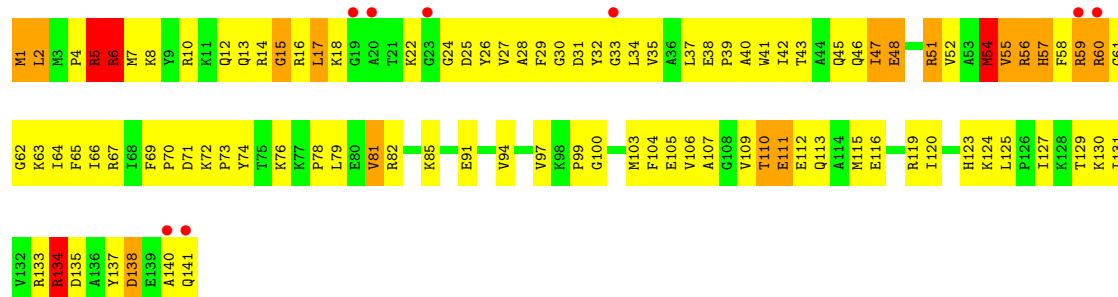
Chain DP:





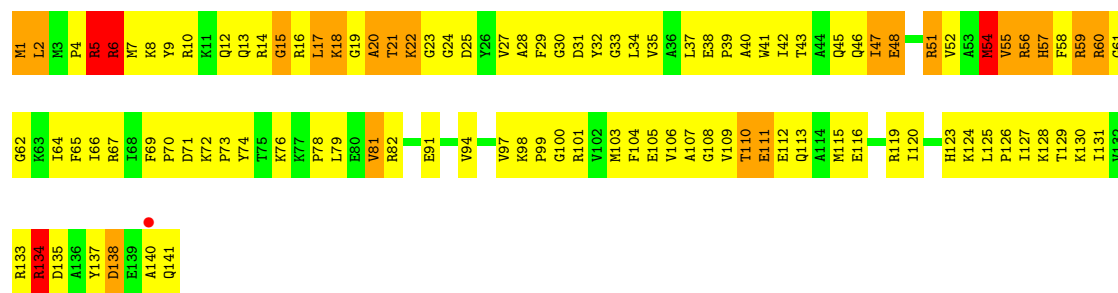
- Molecule 37: 50S ribosomal protein L16

Chain BQ:



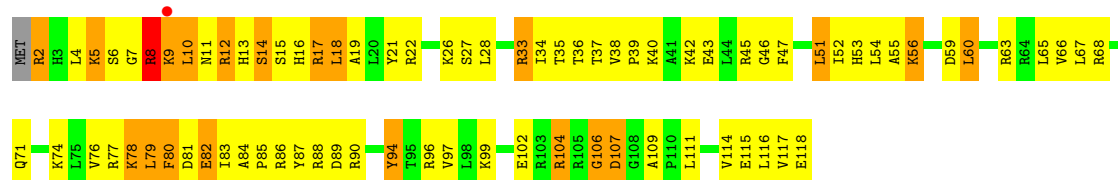
- Molecule 37: 50S ribosomal protein L16

Chain DQ:



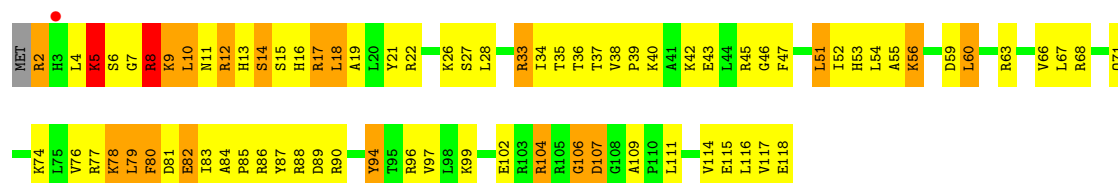
- Molecule 38: 50S ribosomal protein L17

Chain BR:



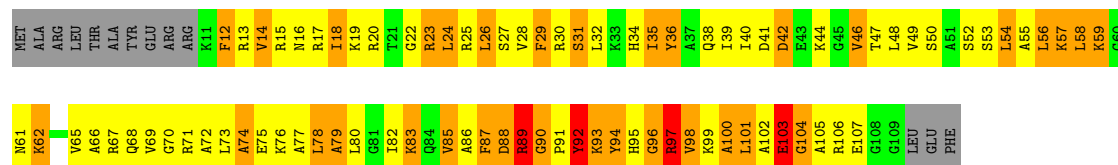
- Molecule 38: 50S ribosomal protein L17

Chain DR:



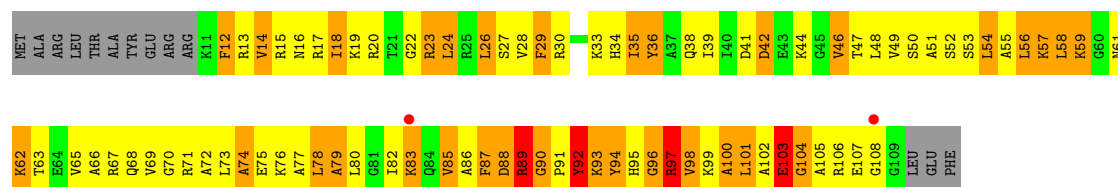
- Molecule 39: 50S ribosomal protein L18

Chain BS:



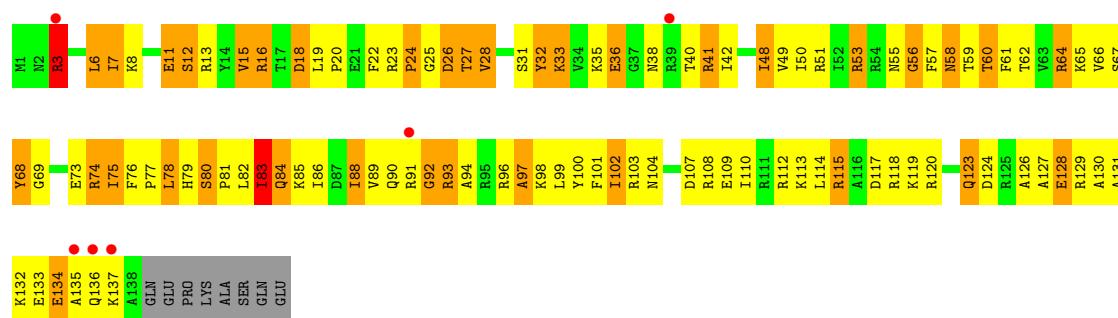
- Molecule 39: 50S ribosomal protein L18

Chain DS:



- Molecule 40: 50S ribosomal protein L19

Chain BT:



- Molecule 40: 50S ribosomal protein L19

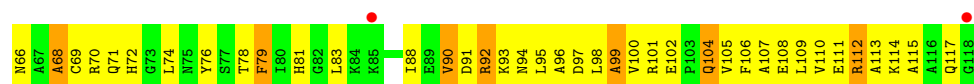
Chain DT:



- Molecule 41: 50S ribosomal protein L20

Chain BU:





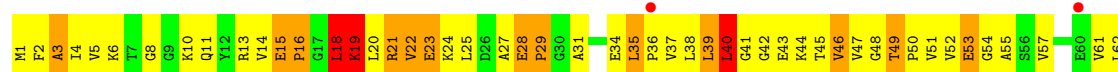
• Molecule 41: 50S ribosomal protein L20

Chain DU:



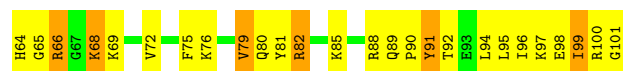
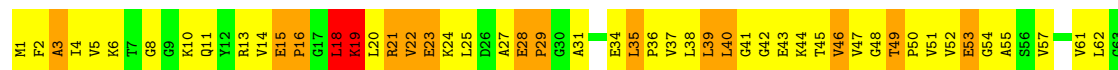
• Molecule 42: 50S ribosomal protein L21

Chain BV:



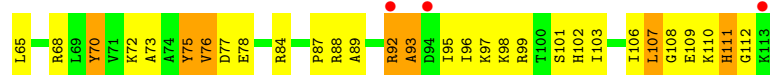
• Molecule 42: 50S ribosomal protein L21

Chain DV:



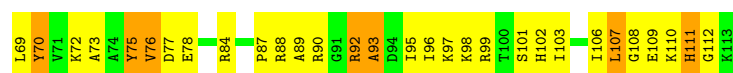
• Molecule 43: 50S ribosomal protein L22

Chain BW:



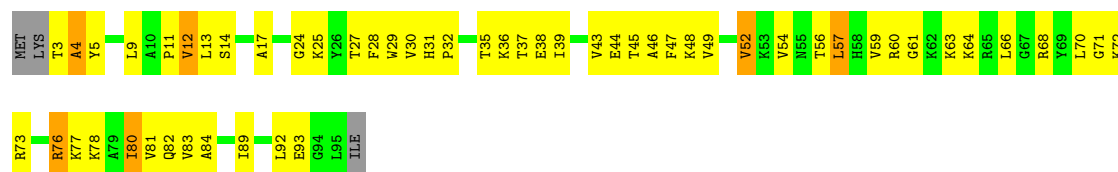
• Molecule 43: 50S ribosomal protein L22

Chain DW:



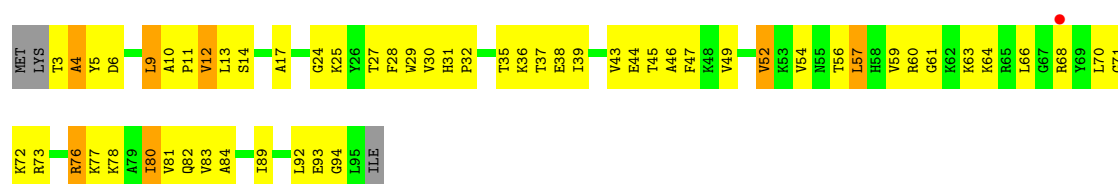
- Molecule 44: 50S ribosomal protein L23

Chain BX:



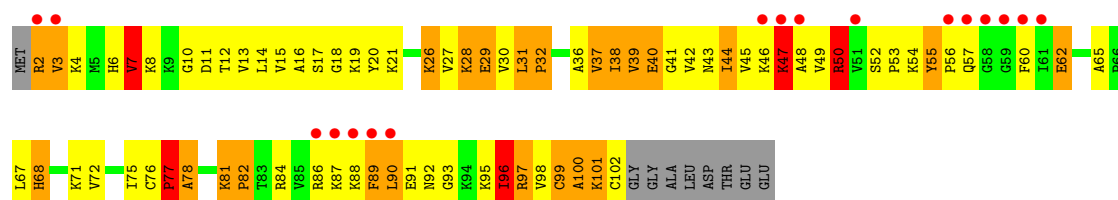
- Molecule 44: 50S ribosomal protein L23

Chain DX:



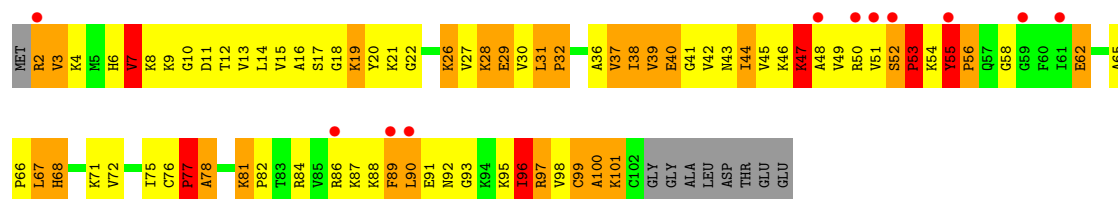
- Molecule 45: 50S ribosomal protein L24

Chain BY:



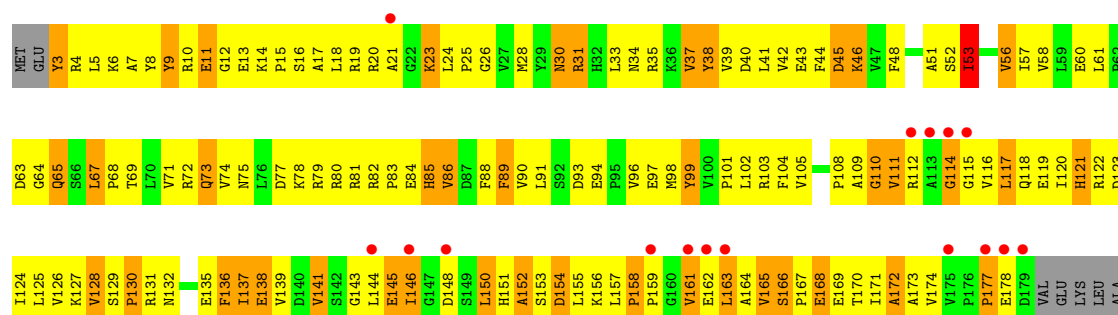
- Molecule 45: 50S ribosomal protein L24

Chain DY:



- Molecule 46: 50S ribosomal protein L25

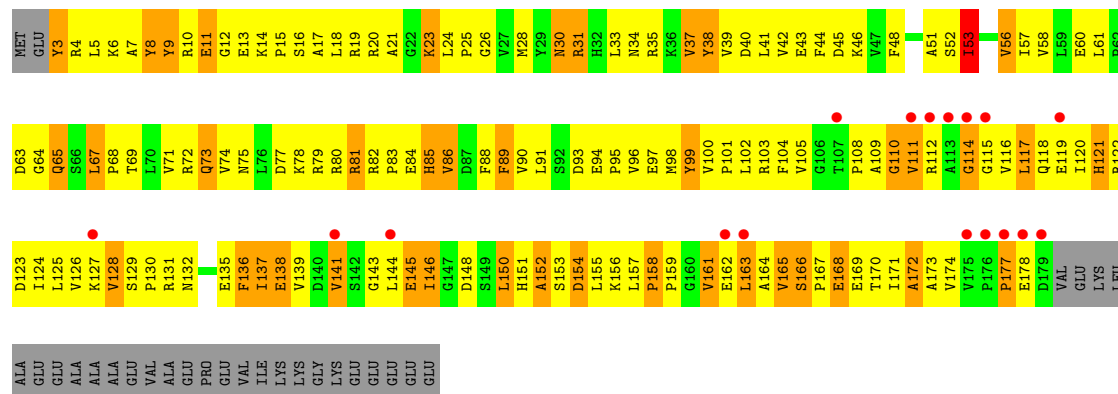
Chain BZ:



GLU
GLU
ALA
ALA
ALA
GLU
VAL
ALA
GLU
PRO
GLU
GLU
ILE
LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU

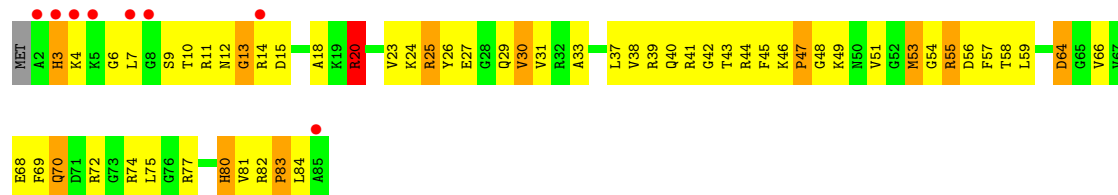
• Molecule 46: 50S ribosomal protein L25

Chain DZ:



