



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:18 PM BST

PDB ID : 4V7W
Title : Structure of the *Thermus thermophilus* ribosome complexed with chloramphenicol.
Authors : Bulkley, D.P.; Innis, C.A.; Blaha, G.; Steitz, T.A.
Deposited on : 2010-08-16
Resolution : 3.00 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>

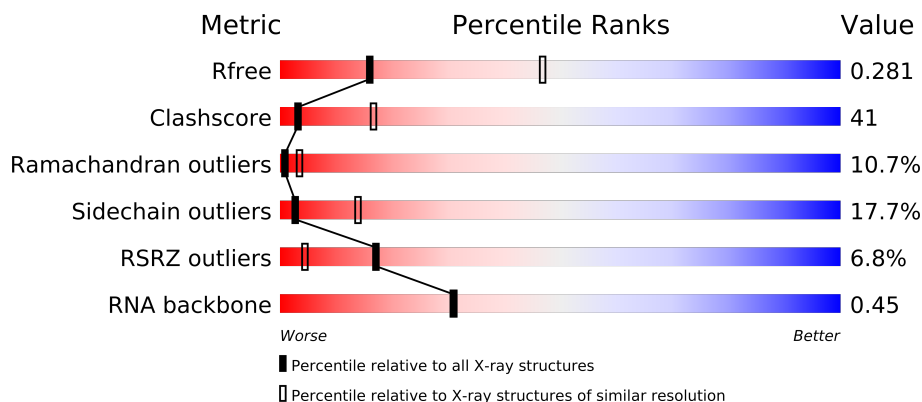
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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	135	
12	CL	135	
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	B0	85	
22	D0	85	
23	B1	98	
23	D1	98	
24	B2	72	
24	D2	72	
25	B3	60	
25	D3	60	
26	B4	71	
26	D4	71	
27	B5	60	
27	D5	60	

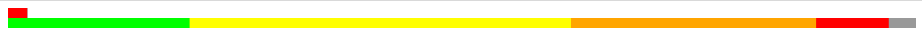
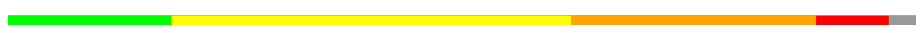


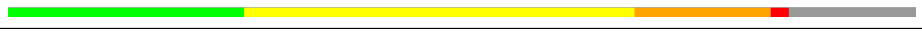

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Mol	Chain	Length	Quality of chain
28	B6	54	
28	D6	54	
29	B7	49	
29	D7	49	
30	B8	65	
30	D8	65	
31	BA	2787	
31	DA	2787	
32	BB	122	
32	DB	122	
33	BD	276	
33	DD	276	
34	BE	206	
34	DE	206	
35	BF	210	
35	DF	210	
36	BG	182	
36	DG	182	
37	BH	180	
37	DH	180	
38	BI	148	
38	DI	148	
39	BN	140	
39	DN	140	
40	BO	122	
40	DO	122	
41	BP	150	
41	DP	150	
42	BQ	141	
42	DQ	141	
43	BR	118	
43	DR	118	
44	BS	112	
44	DS	112	
45	BT	146	
45	DT	146	
46	BU	118	
46	DU	118	
47	BV	101	
47	DV	101	
48	BW	113	
48	DW	113	

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Mol	Chain	Length	Quality of chain
49	BX	96	
49	DX	96	
50	BY	110	
50	DY	110	
51	BZ	206	
51	DZ	206	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 277987 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
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- 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			
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
			1011	639	198	174			
9	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	CONFLICT	UNP P80374
CI	58	ARG	HIS	CONFLICT	UNP P80374

- 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			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	2	VAL	-	INSERTION	UNP Q5SHN3
AL	3	ALA	-	INSERTION	UNP Q5SHN3
AL	4	LEU	-	INSERTION	UNP Q5SHN3
CL	2	VAL	-	INSERTION	UNP Q5SHN3
CL	3	ALA	-	INSERTION	UNP Q5SHN3
CL	4	LEU	-	INSERTION	UNP Q5SHN3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			
13	CM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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 protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	B0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			
22	D0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	B1	89	Total	C	N	O	0	0	1
			693	435	140	118			
23	D1	89	Total	C	N	O	0	0	1
			693	435	140	118			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	B2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			
24	D2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	B4	32	Total	C	N	O	0	0	0
			157	93	32	32			
26	D4	32	Total	C	N	O	0	0	0
			157	93	32	32			

- Molecule 27 is a protein called 50S ribosomal protein L32.

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

- Molecule 28 is a protein called 50S ribosomal protein L33.

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

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BA	2725	Total	C	N	O	P	0	0	0
			58698	26124	10986	18864	2724			
31	DA	2725	Total	C	N	O	P	0	0	0
			58698	26124	10986	18864	2724			

- Molecule 32 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 33 is a protein called 50S ribosomal protein L2.

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

- Molecule 34 is a protein called 50S ribosomal protein L3.

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

- Molecule 35 is a protein called 50S ribosomal protein L4.

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

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

- Molecule 36 is a protein called 50S ribosomal protein L5.

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

- Molecule 37 is a protein called 50S ribosomal protein L6.

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

- Molecule 38 is a protein called 50S ribosomal protein L9.

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

- Molecule 39 is a protein called 50S ribosomal protein L13.

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

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

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

- Molecule 42 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			
42	DQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

- Molecule 45 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BT	132	Total	C	N	O	S	0	0	0
			1100	686	227	186	1			
45	DT	132	Total	C	N	O	S	0	0	0
			1100	686	227	186	1			

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

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

- Molecule 49 is a protein called 50S ribosomal protein L23.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	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
51	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	BA	368	Total	Mg	0	0
			368	368		
52	CA	53	Total	Mg	0	0
			53	53		
52	DQ	1	Total	Mg	0	0
			1	1		
52	DF	1	Total	Mg	0	0
			1	1		
52	BE	1	Total	Mg	0	0
			1	1		
52	DU	1	Total	Mg	0	0
			1	1		
52	B1	1	Total	Mg	0	0
			1	1		
52	BP	2	Total	Mg	0	0
			2	2		
52	DR	1	Total	Mg	0	0
			1	1		
52	B5	2	Total	Mg	0	0
			2	2		
52	BB	7	Total	Mg	0	0
			7	7		
52	BF	1	Total	Mg	0	0
			1	1		
52	BX	1	Total	Mg	0	0
			1	1		
52	AA	56	Total	Mg	0	0
			56	56		
52	BQ	2	Total	Mg	0	0
			2	2		
52	BU	1	Total	Mg	0	0
			1	1		
52	DD	1	Total	Mg	0	0
			1	1		
52	BR	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	DA	332	Total 332	Mg 332	0	0
52	DE	1	Total 1	Mg 1	0	0
52	D1	1	Total 1	Mg 1	0	0
52	DX	1	Total 1	Mg 1	0	0
52	DP	1	Total 1	Mg 1	0	0
52	D5	2	Total 2	Mg 2	0	0
52	BD	1	Total 1	Mg 1	0	0
52	DB	4	Total 4	Mg 4	0	0