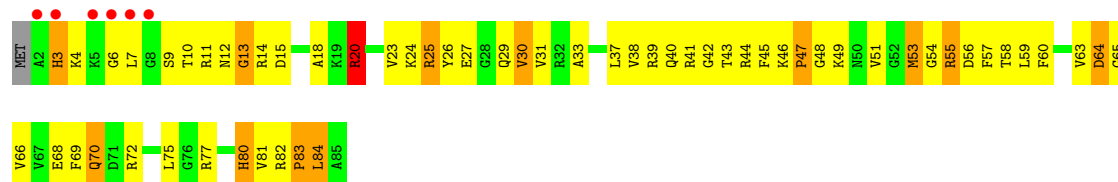
• Molecule 47: 50S ribosomal protein L27

Chain B0:



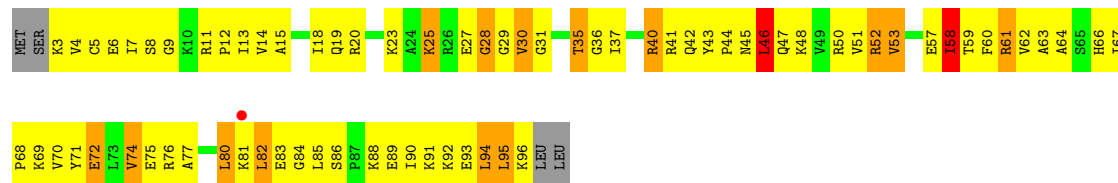
• Molecule 47: 50S ribosomal protein L27

Chain D0:



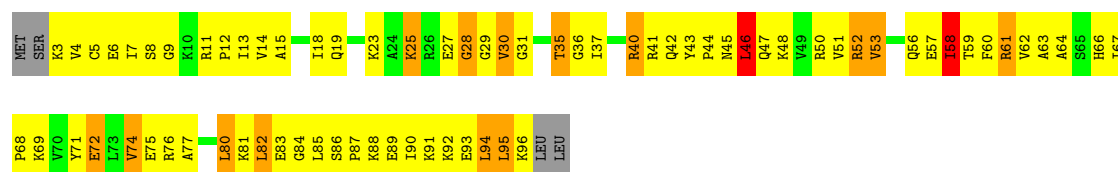
• Molecule 48: 50S ribosomal protein L28

Chain B1:



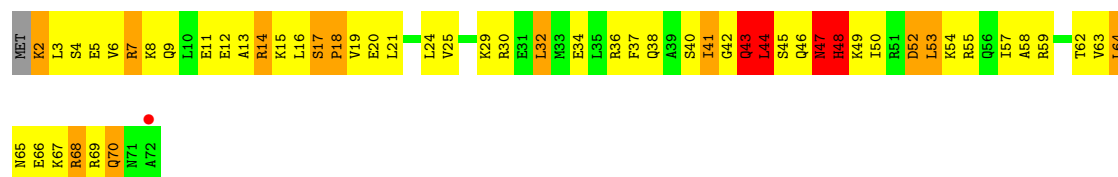
• Molecule 48: 50S ribosomal protein L28

Chain D1:



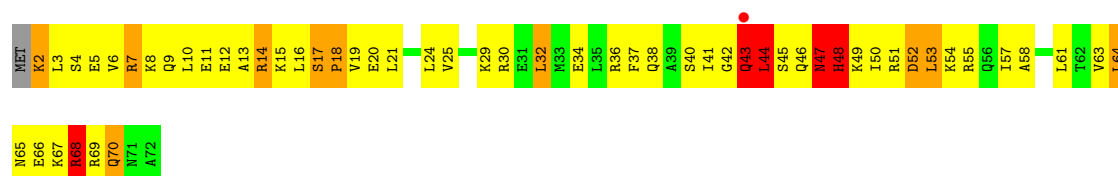
• Molecule 49: 50S ribosomal protein L29

Chain B2:



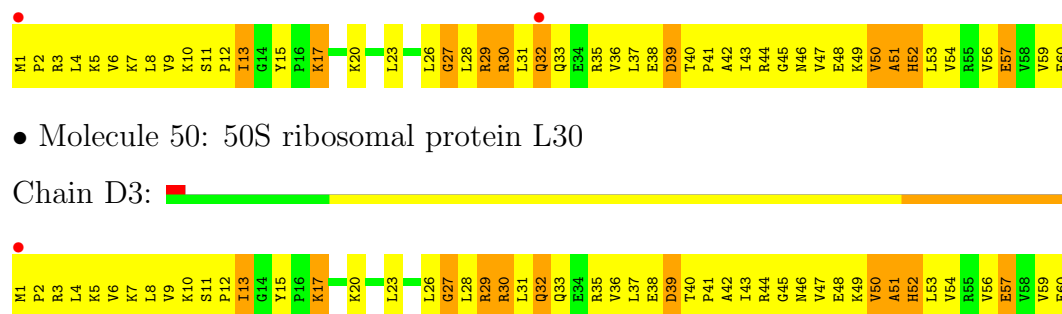
• Molecule 49: 50S ribosomal protein L29

Chain D2:



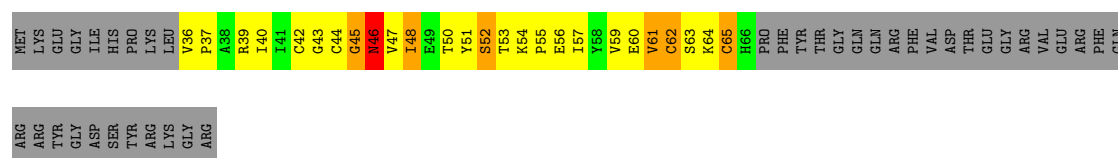
• Molecule 50: 50S ribosomal protein L30

Chain B3:



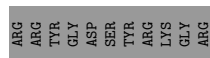
• Molecule 50: 50S ribosomal protein L30

Chain D3:



• Molecule 51: 50S ribosomal protein L31

Chain D4:



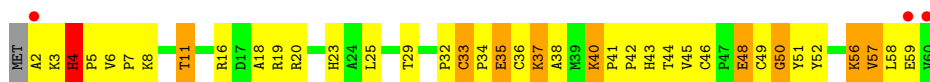
- Molecule 52: 50S ribosomal protein L32

Chain B5:



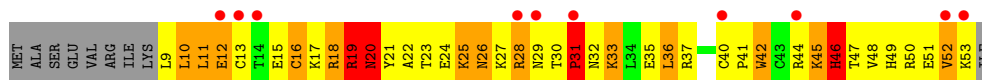
- Molecule 52: 50S ribosomal protein L32

Chain D5:



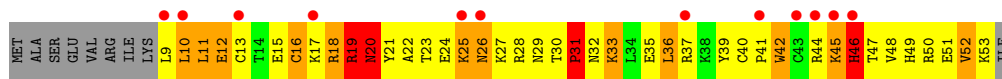
- Molecule 53: 50S ribosomal protein L33

Chain B6:



- Molecule 53: 50S ribosomal protein L33

Chain D6:



- Molecule 54: 50S ribosomal protein L34

Chain B7:



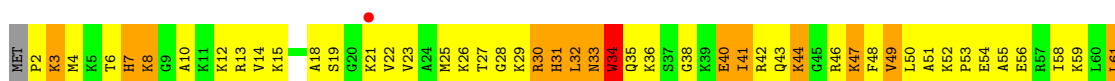
- Molecule 54: 50S ribosomal protein L34

Chain D7:



- Molecule 55: 50S ribosomal protein L35

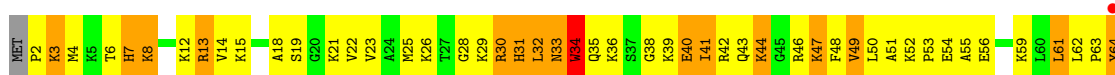
Chain B8:





- Molecule 55: 50S ribosomal protein L35

Chain D8:



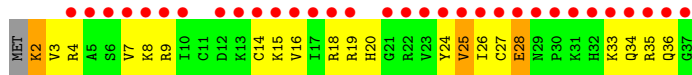
- Molecule 56: 50S ribosomal protein L36

Chain B9:



- Molecule 56: 50S ribosomal protein L36

Chain D9:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.20Å 446.16Å 620.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 34.93 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-3.90) 95.2 (34.93-4.00)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.242 , 0.269 0.253 , 0.277	Depositor DCC
R_{free} test set	20475 reflections (4.61%)	DCC
Wilson B-factor (Å ²)	115.4	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 464342 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	292667	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: ZN, MG, PAR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.53	1/36186 (0.0%)	1.07	56/56479 (0.1%)
1	CA	0.57	0/36161	1.11	53/56440 (0.1%)
2	AB	0.36	0/1936	0.63	0/2611
2	CB	0.35	0/1936	0.62	0/2611
3	AC	0.35	0/1637	0.60	0/2207
3	CC	0.35	0/1637	0.59	0/2207
4	AD	0.39	0/1733	0.66	0/2318
4	CD	0.38	0/1733	0.65	0/2318
5	AE	0.41	0/1163	0.66	0/1566
5	CE	0.41	0/1163	0.66	0/1566
6	AF	0.35	0/856	0.63	0/1154
6	CF	0.36	0/856	0.65	0/1154
7	AG	0.34	0/1276	0.57	0/1709
7	CG	0.34	0/1276	0.57	0/1709
8	AH	0.34	0/1136	0.65	0/1527
8	CH	0.34	0/1136	0.64	0/1527
9	AI	0.35	0/1029	0.62	0/1379
9	CI	0.35	0/1029	0.63	0/1379
10	AJ	0.38	0/808	0.65	0/1087
10	CJ	0.38	0/808	0.64	0/1087
11	AK	0.36	0/900	0.66	0/1213
11	CK	0.36	0/900	0.66	0/1213
12	AL	0.45	0/987	0.78	1/1322 (0.1%)
12	CL	0.43	0/987	0.78	0/1322
13	AM	0.40	0/999	0.72	0/1338
13	CM	0.34	0/999	0.68	1/1338 (0.1%)
14	AN	0.37	0/501	0.63	0/664
14	CN	0.37	0/501	0.63	0/664
15	AO	0.36	0/745	0.58	0/992
15	CO	0.35	0/745	0.58	0/992
16	AP	0.39	0/717	0.65	0/965
16	CP	0.38	0/717	0.63	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.40	0/837	0.65	0/1119
17	CQ	0.36	0/837	0.61	0/1119
18	AR	0.39	0/579	0.71	0/768
18	CR	0.40	0/579	0.70	0/768
19	AS	0.38	0/643	0.68	0/867
19	CS	0.37	0/643	0.62	0/867
20	AT	0.36	0/765	0.66	0/1007
20	CT	0.34	0/765	0.66	0/1007
21	AU	0.71	0/213	0.84	0/279
21	CU	0.75	0/213	0.78	0/279
22	AW	0.51	0/1809	1.00	3/2819 (0.1%)
22	AY	0.74	0/408	1.23	0/634
22	CW	0.53	0/1809	0.99	6/2819 (0.2%)
22	CY	0.85	0/408	1.39	3/634 (0.5%)
23	AV	0.80	0/1836	1.30	11/2859 (0.4%)
23	CV	0.81	0/1836	1.29	9/2859 (0.3%)
24	AX	0.78	0/188	1.33	2/290 (0.7%)
24	CX	0.97	0/235	1.28	2/364 (0.5%)
25	BA	0.52	1/67620 (0.0%)	0.74	24/105555 (0.0%)
25	DA	0.52	2/67620 (0.0%)	0.74	23/105555 (0.0%)
26	BB	0.41	0/2853	0.71	1/4451 (0.0%)
26	DB	0.42	0/2853	0.72	1/4451 (0.0%)
27	BC	0.37	0/1145	0.67	7/1556 (0.4%)
27	DC	0.38	0/1145	0.67	7/1556 (0.4%)
28	BD	0.52	0/2155	0.82	0/2907
28	DD	0.53	0/2155	0.83	0/2907
29	BE	0.44	0/1597	0.78	2/2155 (0.1%)
29	DE	0.44	0/1597	0.77	1/2155 (0.0%)
30	BF	0.45	0/1659	0.74	0/2246
30	DF	0.45	0/1659	0.73	0/2246
31	BG	0.41	0/1499	0.73	1/2016 (0.0%)
31	DG	0.41	0/1499	0.74	1/2016 (0.0%)
32	BH	0.37	0/1246	0.70	2/1684 (0.1%)
32	DH	0.37	0/1246	0.70	2/1684 (0.1%)
33	BI	0.35	0/1147	0.71	0/1553
33	DI	0.37	0/1147	0.71	0/1553
34	BN	0.40	0/1132	0.74	1/1527 (0.1%)
34	DN	0.39	0/1132	0.75	1/1527 (0.1%)
35	BO	0.66	0/943	0.68	0/1269
35	DO	0.82	0/943	0.71	0/1269
36	BP	0.47	0/1131	0.84	0/1504
36	DP	0.45	0/1131	0.82	1/1504 (0.1%)
37	BQ	0.41	0/1143	0.69	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DQ	0.40	0/1143	0.68	0/1527
38	BR	0.40	0/974	0.76	0/1302
38	DR	0.40	0/974	0.77	0/1302
39	BS	0.41	0/779	0.72	0/1038
39	DS	0.38	0/779	0.71	0/1038
40	BT	0.58	0/1156	0.68	0/1544
40	DT	0.65	0/1156	0.70	1/1544 (0.1%)
41	BU	0.39	0/975	0.70	0/1297
41	DU	0.39	0/975	0.70	0/1297
42	BV	0.38	0/790	0.70	0/1057
42	DV	0.39	0/790	0.71	0/1057
43	BW	0.41	0/907	0.69	0/1216
43	DW	0.41	0/907	0.69	0/1216
44	BX	0.49	0/740	0.72	0/995
44	DX	0.49	0/740	0.72	0/995
45	BY	0.49	0/789	0.77	0/1053
45	DY	0.45	0/789	0.79	1/1053 (0.1%)
46	BZ	0.38	0/1436	0.66	0/1951
46	DZ	0.37	0/1436	0.67	0/1951
47	B0	0.39	0/671	0.67	0/892
47	D0	0.39	0/671	0.67	0/892
48	B1	0.46	0/739	0.84	1/983 (0.1%)
48	D1	0.45	0/739	0.84	1/983 (0.1%)
49	B2	0.43	0/600	0.69	0/793
49	D2	0.44	0/600	0.71	0/793
50	B3	0.38	0/473	0.67	0/636
50	D3	0.38	0/473	0.67	0/636
51	B4	0.44	0/229	0.66	0/311
51	D4	0.45	0/229	0.66	0/311
52	B5	0.38	0/473	0.68	0/639
52	D5	0.38	0/473	0.68	0/639
53	B6	0.47	0/388	0.65	0/520
53	D6	0.48	0/388	0.65	0/520
54	B7	0.56	0/427	0.75	0/563
54	D7	0.56	0/427	0.75	0/563
55	B8	0.51	0/516	0.85	0/681
55	D8	0.52	0/516	0.85	0/681
56	B9	0.31	0/302	0.58	0/397
56	D9	0.31	0/302	0.58	0/397
All	All	0.50	4/317064 (0.0%)	0.84	226/474017 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1480	A	N9-C4	5.60	1.41	1.37
25	DA	2307	G	O3'-P	5.54	1.67	1.61
25	BA	271(U)	G	O3'-P	5.17	1.67	1.61
25	DA	271(U)	G	O3'-P	5.13	1.67	1.61

The worst 5 of 226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BE	52	LEU	C-N-CD	-8.27	102.41	120.60
45	DY	55	TYR	C-N-CD	-6.12	107.12	120.60
13	CM	112	GLY	C-N-CD	-6.03	107.34	120.60
23	CV	72	C	N3-C4-C5	-6.00	119.50	121.90
1	CA	1164	A	C8-N9-C4	5.99	108.19	105.80

There are no chirality outliers.

There are no planarity outliers.

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	32326	0	16316	985	0
1	CA	32304	0	16306	977	0
2	AB	1901	0	1951	288	0
2	CB	1901	0	1951	297	0
3	AC	1613	0	1677	215	0
3	CC	1613	0	1677	202	1
4	AD	1703	0	1765	202	0
4	CD	1703	0	1764	152	4
5	AE	1147	0	1207	147	0
5	CE	1147	0	1207	156	0
6	AF	843	0	857	81	0
6	CF	843	0	856	108	0
7	AG	1257	0	1296	137	0
7	CG	1257	0	1296	142	0
8	AH	1116	0	1177	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	CH	1116	0	1177	169	0
9	AI	1010	0	1037	169	0
9	CI	1010	0	1037	135	0
10	AJ	795	0	840	143	0
10	CJ	795	0	840	137	0
11	AK	885	0	904	104	1
11	CK	885	0	904	120	0
12	AL	971	0	1057	129	0
12	CL	971	0	1057	134	0
13	AM	988	0	1059	197	0
13	CM	988	0	1059	203	0
14	AN	492	0	531	88	0
14	CN	492	0	532	92	0
15	AO	734	0	771	70	0
15	CO	734	0	771	71	0
16	AP	701	0	720	56	0
16	CP	701	0	720	58	0
17	AQ	824	0	891	77	0
17	CQ	824	0	891	74	0
18	AR	574	0	644	61	0
18	CR	574	0	644	63	0
19	AS	630	0	652	102	0
19	CS	630	0	652	119	0
20	AT	763	0	861	114	0
20	CT	763	0	861	153	0
21	AU	209	0	221	10	0
21	CU	209	0	221	20	0
22	AW	1619	0	822	155	0
22	AY	365	0	185	55	0
22	CW	1619	0	822	203	0
22	CY	365	0	185	45	0
23	AV	1644	0	836	169	0
23	CV	1644	0	836	173	0
24	AX	169	0	86	17	0
24	CX	210	0	109	24	0
25	BA	60378	0	30440	2704	3
25	DA	60378	0	30441	2817	12
26	BB	2551	0	1295	140	1
26	DB	2551	0	1295	193	1
27	BC	1142	0	865	103	0
27	DC	1142	0	865	135	0
28	BD	2105	0	2182	296	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	DD	2105	0	2182	328	0
29	BE	1564	0	1629	269	0
29	DE	1564	0	1629	280	0
30	BF	1624	0	1677	241	0
30	DF	1624	0	1677	234	0
31	BG	1474	0	1535	318	0
31	DG	1474	0	1535	292	0
32	BH	1223	0	1282	198	0
32	DH	1223	0	1282	236	2
33	BI	1132	0	1218	217	0
33	DI	1132	0	1218	214	0
34	BN	1105	0	1180	169	0
34	DN	1105	0	1180	170	0
35	BO	933	0	995	88	0
35	DO	933	0	996	78	0
36	BP	1114	0	1187	318	0
36	DP	1114	0	1187	299	8
37	BQ	1122	0	1179	154	0
37	DQ	1122	0	1179	184	0
38	BR	960	0	1021	143	0
38	DR	960	0	1021	144	0
39	BS	771	0	832	194	0
39	DS	771	0	832	196	0
40	BT	1142	0	1202	149	0
40	DT	1142	0	1202	225	0
41	BU	958	0	1015	170	0
41	DU	958	0	1015	173	0
42	BV	779	0	852	169	0
42	DV	779	0	852	174	3
43	BW	896	0	953	107	1
43	DW	896	0	953	112	0
44	BX	726	0	778	72	0
44	DX	726	0	778	74	0
45	BY	776	0	870	158	11
45	DY	776	0	870	184	2
46	BZ	1404	0	1432	219	0
46	DZ	1404	0	1432	230	0
47	B0	662	0	688	79	0
47	D0	662	0	688	77	0
48	B1	732	0	808	98	0
48	D1	732	0	808	91	0
49	B2	598	0	653	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	D2	598	0	653	86	1
50	B3	468	0	523	67	8
50	D3	468	0	523	73	0
51	B4	226	0	229	46	0
51	D4	226	0	229	37	0
52	B5	459	0	480	64	0
52	D5	459	0	480	60	3
53	B6	381	0	391	74	0
53	D6	381	0	391	75	0
54	B7	419	0	467	42	0
54	D7	419	0	467	45	0
55	B8	508	0	576	109	0
55	D8	508	0	576	104	0
56	B9	299	0	326	24	0
56	D9	299	0	326	21	0
57	AA	93	0	0	0	0
57	AX	2	0	0	0	0
57	B1	1	0	0	0	0
57	B3	1	0	0	0	0
57	B5	2	0	0	0	0
57	BA	261	0	0	7	0
57	BB	4	0	0	0	0
57	BE	1	0	0	0	0
57	BF	2	0	0	0	0
57	BO	1	0	0	0	0
57	BU	1	0	0	0	0
57	CA	94	0	0	0	0
57	CV	2	0	0	0	0
57	D0	1	0	0	0	0
57	D5	2	0	0	0	0
57	DA	268	0	0	0	0
57	DB	2	0	0	0	0
57	DD	1	0	0	0	0
57	DE	1	0	0	0	0
58	AA	42	0	45	3	0
58	CA	42	0	45	1	0
59	AD	1	0	0	1	0
59	AN	1	0	0	2	0
59	CD	1	0	0	0	0
59	CN	1	0	0	0	0
All	All	292667	0	198350	20561	33

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 42.

The worst 5 of 20561 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:CM:93:ARG:CD	25:DA:888:C:H5'	1.15	1.61
4:AD:167:GLY:CA	28:DD:135:PHE:CE2	1.85	1.56
25:BA:2584:U:C2'	25:BA:2585:U:H5''	1.38	1.54
25:DA:2584:U:C2'	25:DA:2585:U:H5''	1.38	1.54
4:AD:167:GLY:HA3	28:DD:135:PHE:CE2	1.43	1.50

The worst 5 of 33 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
45:BY:55:TYR:CZ	25:DA:355:G:O2'[3_555]	0.78	1.42
45:BY:55:TYR:OH	25:DA:355:G:C2'[3_555]	1.05	1.15
50:B3:1:MET:CB	36:DP:122:PRO:CG[3_455]	1.20	1.00
50:B3:1:MET:CG	36:DP:122:PRO:CB[3_455]	1.33	0.87
45:BY:55:TYR:CE2	25:DA:355:G:O2'[3_555]	1.37	0.83

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	233/256 (91%)	148 (64%)	65 (28%)	20 (9%)	1	25
2	CB	233/256 (91%)	148 (64%)	65 (28%)	20 (9%)	1	25
3	AC	205/239 (86%)	136 (66%)	45 (22%)	24 (12%)	1	14
3	CC	205/239 (86%)	137 (67%)	43 (21%)	25 (12%)	1	14
4	AD	206/209 (99%)	145 (70%)	40 (19%)	21 (10%)	1	19
4	CD	206/209 (99%)	144 (70%)	40 (19%)	22 (11%)	1	17
5	AE	149/162 (92%)	114 (76%)	19 (13%)	16 (11%)	1	17
5	CE	149/162 (92%)	114 (76%)	19 (13%)	16 (11%)	1	17
6	AF	99/101 (98%)	82 (83%)	13 (13%)	4 (4%)	5	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	CF	99/101 (98%)	81 (82%)	15 (15%)	3 (3%)	7	59
7	AG	153/156 (98%)	107 (70%)	32 (21%)	14 (9%)	1	24
7	CG	153/156 (98%)	107 (70%)	32 (21%)	14 (9%)	1	24
8	AH	136/138 (99%)	102 (75%)	26 (19%)	8 (6%)	2	38
8	CH	136/138 (99%)	100 (74%)	28 (21%)	8 (6%)	2	38
9	AI	125/128 (98%)	92 (74%)	21 (17%)	12 (10%)	1	21
9	CI	125/128 (98%)	93 (74%)	22 (18%)	10 (8%)	1	28
10	AJ	97/105 (92%)	66 (68%)	22 (23%)	9 (9%)	1	23
10	CJ	97/105 (92%)	67 (69%)	21 (22%)	9 (9%)	1	23
11	AK	117/129 (91%)	94 (80%)	18 (15%)	5 (4%)	4	48
11	CK	117/129 (91%)	92 (79%)	20 (17%)	5 (4%)	4	48
12	AL	123/132 (93%)	86 (70%)	24 (20%)	13 (11%)	1	17
12	CL	123/132 (93%)	85 (69%)	25 (20%)	13 (11%)	1	17
13	AM	123/126 (98%)	79 (64%)	26 (21%)	18 (15%)	0	9
13	CM	123/126 (98%)	84 (68%)	23 (19%)	16 (13%)	0	12
14	AN	58/61 (95%)	37 (64%)	9 (16%)	12 (21%)	0	3
14	CN	58/61 (95%)	37 (64%)	9 (16%)	12 (21%)	0	3
15	AO	86/89 (97%)	62 (72%)	19 (22%)	5 (6%)	3	39
15	CO	86/89 (97%)	63 (73%)	18 (21%)	5 (6%)	3	39
16	AP	82/88 (93%)	57 (70%)	22 (27%)	3 (4%)	5	53
16	CP	82/88 (93%)	58 (71%)	21 (26%)	3 (4%)	5	53
17	AQ	98/105 (93%)	77 (79%)	14 (14%)	7 (7%)	2	32
17	CQ	98/105 (93%)	77 (79%)	13 (13%)	8 (8%)	1	27
18	AR	68/88 (77%)	48 (71%)	15 (22%)	5 (7%)	2	31
18	CR	68/88 (77%)	45 (66%)	17 (25%)	6 (9%)	1	25
19	AS	77/93 (83%)	55 (71%)	11 (14%)	11 (14%)	0	10
19	CS	77/93 (83%)	55 (71%)	12 (16%)	10 (13%)	0	12
20	AT	97/106 (92%)	72 (74%)	14 (14%)	11 (11%)	1	16
20	CT	97/106 (92%)	72 (74%)	15 (16%)	10 (10%)	1	19
21	AU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	6
21	CU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	1	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	BC	183/229 (80%)	84 (46%)	45 (25%)	54 (30%)	0	1
27	DC	183/229 (80%)	84 (46%)	44 (24%)	55 (30%)	0	1
28	BD	270/276 (98%)	212 (78%)	33 (12%)	25 (9%)	1	23
28	DD	270/276 (98%)	209 (77%)	36 (13%)	25 (9%)	1	23
29	BE	203/206 (98%)	130 (64%)	35 (17%)	38 (19%)	0	4
29	DE	203/206 (98%)	129 (64%)	36 (18%)	38 (19%)	0	4
30	BF	206/210 (98%)	129 (63%)	54 (26%)	23 (11%)	1	16
30	DF	206/210 (98%)	128 (62%)	55 (27%)	23 (11%)	1	16
31	BG	179/182 (98%)	115 (64%)	39 (22%)	25 (14%)	0	10
31	DG	179/182 (98%)	114 (64%)	39 (22%)	26 (14%)	0	9
32	BH	158/180 (88%)	93 (59%)	31 (20%)	34 (22%)	0	3
32	DH	158/180 (88%)	95 (60%)	31 (20%)	32 (20%)	0	4
33	BI	144/148 (97%)	89 (62%)	28 (19%)	27 (19%)	0	4
33	DI	144/148 (97%)	87 (60%)	30 (21%)	27 (19%)	0	4
34	BN	137/140 (98%)	84 (61%)	33 (24%)	20 (15%)	0	9
34	DN	137/140 (98%)	84 (61%)	33 (24%)	20 (15%)	0	9
35	BO	120/122 (98%)	88 (73%)	25 (21%)	7 (6%)	3	39
35	DO	120/122 (98%)	94 (78%)	16 (13%)	10 (8%)	1	27
36	BP	144/150 (96%)	83 (58%)	32 (22%)	29 (20%)	0	4
36	DP	144/150 (96%)	81 (56%)	33 (23%)	30 (21%)	0	3
37	BQ	139/141 (99%)	104 (75%)	19 (14%)	16 (12%)	1	15
37	DQ	139/141 (99%)	104 (75%)	17 (12%)	18 (13%)	0	13
38	BR	115/118 (98%)	83 (72%)	22 (19%)	10 (9%)	1	25
38	DR	115/118 (98%)	83 (72%)	21 (18%)	11 (10%)	1	21
39	BS	97/112 (87%)	38 (39%)	27 (28%)	32 (33%)	0	0
39	DS	97/112 (87%)	38 (39%)	27 (28%)	32 (33%)	0	0
40	BT	136/146 (93%)	82 (60%)	31 (23%)	23 (17%)	0	6
40	DT	136/146 (93%)	88 (65%)	33 (24%)	15 (11%)	1	16
41	BU	115/118 (98%)	70 (61%)	34 (30%)	11 (10%)	1	21
41	DU	115/118 (98%)	70 (61%)	34 (30%)	11 (10%)	1	21
42	BV	99/101 (98%)	63 (64%)	19 (19%)	17 (17%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	DV	99/101 (98%)	64 (65%)	19 (19%)	16 (16%)	0	7
43	BW	111/113 (98%)	75 (68%)	24 (22%)	12 (11%)	1	17
43	DW	111/113 (98%)	75 (68%)	24 (22%)	12 (11%)	1	17
44	BX	91/96 (95%)	66 (72%)	20 (22%)	5 (6%)	3	41
44	DX	91/96 (95%)	66 (72%)	20 (22%)	5 (6%)	3	41
45	BY	99/110 (90%)	54 (54%)	18 (18%)	27 (27%)	0	1
45	DY	99/110 (90%)	53 (54%)	16 (16%)	30 (30%)	0	1
46	BZ	175/206 (85%)	103 (59%)	35 (20%)	37 (21%)	0	3
46	DZ	175/206 (85%)	103 (59%)	35 (20%)	37 (21%)	0	3
47	B0	82/85 (96%)	63 (77%)	12 (15%)	7 (8%)	1	26
47	D0	82/85 (96%)	63 (77%)	12 (15%)	7 (8%)	1	26
48	B1	92/98 (94%)	64 (70%)	19 (21%)	9 (10%)	1	21
48	D1	92/98 (94%)	64 (70%)	19 (21%)	9 (10%)	1	21
49	B2	69/72 (96%)	47 (68%)	13 (19%)	9 (13%)	0	12
49	D2	69/72 (96%)	51 (74%)	9 (13%)	9 (13%)	0	12
50	B3	58/60 (97%)	41 (71%)	7 (12%)	10 (17%)	0	6
50	D3	58/60 (97%)	41 (71%)	7 (12%)	10 (17%)	0	6
51	B4	29/71 (41%)	15 (52%)	7 (24%)	7 (24%)	0	2
51	D4	29/71 (41%)	15 (52%)	7 (24%)	7 (24%)	0	2
52	B5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	1	14
52	D5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	1	14
53	B6	43/54 (80%)	20 (46%)	12 (28%)	11 (26%)	0	2
53	D6	43/54 (80%)	20 (46%)	12 (28%)	11 (26%)	0	2
54	B7	47/49 (96%)	44 (94%)	2 (4%)	1 (2%)	11	66
54	D7	47/49 (96%)	44 (94%)	2 (4%)	1 (2%)	11	66
55	B8	62/65 (95%)	40 (64%)	13 (21%)	9 (14%)	0	9
55	D8	62/65 (95%)	39 (63%)	14 (23%)	9 (14%)	0	9
56	B9	34/37 (92%)	27 (79%)	6 (18%)	1 (3%)	7	59
56	D9	34/37 (92%)	27 (79%)	6 (18%)	1 (3%)	7	59
All	All	11698/12586 (93%)	7854 (67%)	2318 (20%)	1526 (13%)	0	12