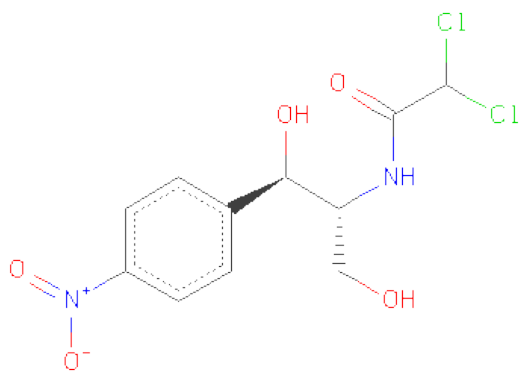
- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 54 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	1	Total 1	K 1	0	0
54	DA	1	Total 1	K 1	0	0

- Molecule 55 is CHLORAMPHENICOL (three-letter code: CLM) (formula: C₁₁H₁₂Cl₂N₂O₅).

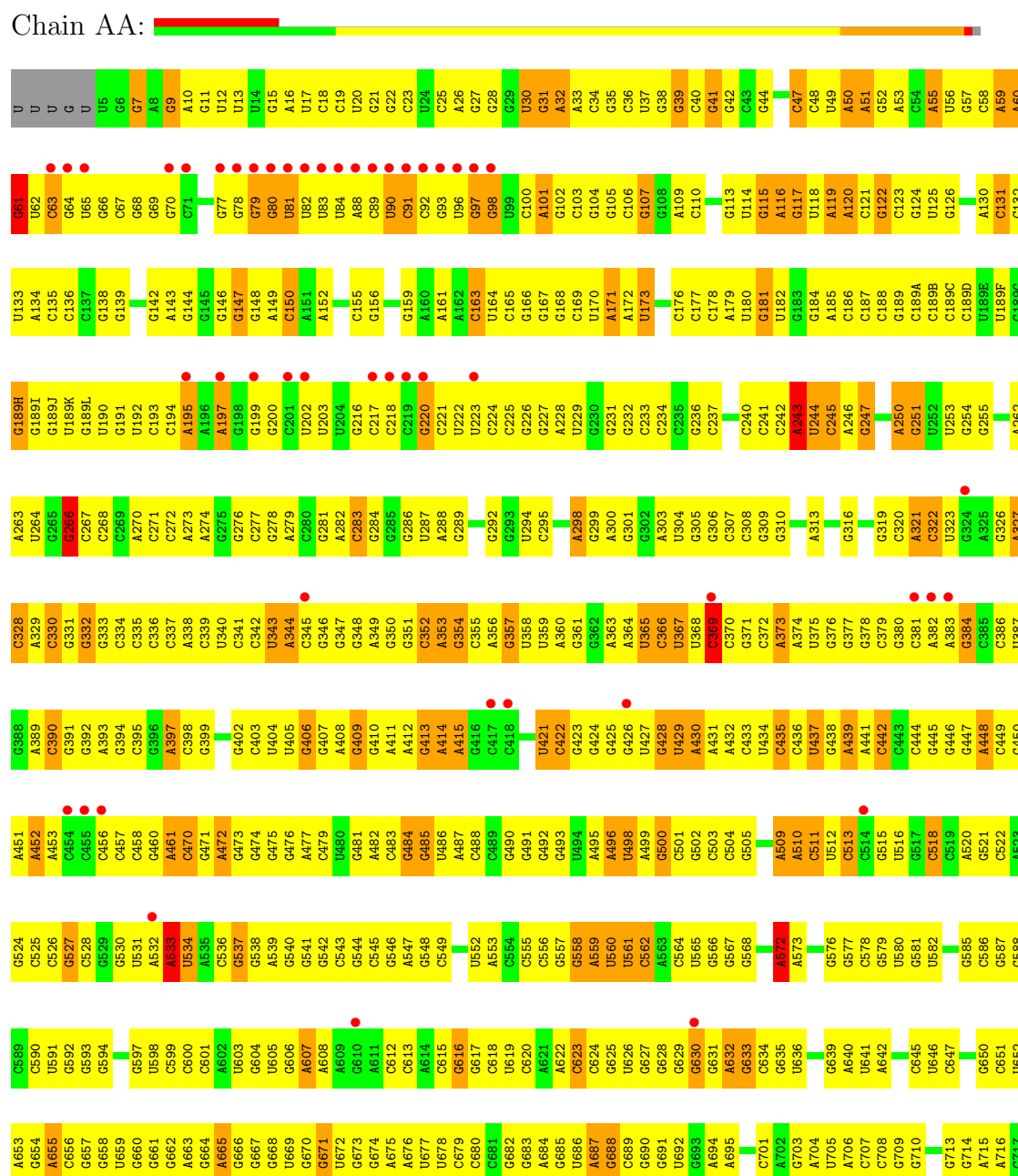


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	BA	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
55	DA	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