5 of 1526 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL
2	AB	20	GLU
2	AB	88	ALA
2	AB	195	ASP

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	202/220 (92%)	177 (88%)	25 (12%)	7	41
2	CB	202/220 (92%)	179 (89%)	23 (11%)	8	44
3	AC	160/188 (85%)	149 (93%)	11 (7%)	22	69
3	CC	160/188 (85%)	149 (93%)	11 (7%)	22	69
4	AD	180/181 (99%)	161 (89%)	19 (11%)	10	49
4	CD	180/181 (99%)	161 (89%)	19 (11%)	10	49
5	AE	115/123 (94%)	101 (88%)	14 (12%)	7	41
5	CE	115/123 (94%)	101 (88%)	14 (12%)	7	41
6	AF	90/90 (100%)	83 (92%)	7 (8%)	18	64
6	CF	90/90 (100%)	85 (94%)	5 (6%)	30	77
7	AG	126/127 (99%)	117 (93%)	9 (7%)	21	69
7	CG	126/127 (99%)	117 (93%)	9 (7%)	21	69
8	AH	119/119 (100%)	112 (94%)	7 (6%)	28	75
8	CH	119/119 (100%)	110 (92%)	9 (8%)	19	66
9	AI	98/99 (99%)	86 (88%)	12 (12%)	7	41
9	CI	98/99 (99%)	83 (85%)	15 (15%)	4	29
10	AJ	88/92 (96%)	76 (86%)	12 (14%)	5	36
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	7	40
11	AK	90/99 (91%)	82 (91%)	8 (9%)	14	58
11	CK	90/99 (91%)	82 (91%)	8 (9%)	14	58
12	AL	104/109 (95%)	94 (90%)	10 (10%)	12	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	CL	104/109 (95%)	92 (88%)	12 (12%)	8	44
13	AM	99/101 (98%)	81 (82%)	18 (18%)	2	19
13	CM	99/101 (98%)	83 (84%)	16 (16%)	3	26
14	AN	49/50 (98%)	40 (82%)	9 (18%)	2	18
14	CN	49/50 (98%)	42 (86%)	7 (14%)	5	33
15	AO	79/80 (99%)	73 (92%)	6 (8%)	19	66
15	CO	79/80 (99%)	73 (92%)	6 (8%)	19	66
16	AP	72/74 (97%)	64 (89%)	8 (11%)	9	46
16	CP	72/74 (97%)	66 (92%)	6 (8%)	16	62
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	12	54
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	20	67
18	AR	61/77 (79%)	57 (93%)	4 (7%)	24	72
18	CR	61/77 (79%)	57 (93%)	4 (7%)	24	72
19	AS	69/80 (86%)	58 (84%)	11 (16%)	4	27
19	CS	69/80 (86%)	58 (84%)	11 (16%)	4	27
20	AT	76/82 (93%)	71 (93%)	5 (7%)	24	72
20	CT	76/82 (93%)	69 (91%)	7 (9%)	13	56
21	AU	19/22 (86%)	18 (95%)	1 (5%)	32	79
21	CU	19/22 (86%)	14 (74%)	5 (26%)	1	7
27	BC	61/181 (34%)	56 (92%)	5 (8%)	17	62
27	DC	61/181 (34%)	56 (92%)	5 (8%)	17	62
28	BD	213/218 (98%)	179 (84%)	34 (16%)	3	27
28	DD	213/218 (98%)	180 (84%)	33 (16%)	4	28
29	BE	165/166 (99%)	140 (85%)	25 (15%)	4	30
29	DE	165/166 (99%)	139 (84%)	26 (16%)	4	28
30	BF	165/166 (99%)	146 (88%)	19 (12%)	8	44
30	DF	165/166 (99%)	146 (88%)	19 (12%)	8	44
31	BG	155/156 (99%)	138 (89%)	17 (11%)	9	47
31	DG	155/156 (99%)	138 (89%)	17 (11%)	9	47
32	BH	132/148 (89%)	119 (90%)	13 (10%)	12	53
32	DH	132/148 (89%)	119 (90%)	13 (10%)	12	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	BI	122/124 (98%)	102 (84%)	20 (16%)	3	25
33	DI	122/124 (98%)	107 (88%)	15 (12%)	7	41
34	BN	117/119 (98%)	96 (82%)	21 (18%)	2	20
34	DN	117/119 (98%)	96 (82%)	21 (18%)	2	20
35	BO	100/100 (100%)	92 (92%)	8 (8%)	17	64
35	DO	100/100 (100%)	83 (83%)	17 (17%)	3	23
36	BP	112/116 (97%)	86 (77%)	26 (23%)	1	9
36	DP	112/116 (97%)	89 (80%)	23 (20%)	2	13
37	BQ	111/111 (100%)	96 (86%)	15 (14%)	6	36
37	DQ	111/111 (100%)	94 (85%)	17 (15%)	4	29
38	BR	100/101 (99%)	87 (87%)	13 (13%)	6	38
38	DR	100/101 (99%)	87 (87%)	13 (13%)	6	38
39	BS	77/88 (88%)	66 (86%)	11 (14%)	5	33
39	DS	77/88 (88%)	67 (87%)	10 (13%)	6	38
40	BT	120/127 (94%)	90 (75%)	30 (25%)	1	8
40	DT	120/127 (94%)	85 (71%)	35 (29%)	0	5
41	BU	92/94 (98%)	85 (92%)	7 (8%)	19	66
41	DU	92/94 (98%)	85 (92%)	7 (8%)	19	66
42	BV	82/82 (100%)	72 (88%)	10 (12%)	7	41
42	DV	82/82 (100%)	72 (88%)	10 (12%)	7	41
43	BW	91/92 (99%)	82 (90%)	9 (10%)	11	52
43	DW	91/92 (99%)	81 (89%)	10 (11%)	9	47
44	BX	74/78 (95%)	67 (90%)	7 (10%)	12	54
44	DX	74/78 (95%)	67 (90%)	7 (10%)	12	54
45	BY	84/91 (92%)	72 (86%)	12 (14%)	5	33
45	DY	84/91 (92%)	70 (83%)	14 (17%)	3	24
46	BZ	155/179 (87%)	138 (89%)	17 (11%)	9	47
46	DZ	155/179 (87%)	137 (88%)	18 (12%)	8	44
47	B0	66/67 (98%)	58 (88%)	8 (12%)	7	41
47	D0	66/67 (98%)	58 (88%)	8 (12%)	7	41
48	B1	78/83 (94%)	67 (86%)	11 (14%)	5	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	D1	78/83 (94%)	67 (86%)	11 (14%)	5	34
49	B2	66/67 (98%)	55 (83%)	11 (17%)	3	24
49	D2	66/67 (98%)	55 (83%)	11 (17%)	3	24
50	B3	51/52 (98%)	49 (96%)	2 (4%)	43	85
50	D3	51/52 (98%)	49 (96%)	2 (4%)	43	85
51	B4	27/63 (43%)	24 (89%)	3 (11%)	9	46
51	D4	27/63 (43%)	24 (89%)	3 (11%)	9	46
52	B5	51/52 (98%)	45 (88%)	6 (12%)	8	43
52	D5	51/52 (98%)	45 (88%)	6 (12%)	8	43
53	B6	43/52 (83%)	32 (74%)	11 (26%)	1	8
53	D6	43/52 (83%)	32 (74%)	11 (26%)	1	8
54	B7	41/42 (98%)	37 (90%)	4 (10%)	12	53
54	D7	41/42 (98%)	37 (90%)	4 (10%)	12	53
55	B8	53/55 (96%)	44 (83%)	9 (17%)	3	23
55	D8	53/55 (96%)	43 (81%)	10 (19%)	2	17
56	B9	33/34 (97%)	30 (91%)	3 (9%)	14	57
56	D9	33/34 (97%)	30 (91%)	3 (9%)	14	57
All	All	9654/10428 (93%)	8458 (88%)	1196 (12%)	7	41

5 of 1196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	B1	82	LEU
7	CG	88	PRO
45	DY	77	PRO
51	B4	46	ASN
2	CB	155	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

Mol	Chain	Res	Type
53	B6	20	ASN
6	CF	100	ASN
47	D0	29	GLN
53	B6	26	ASN

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Mol	Chain	Res	Type
2	CB	95	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	291 (19%)	27 (1%)
1	CA	1502/1522 (98%)	290 (19%)	32 (2%)
22	AW	75/76 (98%)	22 (29%)	0
22	AY	16/76 (21%)	9 (56%)	0
22	CW	75/76 (98%)	26 (34%)	0
22	CY	16/76 (21%)	7 (43%)	0
23	AV	76/77 (98%)	37 (48%)	5 (6%)
23	CV	76/77 (98%)	34 (44%)	5 (6%)
24	AX	7/24 (29%)	2 (28%)	0
24	CX	9/24 (37%)	3 (33%)	1 (11%)
25	BA	2796/2916 (95%)	557 (19%)	53 (1%)
25	DA	2796/2916 (95%)	564 (20%)	58 (2%)
26	BB	118/122 (96%)	18 (15%)	1 (0%)
26	DB	118/122 (96%)	19 (16%)	1 (0%)
All	All	9183/9626 (95%)	1879 (20%)	183 (1%)

5 of 1879 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C

5 of 183 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2763	G
1	CA	731	C
25	DA	2263	C
26	BB	66	A
1	CA	262	C

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 746 ligands modelled in this entry, 744 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
58	PAR	AA	1694	-	45,45,45	1.43	8 (17%)	67,67,67	1.27	8 (11%)
58	PAR	CA	1695	-	45,45,45	1.68	11 (24%)	67,67,67	1.40	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	AA	1694	-	-	0/18/94/94	0/4/4/4
58	PAR	CA	1695	-	-	0/18/94/94	0/4/4/4

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	CA	1695	PAR	C34-C24	5.60	1.61	1.53
58	CA	1695	PAR	C52-C42	3.79	1.59	1.52
58	AA	1694	PAR	C52-C42	3.19	1.58	1.52
58	CA	1695	PAR	C64-C54	3.18	1.59	1.51
58	AA	1694	PAR	C34-C24	3.11	1.57	1.53

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
58	CA	1695	PAR	O52-C13-C23	4.74	115.96	107.50
58	CA	1695	PAR	C14-O54-C54	4.55	122.53	113.73
58	CA	1695	PAR	O54-C54-C64	4.09	113.76	105.97
58	AA	1694	PAR	O52-C13-C23	3.94	114.53	107.50
58	AA	1694	PAR	O54-C54-C64	3.86	113.32	105.97

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	1504/1522 (98%)	0.11	49 (3%) 44 34	7, 49, 127, 206	0
1	CA	1503/1522 (98%)	0.09	43 (2%) 49 37	2, 41, 123, 215	0
2	AB	235/256 (91%)	0.36	8 (3%) 43 33	44, 88, 131, 174	0
2	CB	235/256 (91%)	0.39	10 (4%) 34 27	40, 81, 123, 166	0
3	AC	207/239 (86%)	0.27	7 (3%) 43 33	38, 71, 111, 143	0
3	CC	207/239 (86%)	0.27	2 (0%) 79 64	28, 62, 104, 145	0
4	AD	208/209 (99%)	0.19	2 (0%) 79 64	28, 59, 107, 141	0
4	CD	208/209 (99%)	0.31	4 (1%) 64 48	21, 52, 103, 125	0
5	AE	151/162 (93%)	0.24	1 (0%) 84 71	7, 52, 95, 111	0
5	CE	151/162 (93%)	0.33	3 (1%) 62 46	4, 46, 92, 114	0
6	AF	101/101 (100%)	0.17	1 (0%) 79 64	16, 53, 101, 141	0
6	CF	101/101 (100%)	0.44	2 (1%) 62 46	12, 55, 104, 131	0
7	AG	155/156 (99%)	0.38	11 (7%) 16 15	34, 66, 111, 154	0
7	CG	155/156 (99%)	0.36	7 (4%) 32 26	27, 64, 114, 148	0
8	AH	138/138 (100%)	0.25	3 (2%) 59 44	19, 59, 87, 125	0
8	CH	138/138 (100%)	0.19	1 (0%) 84 71	12, 49, 82, 122	0
9	AI	127/128 (99%)	0.52	4 (3%) 47 36	31, 75, 120, 153	0
9	CI	127/128 (99%)	0.66	11 (8%) 10 12	27, 75, 114, 148	0
10	AJ	99/105 (94%)	0.80	10 (10%) 7 9	41, 85, 128, 142	0
10	CJ	99/105 (94%)	0.87	17 (17%) 2 4	27, 77, 128, 143	0
11	AK	119/129 (92%)	0.32	6 (5%) 28 23	13, 49, 98, 129	0
11	CK	119/129 (92%)	0.38	4 (3%) 43 33	8, 46, 98, 121	0
12	AL	125/132 (94%)	0.24	4 (3%) 45 35	2, 39, 88, 141	0
12	CL	125/132 (94%)	0.34	5 (4%) 36 29	0, 27, 75, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.49	6 (4%) 29 24	36, 76, 116, 147	0
13	CM	125/126 (99%)	0.36	4 (3%) 45 35	22, 61, 109, 136	0
14	AN	60/61 (98%)	0.59	1 (1%) 67 51	40, 67, 117, 132	0
14	CN	60/61 (98%)	0.47	1 (1%) 67 51	31, 50, 106, 121	0
15	AO	88/89 (98%)	0.20	1 (1%) 77 61	14, 48, 93, 116	0
15	CO	88/89 (98%)	0.19	2 (2%) 57 43	9, 45, 89, 132	0
16	AP	84/88 (95%)	0.30	0 100 100	30, 51, 101, 137	0
16	CP	84/88 (95%)	0.29	0 100 100	30, 52, 88, 106	0
17	AQ	100/105 (95%)	0.37	3 (3%) 48 36	24, 56, 103, 111	0
17	CQ	100/105 (95%)	0.42	4 (4%) 36 29	18, 53, 110, 121	0
18	AR	70/88 (79%)	0.45	5 (7%) 16 15	17, 54, 98, 118	0
18	CR	70/88 (79%)	0.32	1 (1%) 72 56	12, 47, 88, 116	0
19	AS	79/93 (84%)	0.41	5 (6%) 19 17	37, 76, 126, 161	0
19	CS	79/93 (84%)	0.49	2 (2%) 54 41	26, 55, 121, 146	0
20	AT	99/106 (93%)	0.52	3 (3%) 48 36	11, 59, 105, 121	0
20	CT	99/106 (93%)	0.33	3 (3%) 48 36	3, 58, 106, 125	0
21	AU	25/27 (92%)	1.51	8 (32%) 1 2	41, 69, 87, 97	0
21	CU	25/27 (92%)	1.11	4 (16%) 3 4	31, 55, 91, 125	0
22	AW	76/76 (100%)	1.16	19 (25%) 1 2	23, 129, 187, 208	0
22	AY	17/76 (22%)	1.11	2 (11%) 5 7	29, 51, 105, 123	0
22	CW	76/76 (100%)	1.27	18 (23%) 1 3	12, 118, 185, 207	0
22	CY	17/76 (22%)	0.57	1 (5%) 22 19	10, 37, 117, 125	0
23	AV	77/77 (100%)	0.13	1 (1%) 74 58	16, 67, 122, 137	0
23	CV	77/77 (100%)	0.19	4 (5%) 26 22	10, 55, 109, 155	0
24	AX	8/24 (33%)	0.25	1 (12%) 5 6	15, 33, 63, 66	0
24	CX	10/24 (41%)	0.24	1 (10%) 8 9	9, 26, 96, 134	0
25	BA	2803/2916 (96%)	0.40	127 (4%) 32 26	6, 38, 143, 240	0
25	DA	2803/2916 (96%)	0.35	112 (3%) 36 29	0, 20, 132, 232	0
26	BB	119/122 (97%)	0.49	3 (2%) 54 41	32, 70, 127, 179	0
26	DB	119/122 (97%)	0.30	2 (1%) 67 51	14, 44, 88, 118	0
27	BC	191/229 (83%)	1.58	59 (30%) 1 2	44, 115, 155, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DC	191/229 (83%)	1.82	72 (37%) 1 1	33, 112, 151, 174	0
28	BD	272/276 (98%)	0.17	0 100 100	6, 23, 70, 121	0
28	DD	272/276 (98%)	0.08	1 (0%) 90 81	0, 11, 51, 96	0
29	BE	205/206 (99%)	0.21	5 (2%) 56 42	13, 50, 111, 161	0
29	DE	205/206 (99%)	0.32	4 (1%) 62 46	1, 29, 96, 158	0
30	BF	208/210 (99%)	0.26	5 (2%) 56 42	10, 43, 115, 172	0
30	DF	208/210 (99%)	0.14	3 (1%) 72 56	0, 23, 106, 154	0
31	BG	181/182 (99%)	0.20	6 (3%) 44 34	9, 63, 118, 169	0
31	DG	181/182 (99%)	0.33	8 (4%) 33 26	4, 51, 107, 178	0
32	BH	160/180 (88%)	1.31	38 (23%) 1 3	37, 115, 166, 197	0
32	DH	160/180 (88%)	0.67	11 (6%) 17 16	3, 61, 115, 143	0
33	BI	146/148 (98%)	0.61	14 (9%) 8 10	19, 68, 125, 152	0
33	DI	146/148 (98%)	0.37	2 (1%) 72 56	6, 64, 119, 168	0
34	BN	139/140 (99%)	0.30	2 (1%) 72 56	23, 58, 106, 176	0
34	DN	139/140 (99%)	0.09	0 100 100	2, 29, 83, 139	0
35	BO	122/122 (100%)	-0.05	0 100 100	17, 42, 82, 99	0
35	DO	122/122 (100%)	-0.16	0 100 100	0, 22, 61, 74	0
36	BP	146/150 (97%)	0.49	4 (2%) 52 39	8, 49, 108, 157	0
36	DP	146/150 (97%)	0.39	2 (1%) 72 56	0, 43, 108, 167	0
37	BQ	141/141 (100%)	0.43	8 (5%) 23 19	7, 50, 102, 180	0
37	DQ	141/141 (100%)	0.18	1 (0%) 84 71	1, 25, 75, 167	0
38	BR	117/118 (99%)	0.16	1 (0%) 81 67	18, 39, 91, 120	0
38	DR	117/118 (99%)	0.08	1 (0%) 81 67	4, 22, 64, 109	0
39	BS	99/112 (88%)	0.43	0 100 100	15, 67, 116, 158	0
39	DS	99/112 (88%)	0.31	2 (2%) 62 46	11, 41, 91, 147	0
40	BT	138/146 (94%)	0.26	6 (4%) 34 27	24, 57, 109, 142	0
40	DT	138/146 (94%)	0.13	5 (3%) 41 32	3, 39, 96, 120	0
41	BU	117/118 (99%)	0.27	2 (1%) 67 51	14, 48, 114, 142	0
41	DU	117/118 (99%)	0.08	0 100 100	2, 19, 65, 93	0
42	BV	101/101 (100%)	0.49	3 (2%) 48 36	15, 72, 122, 175	0
42	DV	101/101 (100%)	0.21	0 100 100	1, 39, 86, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BW	113/113 (100%)	0.41	6 (5%) 25 21	11, 32, 89, 159	0
43	DW	113/113 (100%)	0.15	0 100 100	2, 17, 64, 110	0
44	BX	93/96 (96%)	0.27	0 100 100	15, 35, 72, 98	0
44	DX	93/96 (96%)	0.21	1 (1%) 77 61	2, 20, 73, 84	0
45	BY	101/110 (91%)	0.87	17 (16%) 2 4	20, 63, 128, 197	0
45	DY	101/110 (91%)	0.60	11 (10%) 6 8	6, 54, 131, 226	0
46	BZ	177/206 (85%)	0.81	16 (9%) 10 11	0, 83, 131, 156	0
46	DZ	177/206 (85%)	0.67	17 (9%) 8 10	4, 66, 131, 155	0
47	B0	84/85 (98%)	0.70	8 (9%) 8 10	11, 44, 92, 147	0
47	D0	84/85 (98%)	0.43	6 (7%) 16 15	4, 23, 85, 144	0
48	B1	94/98 (95%)	0.50	1 (1%) 77 61	6, 33, 89, 106	0
48	D1	94/98 (95%)	0.24	0 100 100	2, 28, 85, 136	0
49	B2	71/72 (98%)	0.17	1 (1%) 72 56	18, 49, 104, 122	0
49	D2	71/72 (98%)	0.31	1 (1%) 72 56	2, 30, 96, 132	0
50	B3	60/60 (100%)	0.47	2 (3%) 44 34	20, 59, 111, 177	0
50	D3	60/60 (100%)	0.36	1 (1%) 67 51	2, 26, 90, 130	0
51	B4	31/71 (43%)	0.03	0 100 100	33, 76, 100, 107	0
51	D4	31/71 (43%)	0.21	0 100 100	8, 66, 113, 156	0
52	B5	59/60 (98%)	0.69	9 (15%) 3 4	1, 43, 128, 147	0
52	D5	59/60 (98%)	0.28	3 (5%) 27 22	0, 29, 112, 160	0
53	B6	45/54 (83%)	1.38	10 (22%) 1 3	26, 85, 131, 153	0
53	D6	45/54 (83%)	1.40	12 (26%) 1 2	15, 78, 124, 159	0
54	B7	49/49 (100%)	0.34	1 (2%) 62 46	0, 18, 70, 86	0
54	D7	49/49 (100%)	0.20	1 (2%) 62 46	0, 3, 44, 108	0
55	B8	64/65 (98%)	0.61	4 (6%) 19 17	0, 39, 92, 121	0
55	D8	64/65 (98%)	0.27	1 (1%) 68 53	0, 21, 71, 121	0
56	B9	36/37 (97%)	3.88	34 (94%) 0 1	79, 117, 145, 155	0
56	D9	36/37 (97%)	3.48	32 (88%) 0 1	45, 105, 140, 163	0
All	All	21119/22212 (95%)	0.37	1019 (4%) 29 24	0, 46, 126, 240	0