3 Residue-property plots

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

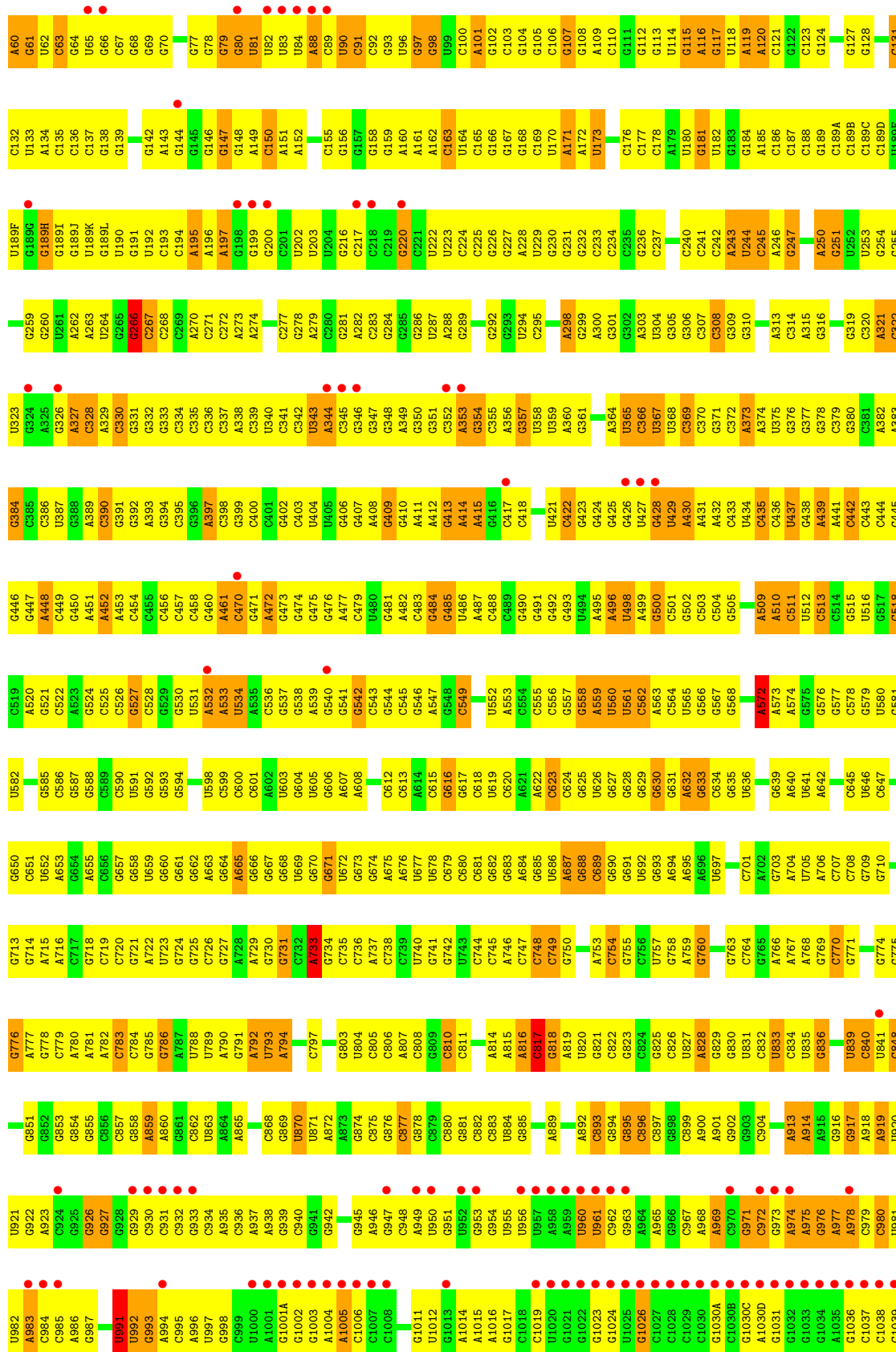
• Molecule 1: 16S rRNA

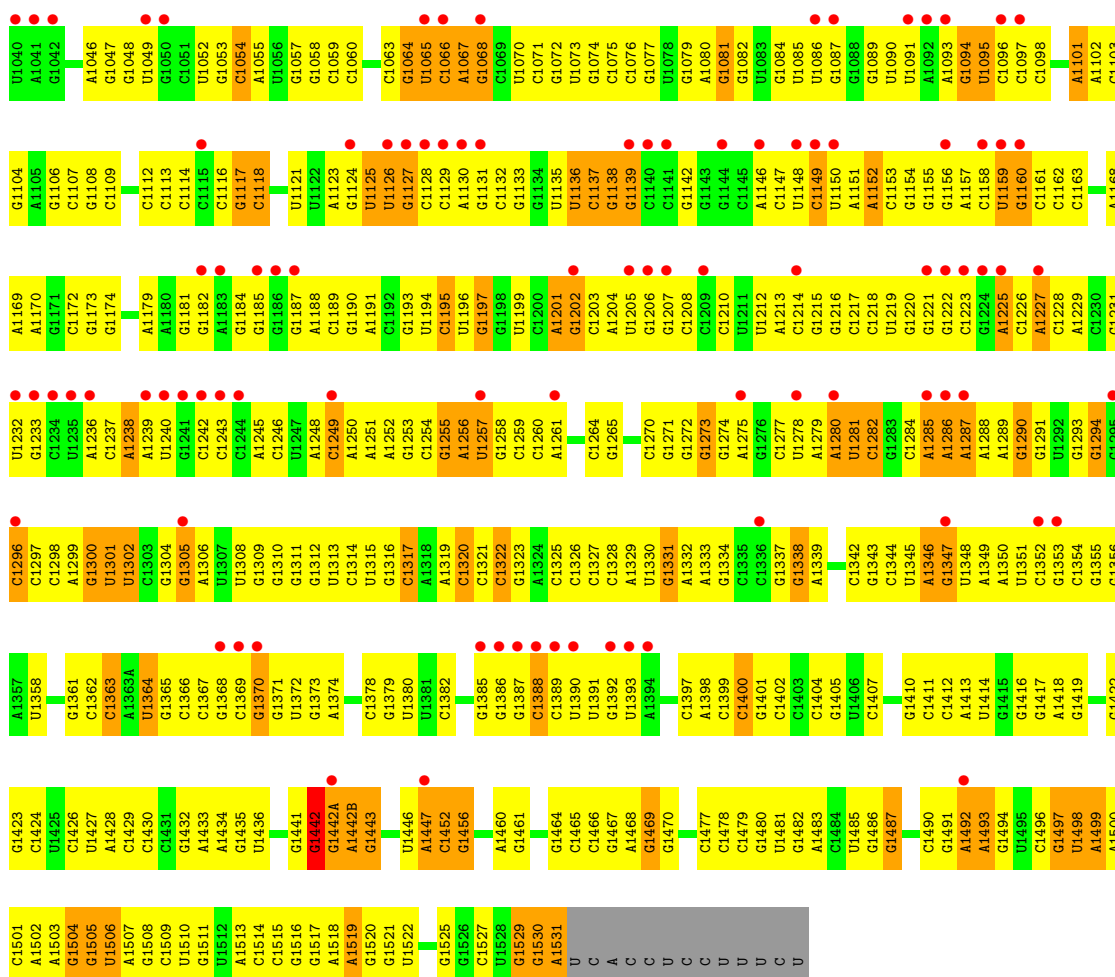


A1500	C1426	A1363A	C1303	U1240	C1113	G1050	A994	G933	C857	C779	G718
C1501	C1427	U1364	G1304	G1241	C1114	C1051	C995	C934	G858	A780	C719
A1502	G1365	G1365	C1305	C1242	C1115	U1052	A996	A935	A859	A781	C720
A1503	A1428	C1366	A1306	C1243	C1116	G1053	U997	C936	A860	A782	G721
G1504	C1429	C1367	U1307	C1244	C1117	C1054	C998	A937	G861	C783	A722
G1505	C1430	G1368	U1308	C1245	C1118	A1055	G999	A938	C862	C784	U723
U1506	C1431	C1369	G1309	U1246	C1119	U1056	U1000	C939	U863	G785	G724
A1507	G1432	G1370	G1310	A1248	C1120	G1057	A1001	C940	A864	G786	G725
U1510	A1433	G1371	G1311	C1249	U1121	G1058	G1001A	G941	A865	A787	C726
G1511	A1434	U1372	G1312	A1250	U1122	C1059	G1002	G942	C868	A728	A728
U1512	G1435	G1373	U1313	A1251	U1123	G1060	G1003	G945	G869	A729	A729
A1513	U1436	A1374	C1314	A1252	G1124	U1061	A1004	A946	U870	G730	G730
C1514	G1441	A1375	U1315	G1253	U1125	C1062	C1005	G947	U871	C731	G731
G1515	U1376	U1376	G1316	C1254	U1126	G1063	C1006	G948	A872	C732	C732
C1516	A1377	A1377	C1317	G1255	G1127	U1064	C1007	G949	A873	A733	A733
G1517	C1378	C1378	A1318	A1256	C1128	U1065	U1008	U950	G874	G734	G734
A1442B	G1379	G1379	U1319	U1257	G1129	C1066	C1008	U951	C875	C735	C735
G1443	U1380	U1380	C1320	G1258	C1130	A1067	G1011	U952	G876	C736	C736
U1518	U1381	U1381	G1321	C1259	G1131	U1068	U1012	U953	C877	A737	A737
C1520	C1382	C1382	C1322	C1260	C1132	U1069	U1013	G954	G878	C738	C738
G1521	C1383	C1383	G1323	A1261	G1133	U1070	A1014	U955	C879	C806	C739
U1522	G1384	G1384	A1324	C1262	G1134	G1071	A1015	U956	C880	A807	U740
G1523	G1385	G1385	C1325	C1263	U1135	U1072	A1016	U957	C881	G741	G741
C1524	G1386	G1386	C1326	G1264	U1136	G1073	U1017	A958	G882	G742	G742
G1525	G1387	G1387	C1327	G1265	C1137	G1074	G1018	A959	C883	U743	U743
U1526	G1388	G1388	C1328	C1266	G1138	C1075	C1019	U960	U884	C744	C744
A1527	C1389	C1389	A1329	C1267	G1139	C1076	U1020	U961	G885	C745	C745
U1528	U1390	U1390	U1330	C1270	C1140	U1077	G1021	C962	A814	A746	A746