The worst 5 of 1019 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	DA	2802	G	13.3
56	B9	14	CYS	12.4
29	DE	205	ALA	12.0
25	BA	2802	G	11.1
22	CW	20	U	10.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
57	MG	BA	3101	1/1	0.09	-	13,13,13,13	0
57	MG	BA	3119	1/1	0.39	-	0,0,0,0	0
57	MG	DA	3196	1/1	0.26	-	3,3,3,3	0
57	MG	AA	1655	1/1	0.19	-	0,0,0,0	0
57	MG	BA	3190	1/1	0.73	-	0,0,0,0	0
57	MG	DA	3106	1/1	0.28	-	0,0,0,0	0
57	MG	BA	3008	1/1	0.14	-	0,0,0,0	0
57	MG	BA	3155	1/1	0.62	-	0,0,0,0	0
57	MG	DA	3099	1/1	0.60	-	0,0,0,0	0
57	MG	DA	3146	1/1	0.55	-	0,0,0,0	0
57	MG	BA	3197	1/1	0.41	-	0,0,0,0	0
57	MG	DA	3200	1/1	0.85	-	0,0,0,0	0
57	MG	DA	3254	1/1	2.39	-	0,0,0,0	1
57	MG	AA	1688	1/1	1.02	-	0,0,0,0	0
57	MG	AA	1649	1/1	0.07	-	67,67,67,67	0
57	MG	CA	1663	1/1	0.31	-	0,0,0,0	0
57	MG	BA	3079	1/1	0.60	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1650	1/1	1.12	-	0,0,0,0	0
57	MG	BA	3240	1/1	0.44	-	0,0,0,0	0
57	MG	DA	3093	1/1	0.49	-	0,0,0,0	0
57	MG	DA	3232	1/1	0.29	-	0,0,0,0	0
57	MG	CA	1674	1/1	0.58	-	0,0,0,0	0
57	MG	CA	1679	1/1	0.17	-	45,45,45,45	0
57	MG	DA	3026	1/1	0.35	-	0,0,0,0	0
57	MG	BA	3052	1/1	0.17	-	1,1,1,1	0
57	MG	BA	3005	1/1	0.26	-	0,0,0,0	0
57	MG	DA	3055	1/1	0.32	-	0,0,0,0	0
57	MG	DA	3153	1/1	0.43	-	0,0,0,0	0
57	MG	DA	3230	1/1	0.56	-	0,0,0,0	0
57	MG	BA	3237	1/1	1.35	-	3,3,3,3	0
57	MG	CA	1652	1/1	0.33	-	0,0,0,0	0
57	MG	AA	1681	1/1	0.47	-	0,0,0,0	0
57	MG	BA	3033	1/1	0.34	-	0,0,0,0	0
57	MG	CA	1626	1/1	1.23	-	0,0,0,0	0
57	MG	CA	1620	1/1	0.91	-	1,1,1,1	0
57	MG	DA	3069	1/1	0.57	-	0,0,0,0	0
57	MG	AA	1602	1/1	0.16	-	0,0,0,0	0
57	MG	AA	1612	1/1	0.86	-	0,0,0,0	0
57	MG	DA	3157	1/1	0.46	-	0,0,0,0	0
57	MG	BA	3143	1/1	0.46	-	0,0,0,0	0
57	MG	BA	3163	1/1	1.24	-	3,3,3,3	0
57	MG	CA	1669	1/1	0.71	-	0,0,0,0	0
57	MG	CA	1631	1/1	0.11	-	0,0,0,0	0
57	MG	CA	1659	1/1	0.47	-	8,8,8,8	0
57	MG	DA	3186	1/1	1.04	-	0,0,0,0	0
57	MG	BA	3124	1/1	1.19	-	2,2,2,2	1
57	MG	BA	3249	1/1	1.37	-	0,0,0,0	0
57	MG	CA	1681	1/1	0.27	-	1,1,1,1	0
57	MG	DA	3098	1/1	0.91	-	1,1,1,1	0
57	MG	BA	3201	1/1	1.26	-	0,0,0,0	0
57	MG	BA	3160	1/1	0.64	-	0,0,0,0	0
57	MG	DA	3040	1/1	0.84	-	0,0,0,0	0
57	MG	DA	3212	1/1	1.05	-	0,0,0,0	0
57	MG	DA	3060	1/1	0.71	-	11,11,11,11	0
57	MG	CA	1686	1/1	0.50	-	0,0,0,0	0
57	MG	CA	1670	1/1	0.75	-	0,0,0,0	0
57	MG	B3	101	1/1	0.72	-	0,0,0,0	0
57	MG	BA	3071	1/1	0.44	-	0,0,0,0	0
57	MG	DA	3038	1/1	0.51	-	0,0,0,0	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1665	1/1	0.18	-	0,0,0,0	0
57	MG	AA	1609	1/1	0.89	-	3,3,3,3	0
57	MG	DA	3100	1/1	0.83	-	0,0,0,0	0
57	MG	BA	3173	1/1	0.45	-	0,0,0,0	0
57	MG	CA	1616	1/1	0.25	-	0,0,0,0	0
57	MG	DA	3020	1/1	1.04	-	0,0,0,0	0
57	MG	DA	3135	1/1	0.29	-	1,1,1,1	0
57	MG	BA	3100	1/1	0.10	-	73,73,73,73	0
57	MG	BB	203	1/1	0.68	-	0,0,0,0	1
57	MG	DA	3223	1/1	0.23	-	0,0,0,0	0
57	MG	CA	1682	1/1	0.78	-	1,1,1,1	0
57	MG	DA	3039	1/1	0.45	-	0,0,0,0	0
57	MG	BA	3014	1/1	0.19	-	0,0,0,0	0
57	MG	BA	3175	1/1	0.18	-	0,0,0,0	0
57	MG	BA	3128	1/1	0.22	-	4,4,4,4	0
57	MG	DA	3112	1/1	0.81	-	0,0,0,0	0
57	MG	BA	3140	1/1	0.24	-	12,12,12,12	0
57	MG	BA	3042	1/1	0.62	-	0,0,0,0	0
57	MG	DA	3241	1/1	0.99	-	0,0,0,0	0
57	MG	BA	3198	1/1	0.19	-	41,41,41,41	0
57	MG	D5	101	1/1	0.65	-	0,0,0,0	0
57	MG	BA	3091	1/1	1.12	-	0,0,0,0	0
57	MG	DA	3091	1/1	0.70	-	0,0,0,0	0
57	MG	AA	1648	1/1	0.18	-	1,1,1,1	0
57	MG	BA	3026	1/1	0.91	-	0,0,0,0	0
57	MG	CA	1693	1/1	0.44	-	0,0,0,0	0
57	MG	DA	3163	1/1	0.79	-	0,0,0,0	0
57	MG	AA	1628	1/1	1.08	-	0,0,0,0	0
57	MG	BA	3086	1/1	0.18	-	35,35,35,35	0
57	MG	DA	3084	1/1	0.49	-	0,0,0,0	0
57	MG	CA	1601	1/1	0.44	-	0,0,0,0	0
57	MG	DA	3092	1/1	0.34	-	0,0,0,0	0
57	MG	DA	3085	1/1	0.91	-	0,0,0,0	0
57	MG	DA	3082	1/1	0.36	-	0,0,0,0	0
57	MG	DA	3077	1/1	0.65	-	1,1,1,1	0
57	MG	BA	3168	1/1	0.14	-	11,11,11,11	0
57	MG	BA	3185	1/1	0.38	-	13,13,13,13	1
57	MG	BA	3041	1/1	0.45	-	0,0,0,0	1
57	MG	DA	3224	1/1	0.21	-	0,0,0,0	0
57	MG	AA	1641	1/1	0.30	-	0,0,0,0	0
57	MG	DA	3022	1/1	0.64	-	0,0,0,0	0
57	MG	BA	3022	1/1	0.14	-	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1687	1/1	0.58	-	0,0,0,0	0
57	MG	DA	3086	1/1	1.01	-	0,0,0,0	0
57	MG	BA	3215	1/1	0.30	-	18,18,18,18	0
57	MG	DA	3018	1/1	0.77	-	0,0,0,0	0
57	MG	DA	3029	1/1	0.33	-	0,0,0,0	0
57	MG	AA	1613	1/1	0.42	-	0,0,0,0	0
57	MG	BA	3044	1/1	0.95	-	0,0,0,0	0
57	MG	BA	3170	1/1	0.32	-	0,0,0,0	0
57	MG	BA	3227	1/1	0.57	-	0,0,0,0	0
57	MG	BA	3242	1/1	0.88	-	0,0,0,0	0
57	MG	CA	1684	1/1	0.57	-	0,0,0,0	0
57	MG	BA	3235	1/1	0.23	-	0,0,0,0	0
57	MG	BA	3092	1/1	0.40	-	0,0,0,0	0
57	MG	DA	3260	1/1	0.61	-	0,0,0,0	0
57	MG	AA	1605	1/1	0.12	-	26,26,26,26	0
57	MG	BA	3117	1/1	0.88	-	0,0,0,0	0
57	MG	BA	3135	1/1	0.83	-	0,0,0,0	0
57	MG	AA	1619	1/1	0.43	-	1,1,1,1	0
57	MG	BA	3056	1/1	1.20	-	0,0,0,0	0
57	MG	DA	3191	1/1	0.42	-	13,13,13,13	0
57	MG	BA	3049	1/1	0.45	-	0,0,0,0	0
57	MG	BA	3068	1/1	0.94	-	0,0,0,0	0
57	MG	CA	1660	1/1	0.12	-	0,0,0,0	0
57	MG	DA	3079	1/1	0.52	-	0,0,0,0	0
57	MG	BA	3146	1/1	0.23	-	0,0,0,0	0
57	MG	DA	3034	1/1	0.34	-	0,0,0,0	0
57	MG	DA	3072	1/1	1.37	-	1,1,1,1	0
57	MG	CA	1609	1/1	1.50	-	0,0,0,0	0
57	MG	BA	3251	1/1	0.52	-	8,8,8,8	0
57	MG	DA	3213	1/1	0.15	-	0,0,0,0	0
57	MG	BA	3144	1/1	0.39	-	1,1,1,1	0
57	MG	BA	3069	1/1	0.08	-	24,24,24,24	0
57	MG	BA	3060	1/1	0.08	-	28,28,28,28	0
57	MG	AA	1678	1/1	0.61	-	2,2,2,2	0
57	MG	DA	3094	1/1	0.92	-	0,0,0,0	0
57	MG	BA	3132	1/1	0.95	-	0,0,0,0	0
57	MG	DA	3154	1/1	0.25	-	0,0,0,0	0
57	MG	BA	3121	1/1	0.53	-	0,0,0,0	0
57	MG	DA	3042	1/1	0.46	-	0,0,0,0	0
57	MG	DA	3109	1/1	0.60	-	0,0,0,0	0
57	MG	AA	1693	1/1	0.13	-	5,5,5,5	0
57	MG	DA	3182	1/1	0.40	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3127	1/1	1.40	-	1,1,1,1	0
57	MG	BA	3127	1/1	0.16	-	55,55,55,55	0
57	MG	BA	3172	1/1	0.23	-	0,0,0,0	0
57	MG	AA	1626	1/1	0.38	-	0,0,0,0	0
57	MG	DA	3142	1/1	0.45	-	0,0,0,0	0
57	MG	CA	1640	1/1	0.62	-	0,0,0,0	0
57	MG	DA	3252	1/1	0.28	-	0,0,0,0	0
57	MG	BO	201	1/1	0.32	-	47,47,47,47	0
57	MG	BA	3116	1/1	0.33	-	0,0,0,0	0
57	MG	DA	3027	1/1	0.23	-	1,1,1,1	0
57	MG	BA	3213	1/1	0.46	-	0,0,0,0	0
57	MG	AA	1615	1/1	0.26	-	1,1,1,1	0
57	MG	DA	3134	1/1	0.57	-	0,0,0,0	0
57	MG	BA	3176	1/1	0.20	-	24,24,24,24	0
57	MG	DA	3144	1/1	0.52	-	0,0,0,0	0
57	MG	BA	3057	1/1	0.07	-	29,29,29,29	0
57	MG	DA	3003	1/1	0.45	-	1,1,1,1	0
57	MG	BA	3189	1/1	0.60	-	40,40,40,40	0
57	MG	DA	3175	1/1	0.83	-	0,0,0,0	0
57	MG	CA	1619	1/1	0.46	-	0,0,0,0	0
57	MG	DA	3124	1/1	0.57	-	0,0,0,0	0
57	MG	BA	3196	1/1	0.31	-	0,0,0,0	1
57	MG	DA	3258	1/1	0.62	-	8,8,8,8	0
57	MG	DA	3202	1/1	0.35	-	0,0,0,0	0
57	MG	DA	3114	1/1	0.24	-	0,0,0,0	0
57	MG	CA	1685	1/1	0.34	-	11,11,11,11	0
57	MG	DA	3111	1/1	0.69	-	1,1,1,1	0
57	MG	DA	3177	1/1	0.81	-	1,1,1,1	0
57	MG	DA	3128	1/1	1.55	-	1,1,1,1	0
57	MG	BA	3050	1/1	0.16	-	0,0,0,0	0
57	MG	DA	3044	1/1	0.59	-	0,0,0,0	0
57	MG	BA	3138	1/1	0.82	-	0,0,0,0	0
57	MG	AA	1677	1/1	0.50	-	0,0,0,0	0
57	MG	AA	1618	1/1	0.24	-	7,7,7,7	0
57	MG	CA	1606	1/1	1.08	-	5,5,5,5	0
57	MG	DA	3151	1/1	0.24	-	0,0,0,0	0
57	MG	AA	1674	1/1	1.08	-	16,16,16,16	0
57	MG	AA	1633	1/1	1.06	-	0,0,0,0	0
57	MG	DA	3243	1/1	0.27	-	0,0,0,0	0
57	MG	DA	3043	1/1	0.89	-	0,0,0,0	0
57	MG	CA	1687	1/1	1.02	-	0,0,0,0	1
57	MG	CA	1648	1/1	0.29	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1694	1/1	0.89	-	1,1,1,1	0
57	MG	DA	3074	1/1	0.23	-	0,0,0,0	0
57	MG	BA	3162	1/1	0.21	-	6,6,6,6	0
57	MG	BA	3059	1/1	0.87	-	0,0,0,0	0
57	MG	BA	3207	1/1	0.19	-	0,0,0,0	0
57	MG	DA	3132	1/1	0.96	-	0,0,0,0	0
57	MG	DA	3014	1/1	0.19	-	8,8,8,8	0
57	MG	AA	1663	1/1	0.15	-	4,4,4,4	0
57	MG	CA	1671	1/1	1.06	-	0,0,0,0	0
57	MG	CA	1689	1/1	1.31	-	0,0,0,0	1
57	MG	BA	3181	1/1	1.31	-	8,8,8,8	0
57	MG	AA	1607	1/1	0.16	-	0,0,0,0	0
57	MG	BA	3018	1/1	1.17	-	0,0,0,0	0
57	MG	AA	1662	1/1	0.58	-	26,26,26,26	0
57	MG	BA	3089	1/1	0.37	-	0,0,0,0	0
57	MG	BA	3070	1/1	0.28	-	0,0,0,0	0
57	MG	AA	1640	1/1	0.43	-	0,0,0,0	0
57	MG	DA	3149	1/1	0.44	-	0,0,0,0	0
57	MG	DA	3234	1/1	1.00	-	0,0,0,0	0
57	MG	BA	3084	1/1	0.72	-	0,0,0,0	0
57	MG	BA	3229	1/1	0.31	-	13,13,13,13	0
57	MG	DA	3061	1/1	0.63	-	0,0,0,0	0
57	MG	AA	1689	1/1	0.53	-	0,0,0,0	0
57	MG	BA	3188	1/1	0.59	-	5,5,5,5	0
57	MG	DA	3122	1/1	0.34	-	0,0,0,0	0
57	MG	DA	3159	1/1	0.62	-	0,0,0,0	0
57	MG	CA	1638	1/1	0.57	-	0,0,0,0	0
57	MG	BA	3012	1/1	0.17	-	68,68,68,68	0
57	MG	CA	1683	1/1	1.02	-	1,1,1,1	0
57	MG	BA	3254	1/1	0.84	-	0,0,0,0	0
57	MG	DA	3189	1/1	0.56	-	0,0,0,0	0
57	MG	BA	3191	1/1	0.87	-	0,0,0,0	0
57	MG	BA	3209	1/1	1.47	-	0,0,0,0	0
57	MG	AA	1610	1/1	1.36	-	0,0,0,0	0
57	MG	AA	1680	1/1	1.50	-	0,0,0,0	0
57	MG	DA	3031	1/1	0.35	-	0,0,0,0	0
57	MG	DA	3185	1/1	0.31	-	0,0,0,0	0
57	MG	BA	3193	1/1	0.76	-	0,0,0,0	0
57	MG	DA	3201	1/1	0.50	-	0,0,0,0	0
57	MG	AA	1636	1/1	0.78	-	4,4,4,4	0
57	MG	BA	3141	1/1	0.70	-	0,0,0,0	0
57	MG	BA	3078	1/1	0.15	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3137	1/1	0.23	-	0,0,0,0	0
57	MG	DA	3108	1/1	0.35	-	0,0,0,0	0
57	MG	BA	3067	1/1	0.70	-	0,0,0,0	0
57	MG	DA	3184	1/1	0.68	-	0,0,0,0	1
57	MG	AA	1658	1/1	0.15	-	41,41,41,41	0
57	MG	DA	3015	1/1	0.63	-	0,0,0,0	0
57	MG	BA	3221	1/1	0.12	-	79,79,79,79	0
57	MG	BA	3167	1/1	0.78	-	0,0,0,0	0
57	MG	BF	301	1/1	0.23	-	27,27,27,27	1
57	MG	DA	3245	1/1	0.89	-	0,0,0,0	1
57	MG	BA	3148	1/1	0.37	-	0,0,0,0	0
57	MG	BA	3088	1/1	0.19	-	2,2,2,2	0
57	MG	DA	3242	1/1	0.61	-	1,1,1,1	0
57	MG	CA	1636	1/1	0.52	-	0,0,0,0	0
57	MG	DA	3063	1/1	0.91	-	0,0,0,0	0
57	MG	CA	1627	1/1	0.27	-	3,3,3,3	0
57	MG	BA	3039	1/1	0.39	-	0,0,0,0	0
57	MG	CA	1629	1/1	0.28	-	0,0,0,0	0
57	MG	AA	1664	1/1	0.39	-	0,0,0,0	0
57	MG	BA	3241	1/1	0.31	-	5,5,5,5	0
57	MG	DA	3007	1/1	0.92	-	1,1,1,1	0
57	MG	AA	1620	1/1	0.29	-	1,1,1,1	0
57	MG	BA	3081	1/1	0.42	-	0,0,0,0	0
57	MG	BA	3013	1/1	0.21	-	63,63,63,63	0
57	MG	BA	3034	1/1	0.17	-	2,2,2,2	0
57	MG	AA	1616	1/1	0.78	-	0,0,0,0	0
57	MG	DA	3179	1/1	0.69	-	0,0,0,0	0
57	MG	BA	3073	1/1	0.54	-	0,0,0,0	0
57	MG	DA	3059	1/1	0.27	-	1,1,1,1	0
57	MG	DA	3194	1/1	0.38	-	0,0,0,0	0
57	MG	DA	3064	1/1	0.59	-	0,0,0,0	0
57	MG	BA	3226	1/1	0.28	-	39,39,39,39	0
57	MG	BA	3093	1/1	1.03	-	0,0,0,0	0
57	MG	DA	3214	1/1	1.15	-	0,0,0,0	0
57	MG	AA	1621	1/1	1.03	-	0,0,0,0	0
57	MG	DA	3251	1/1	0.62	-	0,0,0,0	1
57	MG	DA	3129	1/1	0.51	-	0,0,0,0	0
57	MG	DA	3096	1/1	0.43	-	0,0,0,0	0
57	MG	CA	1605	1/1	0.28	-	1,1,1,1	0
57	MG	DA	3156	1/1	0.30	-	0,0,0,0	0
57	MG	DA	3216	1/1	0.62	-	0,0,0,0	0
57	MG	BA	3211	1/1	0.34	-	0,0,0,0	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1657	1/1	0.22	-	0,0,0,0	0
57	MG	DA	3073	1/1	0.47	-	0,0,0,0	0
57	MG	DA	3008	1/1	0.90	-	0,0,0,0	0
57	MG	BA	3174	1/1	0.69	-	0,0,0,0	0
57	MG	CA	1644	1/1	0.38	-	27,27,27,27	0
57	MG	BA	3120	1/1	0.86	-	0,0,0,0	0
57	MG	BA	3222	1/1	0.23	-	4,4,4,4	0
57	MG	CA	1647	1/1	0.91	-	0,0,0,0	1
57	MG	CA	1635	1/1	0.62	-	0,0,0,0	0
57	MG	BA	3217	1/1	0.49	-	0,0,0,0	0
57	MG	DA	3247	1/1	0.58	-	0,0,0,0	1
57	MG	DA	3048	1/1	0.53	-	0,0,0,0	0
57	MG	BA	3001	1/1	1.58	-	17,17,17,17	0
57	MG	DA	3253	1/1	0.47	-	5,5,5,5	0
57	MG	BA	3043	1/1	0.15	-	0,0,0,0	1
57	MG	DA	3033	1/1	1.72	-	1,1,1,1	0
57	MG	DA	3131	1/1	0.29	-	0,0,0,0	0
57	MG	CA	1614	1/1	0.21	-	0,0,0,0	0
57	MG	DA	3187	1/1	0.46	-	0,0,0,0	0
57	MG	DA	3097	1/1	0.41	-	1,1,1,1	0
57	MG	CA	1608	1/1	0.38	-	0,0,0,0	0
57	MG	CA	1654	1/1	0.61	-	0,0,0,0	0
57	MG	AA	1679	1/1	0.56	-	0,0,0,0	1
57	MG	DA	3162	1/1	0.69	-	0,0,0,0	0
57	MG	AA	1614	1/1	0.64	-	2,2,2,2	0
57	MG	BA	3179	1/1	0.26	-	0,0,0,0	0
57	MG	BE	301	1/1	0.52	-	0,0,0,0	0
57	MG	BU	201	1/1	0.42	-	8,8,8,8	0
57	MG	CA	1673	1/1	0.46	-	0,0,0,0	0
57	MG	CA	1664	1/1	0.33	-	0,0,0,0	0
57	MG	CA	1603	1/1	0.38	-	0,0,0,0	0
57	MG	BA	3152	1/1	1.02	-	3,3,3,3	0
57	MG	CA	1612	1/1	0.11	-	8,8,8,8	0
57	MG	BA	3156	1/1	0.45	-	0,0,0,0	0
57	MG	DA	3229	1/1	0.56	-	1,1,1,1	0
57	MG	DA	3065	1/1	0.75	-	0,0,0,0	0
57	MG	BA	3159	1/1	0.46	-	7,7,7,7	0
57	MG	BA	3051	1/1	0.67	-	0,0,0,0	0
57	MG	DA	3125	1/1	0.14	-	0,0,0,0	0
57	MG	DA	3169	1/1	0.82	-	0,0,0,0	0
57	MG	BA	3258	1/1	0.11	-	23,23,23,23	0
57	MG	DA	3002	1/1	1.08	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3052	1/1	0.23	-	0,0,0,0	0
57	MG	DA	3021	1/1	0.40	-	18,18,18,18	0
57	MG	AA	1647	1/1	0.27	-	0,0,0,0	0
57	MG	AA	1684	1/1	0.45	-	0,0,0,0	0
57	MG	BA	3032	1/1	0.14	-	0,0,0,0	0
57	MG	DA	3090	1/1	0.31	-	0,0,0,0	0
57	MG	BA	3230	1/1	0.76	-	0,0,0,0	0
57	MG	AA	1671	1/1	0.46	-	0,0,0,0	0
57	MG	BA	3246	1/1	0.12	-	21,21,21,21	0
57	MG	BA	3029	1/1	0.25	-	0,0,0,0	0
57	MG	BA	3096	1/1	0.33	-	0,0,0,0	0
57	MG	AA	1622	1/1	0.24	-	0,0,0,0	0
57	MG	DA	3262	1/1	0.80	-	0,0,0,0	0
57	MG	BA	3072	1/1	0.52	-	0,0,0,0	0
57	MG	DA	3190	1/1	0.20	-	0,0,0,0	0
57	MG	BA	3108	1/1	1.13	-	0,0,0,0	0
57	MG	BA	3062	1/1	0.06	-	42,42,42,42	0
57	MG	BA	3238	1/1	0.23	-	2,2,2,2	1
57	MG	AA	1652	1/1	2.02	-	0,0,0,0	1
57	MG	CA	1666	1/1	0.56	-	0,0,0,0	0
57	MG	DA	3012	1/1	0.23	-	0,0,0,0	0
57	MG	BA	3200	1/1	0.07	-	64,64,64,64	0
57	MG	BA	3184	1/1	0.76	-	0,0,0,0	0
57	MG	DA	3221	1/1	0.82	-	0,0,0,0	0
57	MG	DA	3062	1/1	0.43	-	1,1,1,1	0
57	MG	DA	3107	1/1	0.55	-	0,0,0,0	0
57	MG	CA	1623	1/1	0.43	-	0,0,0,0	0
57	MG	CA	1632	1/1	1.24	-	0,0,0,0	0
57	MG	DD	301	1/1	0.32	-	0,0,0,0	0
57	MG	BA	3016	1/1	0.57	-	1,1,1,1	0
57	MG	B1	101	1/1	0.20	-	59,59,59,59	1
57	MG	DA	3207	1/1	0.55	-	0,0,0,0	0
57	MG	DA	3204	1/1	0.37	-	0,0,0,0	0
58	PAR	CA	1695	42/42	0.32	-	36,39,47,50	0
57	MG	BA	3153	1/1	0.20	-	0,0,0,0	0
57	MG	BA	3178	1/1	0.66	-	0,0,0,0	0
57	MG	DA	3087	1/1	0.98	-	1,1,1,1	0
57	MG	DA	3249	1/1	0.17	-	0,0,0,0	0
57	MG	DA	3174	1/1	0.50	-	0,0,0,0	0
57	MG	BA	3076	1/1	0.24	-	34,34,34,34	0
57	MG	AA	1643	1/1	0.13	-	35,35,35,35	0
57	MG	BA	3134	1/1	1.45	-	0,0,0,0	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3257	1/1	0.60	-	0,0,0,0	0
57	MG	DA	3080	1/1	0.38	-	0,0,0,0	0
57	MG	BA	3248	1/1	0.64	-	7,7,7,7	0
57	MG	AA	1611	1/1	0.39	-	0,0,0,0	0
57	MG	AA	1645	1/1	0.79	-	0,0,0,0	0
57	MG	DA	3240	1/1	0.42	-	0,0,0,0	0
57	MG	AA	1668	1/1	0.20	-	36,36,36,36	0
57	MG	AA	1685	1/1	1.11	-	0,0,0,0	0
57	MG	BA	3169	1/1	1.19	-	0,0,0,0	0
57	MG	AA	1639	1/1	0.60	-	0,0,0,0	0
57	MG	DA	3158	1/1	0.41	-	0,0,0,0	0
57	MG	BA	3097	1/1	0.47	-	0,0,0,0	0
57	MG	BA	3223	1/1	0.58	-	0,0,0,0	0
57	MG	DA	3217	1/1	0.06	-	31,31,31,31	0
57	MG	BA	3216	1/1	0.25	-	0,0,0,0	1
57	MG	DA	3017	1/1	0.49	-	0,0,0,0	0
57	MG	BA	3220	1/1	0.09	-	16,16,16,16	0
57	MG	BA	3165	1/1	0.44	-	0,0,0,0	0
57	MG	DA	3068	1/1	0.37	-	1,1,1,1	0
57	MG	AA	1635	1/1	1.35	-	0,0,0,0	0
57	MG	AA	1682	1/1	0.14	-	0,0,0,0	0
57	MG	AA	1644	1/1	0.58	-	0,0,0,0	0
57	MG	CA	1651	1/1	0.34	-	0,0,0,0	0
57	MG	DA	3010	1/1	0.62	-	0,0,0,0	0
57	MG	BA	3004	1/1	1.00	-	0,0,0,0	0
57	MG	BA	3015	1/1	0.24	-	0,0,0,0	1
57	MG	DA	3178	1/1	0.38	-	0,0,0,0	1
57	MG	BA	3129	1/1	0.22	-	0,0,0,0	1
57	MG	DA	3267	1/1	0.11	-	0,0,0,0	0
57	MG	BA	3105	1/1	1.18	-	0,0,0,0	0
57	MG	DA	3028	1/1	0.60	-	0,0,0,0	0
57	MG	DA	3004	1/1	1.14	-	1,1,1,1	0
57	MG	AX	102	1/1	0.17	-	29,29,29,29	0
57	MG	BA	3122	1/1	0.45	-	0,0,0,0	0
59	ZN	AD	801	1/1	0.25	-	9,9,9,9	0
57	MG	CA	1641	1/1	1.81	-	0,0,0,0	0
57	MG	BA	3030	1/1	0.23	-	26,26,26,26	0
57	MG	AA	1692	1/1	0.23	-	2,2,2,2	0
57	MG	BA	3107	1/1	0.19	-	12,12,12,12	0
57	MG	DA	3050	1/1	1.31	-	0,0,0,0	0
57	MG	BA	3166	1/1	0.37	-	0,0,0,0	0
57	MG	BA	3045	1/1	0.73	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3019	1/1	0.50	-	0,0,0,0	0
57	MG	DA	3047	1/1	0.67	-	0,0,0,0	0
57	MG	BA	3087	1/1	0.57	-	0,0,0,0	0
57	MG	BA	3187	1/1	0.61	-	5,5,5,5	0
57	MG	BA	3142	1/1	0.61	-	0,0,0,0	0
57	MG	DA	3238	1/1	0.43	-	0,0,0,0	0
57	MG	DA	3168	1/1	0.45	-	37,37,37,37	1
57	MG	BB	201	1/1	0.36	-	0,0,0,0	1
57	MG	CA	1675	1/1	0.37	-	0,0,0,0	0
57	MG	CA	1621	1/1	0.10	-	34,34,34,34	0
57	MG	DA	3126	1/1	0.40	-	0,0,0,0	0
57	MG	BA	3099	1/1	0.85	-	0,0,0,0	0
57	MG	DA	3226	1/1	0.41	-	0,0,0,0	0
57	MG	BA	3054	1/1	0.74	-	0,0,0,0	0
57	MG	DA	3192	1/1	0.90	-	0,0,0,0	0
57	MG	DA	3049	1/1	0.50	-	0,0,0,0	0
57	MG	BA	3147	1/1	0.15	-	0,0,0,0	0
57	MG	BA	3080	1/1	0.23	-	13,13,13,13	0
57	MG	BA	3037	1/1	0.71	-	0,0,0,0	0
57	MG	DA	3102	1/1	0.73	-	0,0,0,0	0
57	MG	BB	202	1/1	0.08	-	29,29,29,29	0
57	MG	CA	1661	1/1	0.48	-	1,1,1,1	0
57	MG	AA	1629	1/1	0.15	-	29,29,29,29	0
57	MG	CA	1642	1/1	1.08	-	0,0,0,0	0
57	MG	DA	3261	1/1	0.17	-	3,3,3,3	0
57	MG	BA	3109	1/1	0.31	-	2,2,2,2	0
57	MG	DA	3053	1/1	0.42	-	0,0,0,0	0
57	MG	DA	3036	1/1	0.69	-	1,1,1,1	0
57	MG	DA	3259	1/1	1.06	-	0,0,0,0	0
57	MG	BA	3025	1/1	0.40	-	0,0,0,0	0
57	MG	BA	3244	1/1	0.82	-	0,0,0,0	0
57	MG	BA	3066	1/1	0.14	-	86,86,86,86	0
57	MG	BA	3231	1/1	0.64	-	0,0,0,0	0
57	MG	DA	3133	1/1	0.43	-	0,0,0,0	0
57	MG	DA	3117	1/1	0.34	-	0,0,0,0	0
57	MG	DA	3141	1/1	0.78	-	0,0,0,0	0
57	MG	DA	3181	1/1	0.74	-	15,15,15,15	0
57	MG	BA	3104	1/1	1.01	-	0,0,0,0	0
57	MG	AA	1601	1/1	1.02	-	0,0,0,0	0
57	MG	DA	3265	1/1	0.73	-	0,0,0,0	0
57	MG	AA	1654	1/1	0.50	-	0,0,0,0	0
57	MG	BA	3195	1/1	0.49	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3182	1/1	0.17	-	17,17,17,17	0
57	MG	AA	1624	1/1	0.70	-	0,0,0,0	0
57	MG	DA	3046	1/1	0.36	-	0,0,0,0	0
57	MG	BA	3256	1/1	0.69	-	0,0,0,0	0
57	MG	DA	3110	1/1	0.61	-	0,0,0,0	0
57	MG	AA	1627	1/1	0.29	-	0,0,0,0	0
57	MG	BA	3219	1/1	0.09	-	0,0,0,0	0
57	MG	AA	1669	1/1	0.72	-	3,3,3,3	1
57	MG	CA	1624	1/1	0.27	-	1,1,1,1	0
57	MG	DA	3205	1/1	0.46	-	0,0,0,0	0
57	MG	AA	1673	1/1	1.35	-	0,0,0,0	0
57	MG	DA	3138	1/1	0.32	-	0,0,0,0	0
57	MG	DA	3183	1/1	0.50	-	0,0,0,0	0
57	MG	D5	102	1/1	0.80	-	0,0,0,0	1
57	MG	BA	3075	1/1	0.74	-	0,0,0,0	0
57	MG	DA	3071	1/1	1.18	-	1,1,1,1	0
57	MG	BA	3074	1/1	0.42	-	0,0,0,0	0
57	MG	DA	3067	1/1	1.34	-	1,1,1,1	0
57	MG	DA	3148	1/1	0.20	-	0,0,0,0	0
57	MG	AX	101	1/1	0.11	-	3,3,3,3	0
57	MG	CA	1611	1/1	0.46	-	0,0,0,0	0
57	MG	DA	3250	1/1	0.27	-	46,46,46,46	0
57	MG	AA	1634	1/1	1.85	-	0,0,0,0	1
57	MG	DA	3220	1/1	0.80	-	0,0,0,0	0
57	MG	AA	1657	1/1	0.23	-	1,1,1,1	0
57	MG	BA	3017	1/1	0.29	-	0,0,0,0	0
57	MG	CA	1639	1/1	0.47	-	1,1,1,1	0
59	ZN	CD	801	1/1	0.30	-	8,8,8,8	0
57	MG	DA	3057	1/1	0.21	-	0,0,0,0	0
57	MG	BB	204	1/1	0.12	-	0,0,0,0	1
57	MG	AA	1608	1/1	0.29	-	0,0,0,0	0
57	MG	DA	3081	1/1	0.25	-	0,0,0,0	0
57	MG	CA	1677	1/1	0.45	-	0,0,0,0	1
57	MG	DA	3227	1/1	0.45	-	0,0,0,0	0
57	MG	DA	3233	1/1	1.38	-	0,0,0,0	0
57	MG	BA	3048	1/1	0.49	-	0,0,0,0	0
57	MG	DA	3210	1/1	0.36	-	15,15,15,15	0
57	MG	BA	3118	1/1	0.33	-	3,3,3,3	0
57	MG	DA	3235	1/1	1.02	-	0,0,0,0	0
59	ZN	CN	101	1/1	0.15	-	125,125,125,125	0
57	MG	CA	1604	1/1	0.35	-	0,0,0,0	0
57	MG	CA	1658	1/1	0.18	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3149	1/1	0.20	-	10,10,10,10	0
57	MG	BA	3154	1/1	0.50	-	0,0,0,0	0
57	MG	BA	3024	1/1	0.58	-	0,0,0,0	0
57	MG	CA	1618	1/1	0.14	-	0,0,0,0	0
57	MG	AA	1642	1/1	0.10	-	46,46,46,46	0
57	MG	AA	1632	1/1	0.17	-	3,3,3,3	0
57	MG	BA	3102	1/1	0.28	-	38,38,38,38	0
57	MG	DA	3116	1/1	0.39	-	0,0,0,0	0
57	MG	CA	1637	1/1	0.31	-	0,0,0,0	0
57	MG	BA	3228	1/1	0.30	-	1,1,1,1	0
57	MG	AA	1659	1/1	0.22	-	0,0,0,0	0
57	MG	DA	3006	1/1	0.57	-	3,3,3,3	0
57	MG	BA	3061	1/1	0.22	-	40,40,40,40	0
57	MG	BA	3095	1/1	0.62	-	0,0,0,0	0
57	MG	BA	3058	1/1	0.31	-	4,4,4,4	0
57	MG	BA	3115	1/1	0.54	-	1,1,1,1	0
57	MG	DA	3198	1/1	0.94	-	0,0,0,0	1
57	MG	BA	3035	1/1	1.57	-	0,0,0,0	0
57	MG	AA	1623	1/1	0.46	-	0,0,0,0	0
57	MG	DA	3218	1/1	0.55	-	0,0,0,0	0
57	MG	DA	3152	1/1	0.26	-	2,2,2,2	0
57	MG	BA	3157	1/1	0.80	-	1,1,1,1	0
57	MG	DA	3197	1/1	0.93	-	1,1,1,1	0
57	MG	AA	1683	1/1	0.20	-	0,0,0,0	0
57	MG	BA	3225	1/1	1.07	-	0,0,0,0	0
57	MG	AA	1638	1/1	0.62	-	9,9,9,9	0
57	MG	DA	3001	1/1	0.61	-	0,0,0,0	0
57	MG	BA	3150	1/1	1.36	-	0,0,0,0	0
57	MG	BA	3218	1/1	0.26	-	0,0,0,0	0
57	MG	DA	3041	1/1	0.26	-	36,36,36,36	0
57	MG	BA	3064	1/1	0.18	-	51,51,51,51	0
57	MG	AA	1617	1/1	0.61	-	0,0,0,0	0
57	MG	DA	3172	1/1	0.24	-	43,43,43,43	0
57	MG	DA	3225	1/1	0.71	-	0,0,0,0	0
57	MG	DA	3105	1/1	0.68	-	0,0,0,0	0
57	MG	CA	1617	1/1	0.91	-	1,1,1,1	0
57	MG	BA	3183	1/1	0.32	-	1,1,1,1	0
57	MG	AA	1651	1/1	0.32	-	0,0,0,0	0
57	MG	DA	3215	1/1	0.29	-	0,0,0,0	0
59	ZN	AN	101	1/1	0.09	-	76,76,76,76	0
57	MG	BA	3123	1/1	0.53	-	0,0,0,0	0
57	MG	AA	1606	1/1	0.53	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1653	1/1	0.28	-	0,0,0,0	0
57	MG	BA	3027	1/1	0.12	-	0,0,0,0	1
57	MG	BA	3090	1/1	0.57	-	0,0,0,0	0
57	MG	DA	3088	1/1	0.73	-	1,1,1,1	0
57	MG	DA	3266	1/1	0.53	-	0,0,0,0	0
57	MG	BA	3253	1/1	0.97	-	0,0,0,0	0
57	MG	DA	3237	1/1	1.34	-	1,1,1,1	0
57	MG	DA	3161	1/1	0.69	-	0,0,0,0	0
57	MG	CA	1692	1/1	0.08	-	0,0,0,0	1
57	MG	DA	3255	1/1	0.42	-	0,0,0,0	0
57	MG	BA	3255	1/1	0.09	-	0,0,0,0	0
57	MG	BA	3180	1/1	0.51	-	0,0,0,0	0
57	MG	BA	3082	1/1	0.27	-	88,88,88,88	0
57	MG	BA	3202	1/1	0.74	-	0,0,0,0	0
57	MG	BA	3047	1/1	0.29	-	0,0,0,0	0
57	MG	DA	3167	1/1	0.69	-	1,1,1,1	0
57	MG	AA	1631	1/1	1.24	-	0,0,0,0	0
57	MG	DA	3143	1/1	0.52	-	1,1,1,1	0
57	MG	BA	3007	1/1	1.29	-	0,0,0,0	0
57	MG	DA	3120	1/1	0.47	-	0,0,0,0	0
57	MG	DA	3203	1/1	0.40	-	0,0,0,0	0
57	MG	BA	3130	1/1	0.23	-	0,0,0,0	0
57	MG	BA	3224	1/1	0.10	-	52,52,52,52	0
57	MG	CA	1630	1/1	0.54	-	1,1,1,1	0
57	MG	DA	3103	1/1	1.30	-	1,1,1,1	0
57	MG	BA	3136	1/1	0.49	-	0,0,0,0	0
57	MG	BA	3023	1/1	0.11	-	43,43,43,43	0
57	MG	BA	3232	1/1	0.40	-	0,0,0,0	0
57	MG	DA	3256	1/1	1.15	-	0,0,0,0	0
57	MG	BA	3171	1/1	0.12	-	6,6,6,6	0
57	MG	AA	1603	1/1	0.08	-	55,55,55,55	0
57	MG	BA	3063	1/1	0.20	-	32,32,32,32	0
57	MG	DA	3070	1/1	0.98	-	0,0,0,0	0
57	MG	DA	3268	1/1	0.89	-	0,0,0,0	1
57	MG	DA	3118	1/1	0.94	-	0,0,0,0	0
57	MG	BA	3151	1/1	0.39	-	0,0,0,0	0
57	MG	AA	1604	1/1	0.35	-	0,0,0,0	0
57	MG	DA	3023	1/1	1.10	-	0,0,0,0	0
57	MG	DA	3263	1/1	0.45	-	0,0,0,0	0
57	MG	BA	3137	1/1	0.10	-	108,108,108,108	0
57	MG	BA	3131	1/1	0.25	-	0,0,0,0	0
57	MG	CA	1665	1/1	0.29	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1675	1/1	0.99	-	0,0,0,0	0
57	MG	BA	3164	1/1	0.13	-	54,54,54,54	0
57	MG	BA	3161	1/1	0.74	-	0,0,0,0	0
57	MG	CA	1613	1/1	0.69	-	0,0,0,0	0
57	MG	DA	3095	1/1	0.94	-	0,0,0,0	0
57	MG	DA	3115	1/1	0.19	-	0,0,0,0	0
57	MG	B5	101	1/1	0.41	-	0,0,0,0	0
57	MG	BA	3021	1/1	1.31	-	0,0,0,0	0
57	MG	CA	1602	1/1	0.29	-	0,0,0,0	0
57	MG	CA	1672	1/1	0.58	-	0,0,0,0	0
57	MG	DA	3101	1/1	0.57	-	0,0,0,0	0
57	MG	BA	3158	1/1	1.00	-	0,0,0,0	0
57	MG	CA	1625	1/1	1.33	-	1,1,1,1	0
57	MG	BA	3259	1/1	0.89	-	0,0,0,0	0
57	MG	CA	1676	1/1	0.21	-	0,0,0,0	0
57	MG	DA	3066	1/1	0.65	-	1,1,1,1	0
57	MG	DA	3206	1/1	0.31	-	36,36,36,36	0
57	MG	BA	3010	1/1	0.45	-	0,0,0,0	0
57	MG	BA	3103	1/1	0.73	-	0,0,0,0	0
57	MG	AA	1661	1/1	0.11	-	1,1,1,1	0
57	MG	DA	3160	1/1	1.11	-	0,0,0,0	0
57	MG	BA	3028	1/1	0.18	-	83,83,83,83	0
57	MG	BA	3002	1/1	0.25	-	13,13,13,13	0
57	MG	AA	1686	1/1	0.95	-	0,0,0,0	0
57	MG	BA	3083	1/1	0.75	-	0,0,0,0	0
57	MG	BA	3126	1/1	0.61	-	0,0,0,0	1
57	MG	DA	3166	1/1	0.41	-	11,11,11,11	0
57	MG	BA	3214	1/1	1.09	-	0,0,0,0	0
57	MG	DA	3195	1/1	0.65	-	32,32,32,32	0
57	MG	DA	3176	1/1	0.91	-	0,0,0,0	0
57	MG	DA	3246	1/1	1.22	-	0,0,0,0	0
57	MG	BA	3234	1/1	0.42	-	0,0,0,0	0
57	MG	DA	3075	1/1	0.50	-	0,0,0,0	0
57	MG	BA	3177	1/1	0.40	-	0,0,0,0	0
57	MG	AA	1660	1/1	0.46	-	2,2,2,2	0
57	MG	BA	3053	1/1	0.44	-	0,0,0,0	0
57	MG	BA	3065	1/1	0.12	-	16,16,16,16	0
57	MG	AA	1656	1/1	0.23	-	9,9,9,9	0
57	MG	DA	3236	1/1	1.47	-	0,0,0,0	0
57	MG	DA	3051	1/1	0.65	-	0,0,0,0	0
57	MG	CV	102	1/1	0.81	-	0,0,0,0	0
57	MG	AA	1630	1/1	0.39	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3016	1/1	0.44	-	0,0,0,0	0
57	MG	DA	3024	1/1	0.42	-	0,0,0,0	0
57	MG	CA	1668	1/1	1.07	-	0,0,0,0	0
57	MG	BA	3199	1/1	0.52	-	0,0,0,0	0
57	MG	BA	3113	1/1	0.31	-	0,0,0,0	0
57	MG	CA	1615	1/1	0.34	-	1,1,1,1	0
57	MG	BA	3077	1/1	0.49	-	0,0,0,0	0
57	MG	DA	3056	1/1	0.77	-	0,0,0,0	0
57	MG	DA	3032	1/1	0.25	-	0,0,0,0	0
57	MG	DA	3165	1/1	1.03	-	0,0,0,0	0
57	MG	CA	1667	1/1	0.61	-	27,27,27,27	0
57	MG	DA	3035	1/1	0.41	-	0,0,0,0	0
57	MG	DA	3248	1/1	0.46	-	0,0,0,0	1
57	MG	DA	3219	1/1	0.67	-	0,0,0,0	0
57	MG	DE	301	1/1	0.26	-	1,1,1,1	0
57	MG	BA	3233	1/1	0.82	-	0,0,0,0	0
57	MG	DA	3083	1/1	0.46	-	1,1,1,1	0
57	MG	B5	102	1/1	1.08	-	0,0,0,0	1
57	MG	BA	3203	1/1	0.62	-	0,0,0,0	0
57	MG	CA	1678	1/1	0.43	-	0,0,0,0	1
57	MG	BA	3036	1/1	0.73	-	0,0,0,0	0
57	MG	BA	3204	1/1	0.48	-	3,3,3,3	0
57	MG	DA	3104	1/1	0.77	-	0,0,0,0	0
57	MG	CA	1690	1/1	0.36	-	3,3,3,3	0
57	MG	BA	3243	1/1	1.00	-	0,0,0,0	0
57	MG	BA	3186	1/1	0.55	-	0,0,0,0	0
57	MG	AA	1676	1/1	0.56	-	0,0,0,0	0
57	MG	DA	3139	1/1	0.56	-	0,0,0,0	0
57	MG	BA	3114	1/1	0.58	-	0,0,0,0	0
57	MG	D0	101	1/1	0.55	-	1,1,1,1	0
57	MG	BA	3192	1/1	0.39	-	0,0,0,0	0
57	MG	DA	3123	1/1	0.44	-	0,0,0,0	0
57	MG	BA	3212	1/1	0.80	-	11,11,11,11	0
57	MG	DA	3054	1/1	0.87	-	0,0,0,0	0
57	MG	DA	3264	1/1	0.74	-	1,1,1,1	0
57	MG	DA	3193	1/1	0.64	-	0,0,0,0	0
57	MG	CA	1650	1/1	0.32	-	0,0,0,0	0
57	MG	DA	3119	1/1	0.50	-	0,0,0,0	0
57	MG	BA	3003	1/1	1.20	-	0,0,0,0	0
57	MG	AA	1670	1/1	0.50	-	0,0,0,0	0
57	MG	BA	3252	1/1	0.27	-	0,0,0,0	0
57	MG	BA	3110	1/1	0.94	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1688	1/1	0.30	-	1,1,1,1	0
57	MG	DA	3058	1/1	1.22	-	0,0,0,0	0
57	MG	CA	1633	1/1	0.41	-	0,0,0,0	0
57	MG	DA	3164	1/1	1.20	-	0,0,0,0	0
57	MG	DA	3030	1/1	0.23	-	0,0,0,0	0
57	MG	CA	1646	1/1	0.40	-	1,1,1,1	0
57	MG	DA	3121	1/1	0.69	-	0,0,0,0	0
57	MG	BA	3046	1/1	0.61	-	0,0,0,0	0
57	MG	DA	3244	1/1	1.06	-	0,0,0,0	0
57	MG	AA	1672	1/1	0.63	-	0,0,0,0	0
57	MG	DA	3045	1/1	0.68	-	0,0,0,0	0
57	MG	CA	1607	1/1	1.27	-	0,0,0,0	0
57	MG	BA	3009	1/1	0.47	-	0,0,0,0	0
57	MG	BA	3055	1/1	0.43	-	0,0,0,0	0
57	MG	DA	3005	1/1	0.74	-	0,0,0,0	0
57	MG	DA	3145	1/1	0.71	-	1,1,1,1	0
57	MG	CA	1634	1/1	1.15	-	0,0,0,0	0
57	MG	DA	3180	1/1	0.26	-	0,0,0,0	0
57	MG	CV	101	1/1	0.10	-	1,1,1,1	0
57	MG	DA	3025	1/1	0.15	-	1,1,1,1	0
57	MG	AA	1625	1/1	0.08	-	3,3,3,3	0
57	MG	BA	3260	1/1	0.19	-	13,13,13,13	0
57	MG	BA	3020	1/1	0.65	-	0,0,0,0	0
57	MG	AA	1646	1/1	0.91	-	0,0,0,0	0
57	MG	BA	3019	1/1	0.67	-	0,0,0,0	0
57	MG	CA	1680	1/1	0.53	-	1,1,1,1	0
57	MG	DA	3199	1/1	0.64	-	1,1,1,1	0
57	MG	DA	3011	1/1	0.13	-	10,10,10,10	0
57	MG	DA	3257	1/1	0.35	-	0,0,0,0	1
57	MG	DB	202	1/1	0.12	-	0,0,0,0	0
57	MG	CA	1610	1/1	0.53	-	0,0,0,0	0
57	MG	BA	3094	1/1	0.61	-	0,0,0,0	0
57	MG	DA	3228	1/1	0.36	-	0,0,0,0	0
57	MG	BA	3245	1/1	0.75	-	0,0,0,0	0
57	MG	DA	3231	1/1	0.30	-	0,0,0,0	0
57	MG	BA	3031	1/1	0.12	-	21,21,21,21	0
57	MG	AA	1690	1/1	0.19	-	23,23,23,23	0
57	MG	BA	3098	1/1	1.19	-	0,0,0,0	0
57	MG	DA	3130	1/1	0.41	-	0,0,0,0	0
57	MG	CA	1662	1/1	0.35	-	13,13,13,13	0
57	MG	DA	3150	1/1	0.34	-	0,0,0,0	0
57	MG	CA	1691	1/1	0.13	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3188	1/1	0.78	-	0,0,0,0	0
57	MG	BA	3236	1/1	0.62	-	0,0,0,0	0
57	MG	BA	3106	1/1	0.21	-	7,7,7,7	0
57	MG	BA	3208	1/1	0.35	-	0,0,0,0	0
57	MG	BA	3145	1/1	1.11	-	0,0,0,0	0
57	MG	DA	3076	1/1	0.30	-	1,1,1,1	0
57	MG	CA	1655	1/1	0.29	-	21,21,21,21	0
57	MG	DA	3113	1/1	0.38	-	0,0,0,0	0
57	MG	DA	3239	1/1	0.21	-	0,0,0,0	0
57	MG	AA	1691	1/1	0.80	-	58,58,58,58	0
57	MG	DA	3222	1/1	1.20	-	1,1,1,1	0
57	MG	BA	3040	1/1	0.62	-	0,0,0,0	0
57	MG	DA	3208	1/1	0.22	-	0,0,0,0	0
57	MG	BA	3133	1/1	0.37	-	0,0,0,0	0
57	MG	DA	3209	1/1	0.41	-	0,0,0,0	0
57	MG	CA	1628	1/1	0.19	-	0,0,0,0	0
57	MG	BA	3205	1/1	0.19	-	33,33,33,33	0
57	MG	BA	3261	1/1	0.32	-	31,31,31,31	0
57	MG	DA	3140	1/1	0.26	-	0,0,0,0	0
57	MG	DA	3089	1/1	0.53	-	0,0,0,0	0
57	MG	DB	201	1/1	0.14	-	0,0,0,0	1
57	MG	BA	3038	1/1	0.50	-	28,28,28,28	0
57	MG	BA	3125	1/1	0.71	-	0,0,0,0	0
57	MG	BA	3085	1/1	1.30	-	0,0,0,0	0
57	MG	AA	1667	1/1	0.40	-	15,15,15,15	0
57	MG	DA	3171	1/1	0.15	-	0,0,0,0	0
57	MG	DA	3173	1/1	0.58	-	0,0,0,0	0
57	MG	CA	1653	1/1	0.58	-	1,1,1,1	0
57	MG	AA	1666	1/1	0.12	-	45,45,45,45	0
57	MG	DA	3037	1/1	0.26	-	0,0,0,0	0
57	MG	CA	1645	1/1	2.05	-	1,1,1,1	0
57	MG	DA	3147	1/1	0.16	-	1,1,1,1	0
57	MG	DA	3009	1/1	0.90	-	0,0,0,0	0
57	MG	BA	3011	1/1	1.86	-	0,0,0,0	0
57	MG	AA	1637	1/1	0.20	-	34,34,34,34	0
57	MG	BA	3111	1/1	0.91	-	2,2,2,2	0
57	MG	BA	3139	1/1	0.32	-	0,0,0,0	0
57	MG	BA	3112	1/1	0.35	-	0,0,0,0	0
57	MG	CA	1649	1/1	0.21	-	0,0,0,0	0
57	MG	BA	3206	1/1	0.24	-	0,0,0,0	0
58	PAR	AA	1694	42/42	0.32	-	11,14,23,25	0
57	MG	DA	3170	1/1	0.57	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3194	1/1	0.64	-	0,0,0,0	0
57	MG	DA	3136	1/1	0.77	-	1,1,1,1	0
57	MG	BA	3210	1/1	0.23	-	0,0,0,0	0
57	MG	CA	1643	1/1	0.34	-	0,0,0,0	0
57	MG	DA	3155	1/1	0.49	-	0,0,0,0	0
57	MG	BA	3250	1/1	1.36	-	0,0,0,0	1
57	MG	CA	1656	1/1	1.32	-	0,0,0,0	0
57	MG	BA	3006	1/1	0.82	-	0,0,0,0	0
57	MG	BA	3247	1/1	0.57	-	7,7,7,7	0
57	MG	DA	3078	1/1	0.24	-	0,0,0,0	0
57	MG	CA	1622	1/1	0.56	-	0,0,0,0	0
57	MG	BA	3239	1/1	0.38	-	0,0,0,0	0
57	MG	DA	3211	1/1	0.53	-	12,12,12,12	0
57	MG	BF	302	1/1	0.36	-	0,0,0,0	0
57	MG	DA	3013	1/1	0.22	-	0,0,0,0	0

6.5 Other polymers ⓘ

There are no such residues in this entry.