G1529	G1391	G1391	G1331	G1271	C1141	U1078	G1022	G963	A815	C747	C747
C1530	C1392	C1392	A1332	C1272	C1142	U1079	G1023	A964	C893	C748	C748
U1531	U1393	U1393	C1333	G1273	U1143	A1081	U1024	A965	C894	C749	C749
U	A1394	A1394	G1334	C1274	A1146	G1082	U1025	G966	C895	G750	G750
C	C1397	C1397	G1335	C1275	C1147	U1083	G1026	C967	C896	U751	U751
A	A1398	A1398	C1336	G1276	U1148	U1084	C1027	A968	U820	G752	G752
C	C1399	C1399	G1337	C1277	C1149	U1085	C1028	A969	C821	A753	A753
U	C1400	C1400	A1338	U1278	U1150	U1086	C1029	C970	A900	G754	G754
C	U1401	U1401	G1339	C1279	A1151	G1087	C1030	G971	A901	G755	G755
C	G1402	G1402	C1340	A1280	A1152	U1088	G1030A	C972	C826	C756	C756
U	C1403	C1403	G1341	U1281	C1153	U1089	G1030B	G973	U827	U757	U757
U	C1404	C1404	C1342	C1282	G1154	U1090	G1030C	A974	A828	G758	G758
U	G1405	G1405	G1343	G1283	U1155	U1091	A1030D	A975	G829	A759	A759
C	U1406	U1406	U1344	C1284	G1156	A1092	G1031	G976	U831	G760	G760
U	C1407	C1407	A1345	A1285	A1157	A1093	G1032	A977	C832	G761	G761
C	U1408	U1408	G1346	C1286	C1158	G1094	G1033	A978	U833	C762	C762
U	A1409	A1409	U1347	A1287	U1159	U1095	G1034	C979	C834	G763	G763
C	C1409	C1409	A1349	A1288	G1160	C1096	A1035	C980	U835	C764	C764
G	G1410	G1410	A1350	C1289	C1161	C1097	C1036	U981	C836	A766	A766
C	C1411	C1411	U1351	U1290	C1162	C1098	C1037	U982	U839	A767	A767
C	C1412	C1412	G1352	G1291	C1163	U1099	C1038	U983	C840	A768	A768
U	A1413	A1413	C1353	U1292	A1163	A1101	C1039	C984	U841	G769	G769
U	U1414	U1414	G1354	G1293	A1168	A1102	U1040	C985	C848	C770	C770
C	G1415	G1415	C1355	C1294	A1169	C1103	A1041	A986	G925	G771	G771
C	U1416	U1416	G1356	G1295	A1170	G1104	C1042	G987	G926	G772	G772
C	G1417	G1417	A1357	C1296	G1171	A1105	C1043	G988	G927	G773	G773
C	A1418	A1418	C1358	C1297	C1172	C1106	A1044	G989	G928	G774	G774
C	G1419	G1419	U1359	C1298	G1173	G1107	C1045	C990	G852	G775	G775
U	U1420	U1420	A1360	A1299	G1174	G1108	A1046	U991	G853	G776	G776
C	G1422	G1422	G1361	G1300	G1175	C1109	G1047	U992	G854	A777	A777
C	A1423	A1423	U1301	U1302	A1179	C1112	U1049	G993	C856	G778	G778
C	C1363	C1363	A1239	U1302	A1179	C1112	U1049	G993	C856	G778	G778

● Molecule 1: 16S rRNA

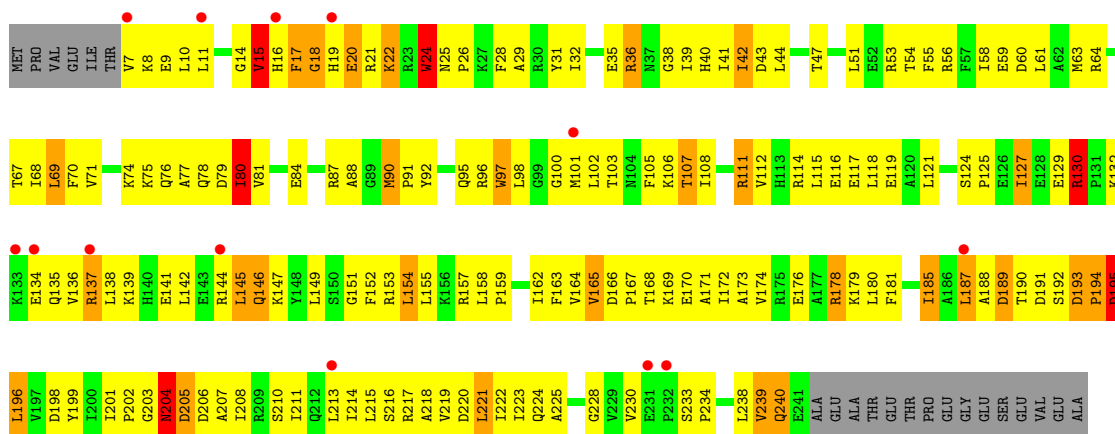
Chain CA:





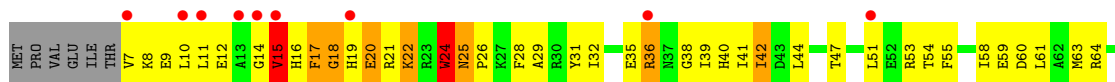
• Molecule 2: 30S ribosomal protein S2

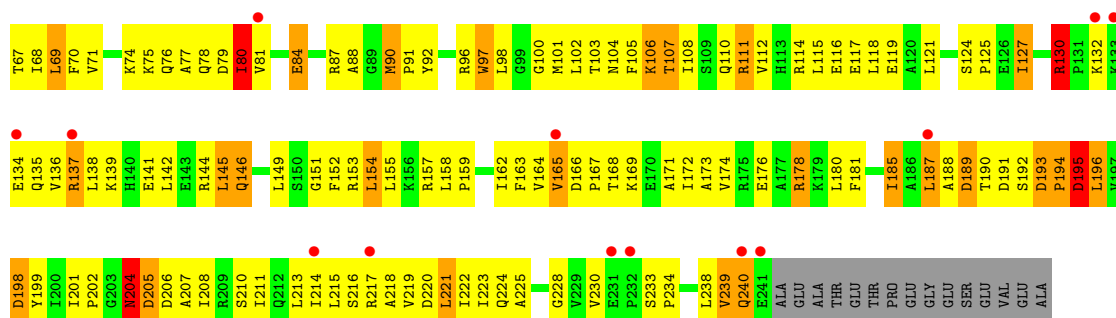
Chain AB:



• Molecule 2: 30S ribosomal protein S2

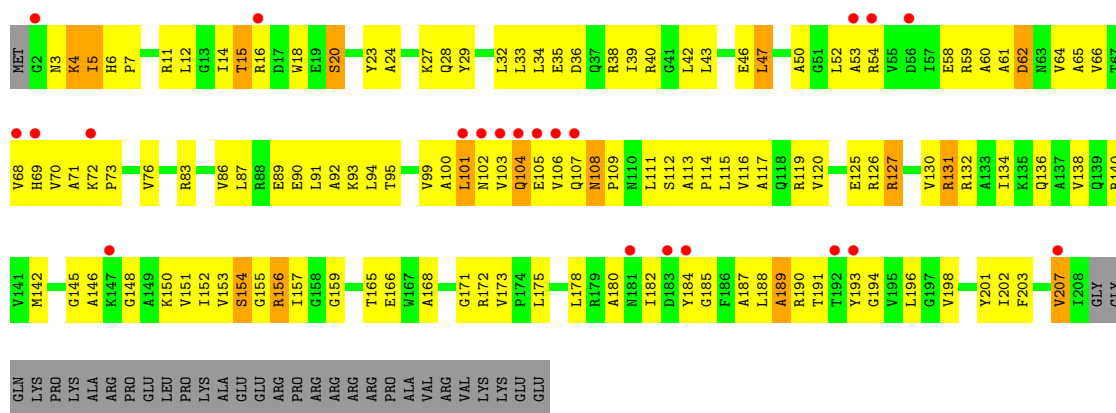
Chain CB:





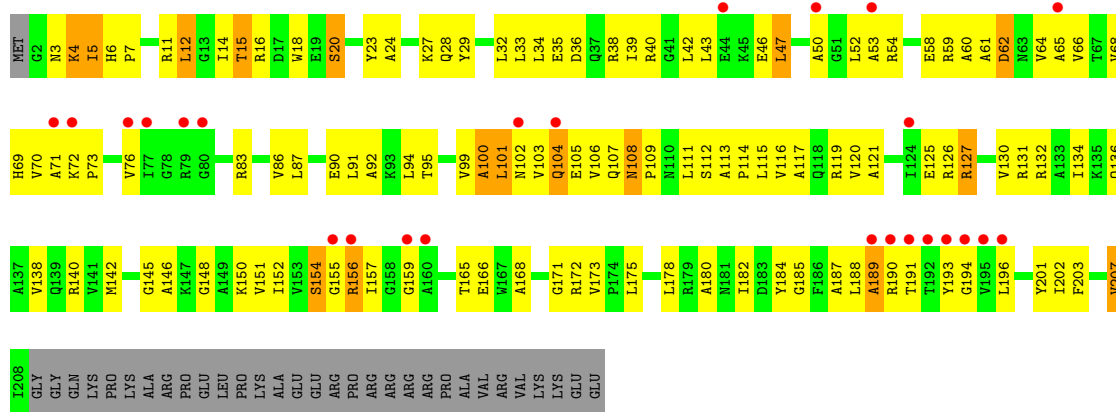
• Molecule 3: 30S ribosomal protein S3

Chain AC:



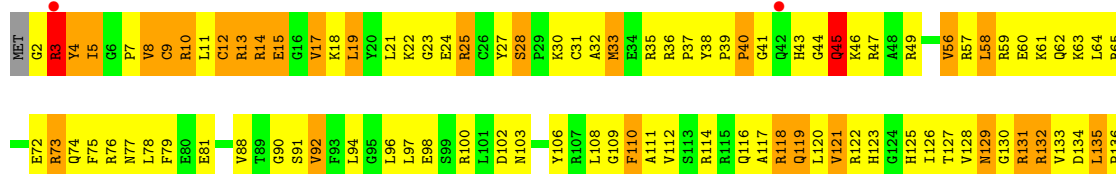
• Molecule 3: 30S ribosomal protein S3

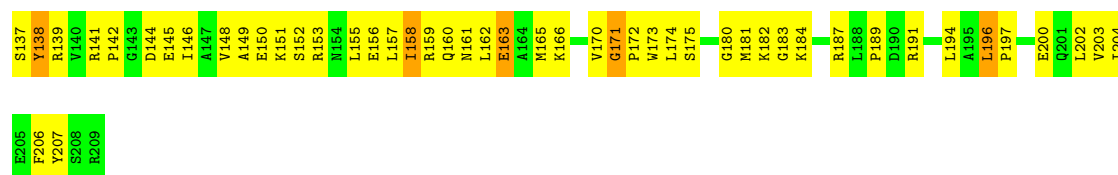
Chain CC:



• Molecule 4: 30S ribosomal protein S4

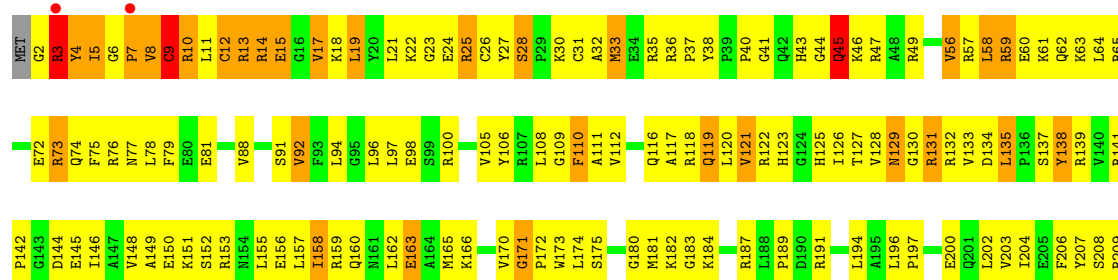
Chain AD:

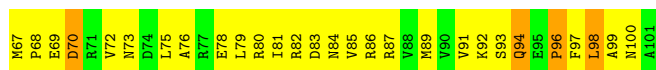




- Molecule 4: 30S ribosomal protein S4

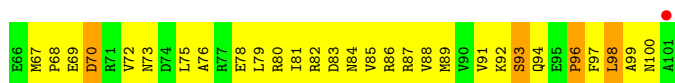
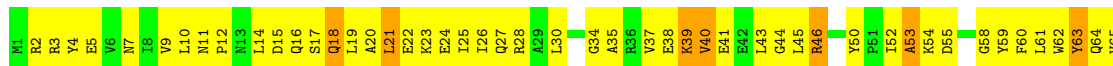
Chain CD:





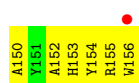
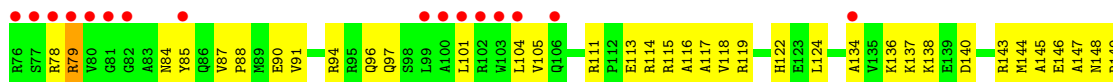
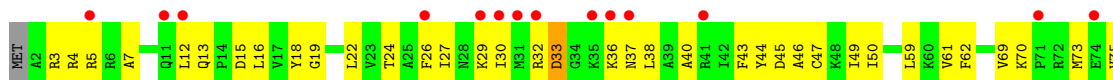
• Molecule 6: 30S ribosomal protein S6

Chain CF:



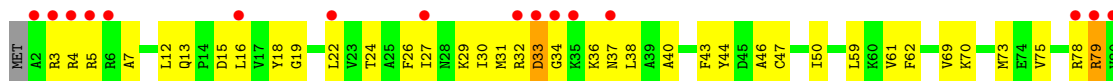
• Molecule 7: 30S ribosomal protein S7

Chain AG:



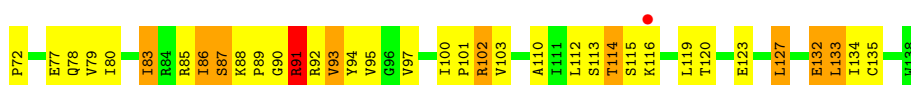
• Molecule 7: 30S ribosomal protein S7

Chain CG:



• Molecule 8: 30S ribosomal protein S8

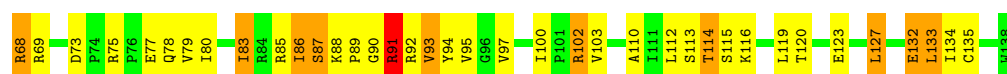
Chain AH:



• Molecule 8: 30S ribosomal protein S8

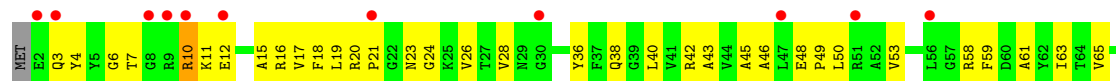
Chain CH:





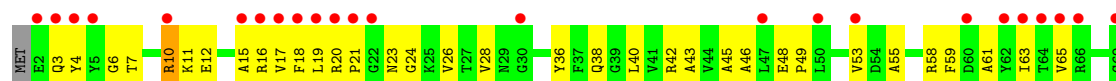
• Molecule 9: 30S ribosomal protein S9

Chain AI:



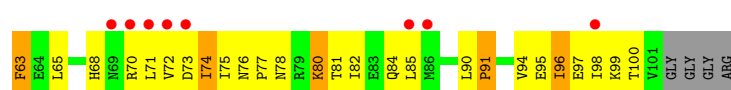
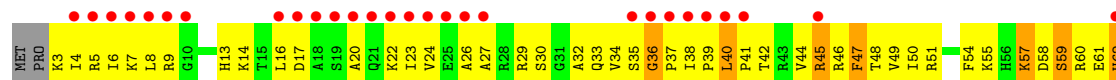
• Molecule 9: 30S ribosomal protein S9

Chain CI:



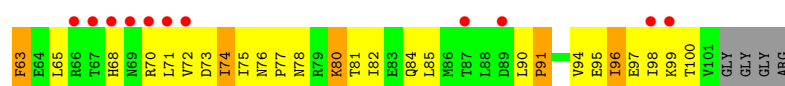
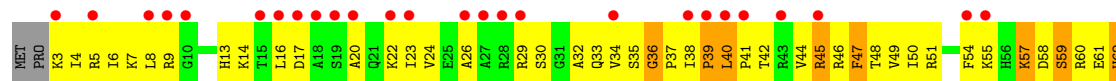
• Molecule 10: 30S ribosomal protein S10

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:



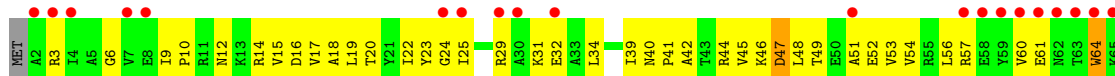
- Molecule 12: 30S ribosomal protein S12

Chain CL:



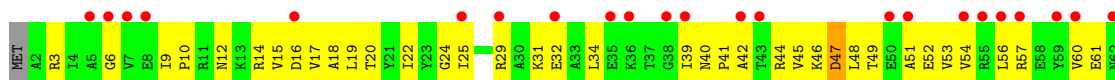
- Molecule 13: 30S ribosomal protein S13

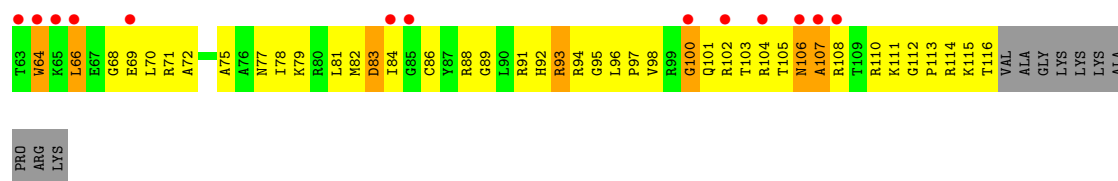
Chain AM:



- 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

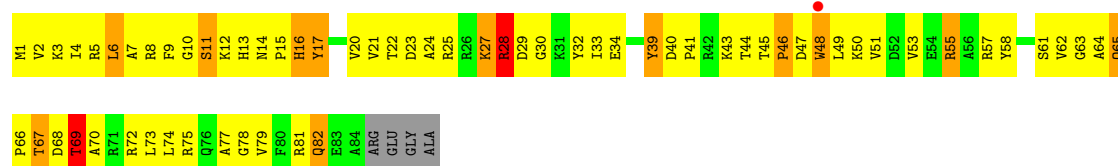
Chain CO:

- Molecule 16: 30S ribosomal protein S16

Chain AP:

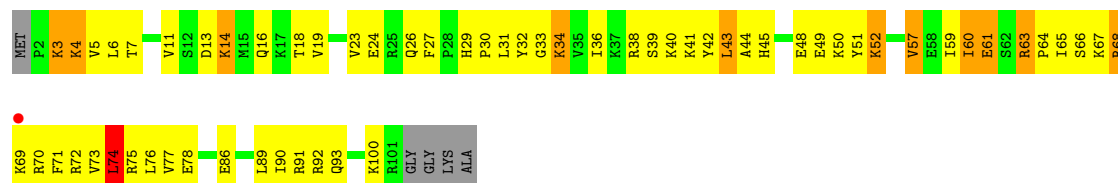
- Molecule 16: 30S ribosomal protein S16

Chain CP:



• Molecule 17: 30S ribosomal protein S17

Chain AQ:



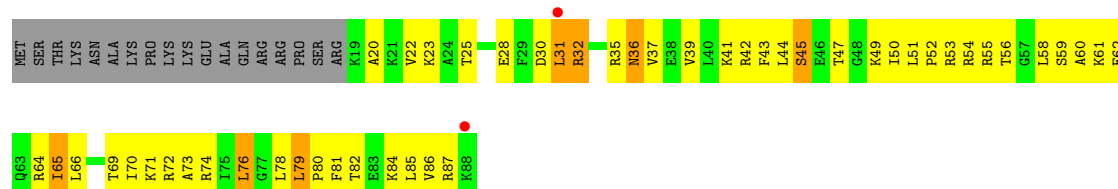
• Molecule 17: 30S ribosomal protein S17

Chain CQ:



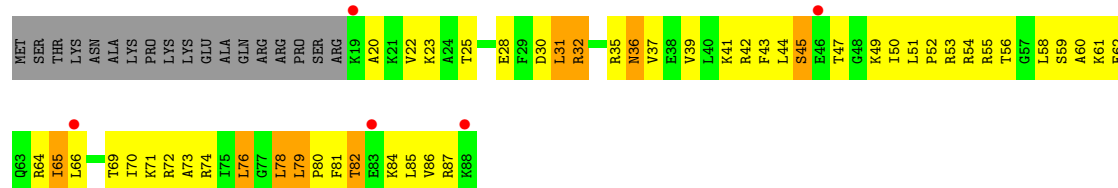
• Molecule 18: 30S ribosomal protein S18

Chain AR:



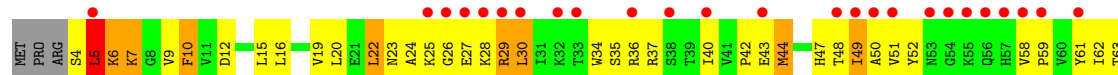
• Molecule 18: 30S ribosomal protein S18

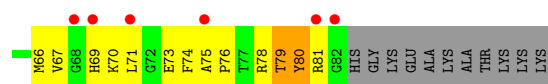
Chain CR:



• Molecule 19: 30S ribosomal protein S19

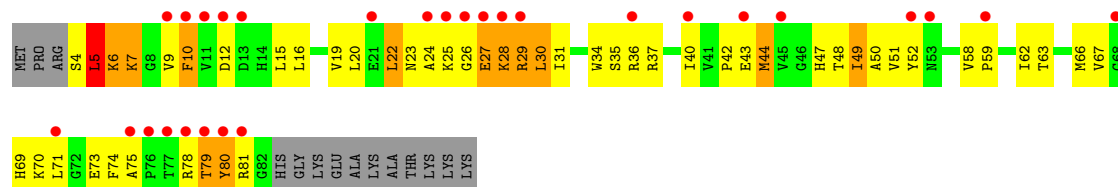
Chain AS:





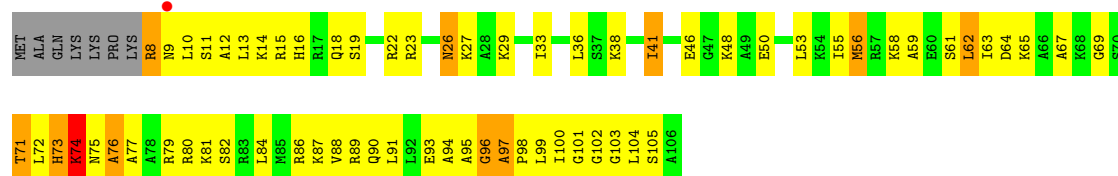
- Molecule 19: 30S ribosomal protein S19

Chain CS:



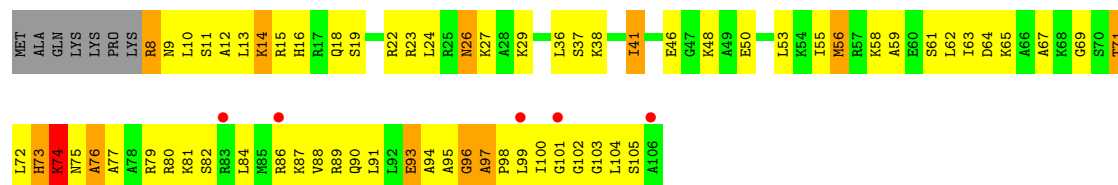
- Molecule 20: 30S ribosomal protein S20

Chain AT:



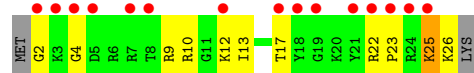
- Molecule 20: 30S ribosomal protein S20

Chain CT:



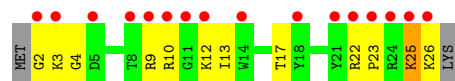
- Molecule 21: 30S ribosomal protein Thx

Chain AU:



- Molecule 21: 30S ribosomal protein Thx

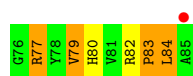
Chain CU:



- Molecule 22: 50S ribosomal protein L27

Chain B0:





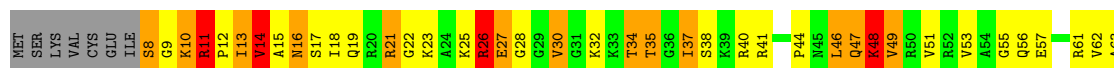
- Molecule 22: 50S ribosomal protein L27

Chain D0:



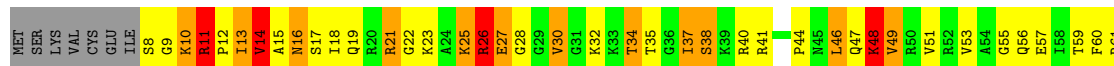
- Molecule 23: 50S ribosomal protein L28

Chain B1:



- Molecule 23: 50S ribosomal protein L28

Chain D1:



- Molecule 24: 50S ribosomal protein L29

Chain B2:

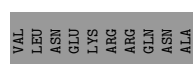


- Molecule 24: 50S ribosomal protein L29

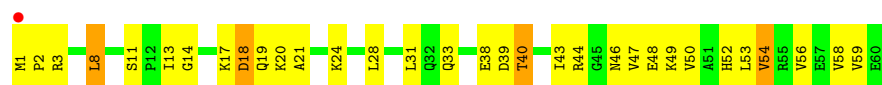
Chain D2:



- Molecule 25: 50S ribosomal protein L30

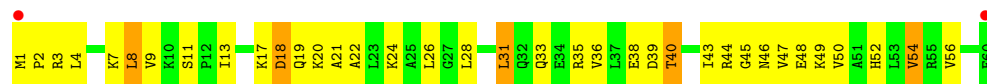


Chain B3: 



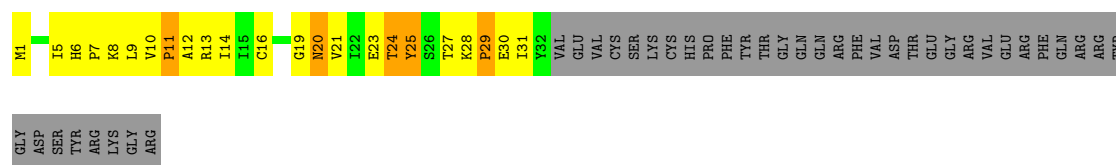
- Molecule 25: 50S ribosomal protein L30

Chain D3: 



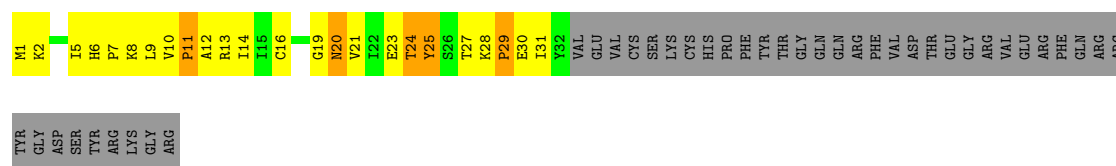
- Molecule 26: 50S ribosomal protein L31

Chain B4: 



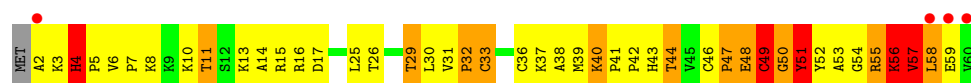
- Molecule 26: 50S ribosomal protein L31

Chain D4: 



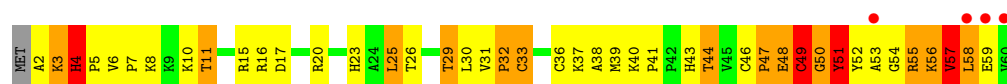
- Molecule 27: 50S ribosomal protein L32

Chain B5: 



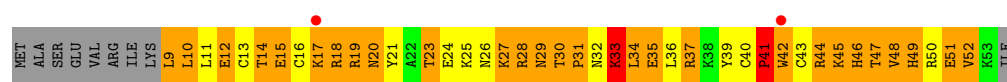
- Molecule 27: 50S ribosomal protein L32

Chain D5: 



- Molecule 28: 50S ribosomal protein L33

Chain B6: 



- Molecule 28: 50S ribosomal protein L33

Chain D6: 



- Molecule 29: 50S ribosomal protein L34

Chain B7: 



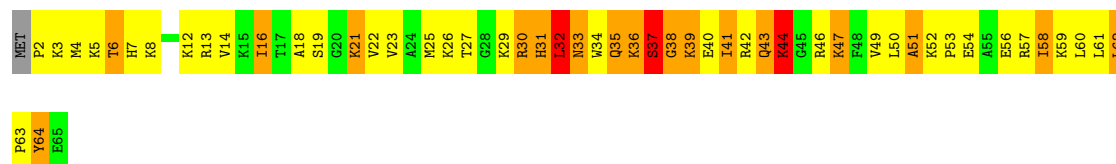
- Molecule 29: 50S ribosomal protein L34

Chain D7: 



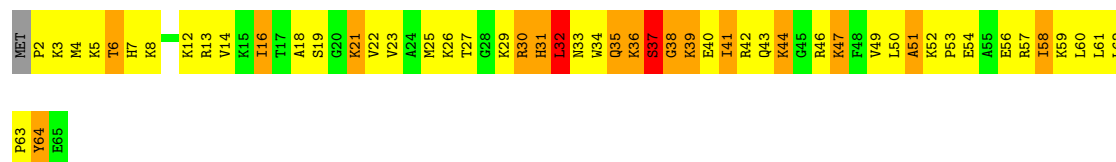
- Molecule 30: 50S ribosomal protein L35

Chain B8: 



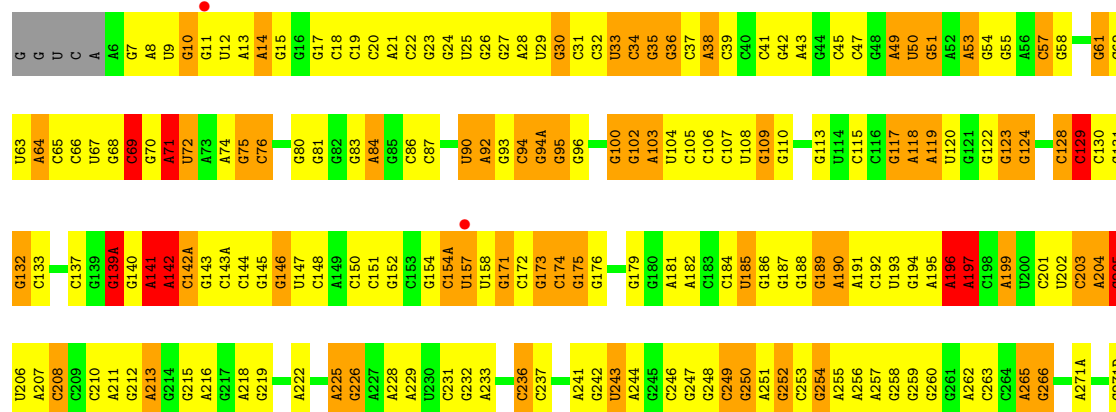
- Molecule 30: 50S ribosomal protein L35

Chain D8: 



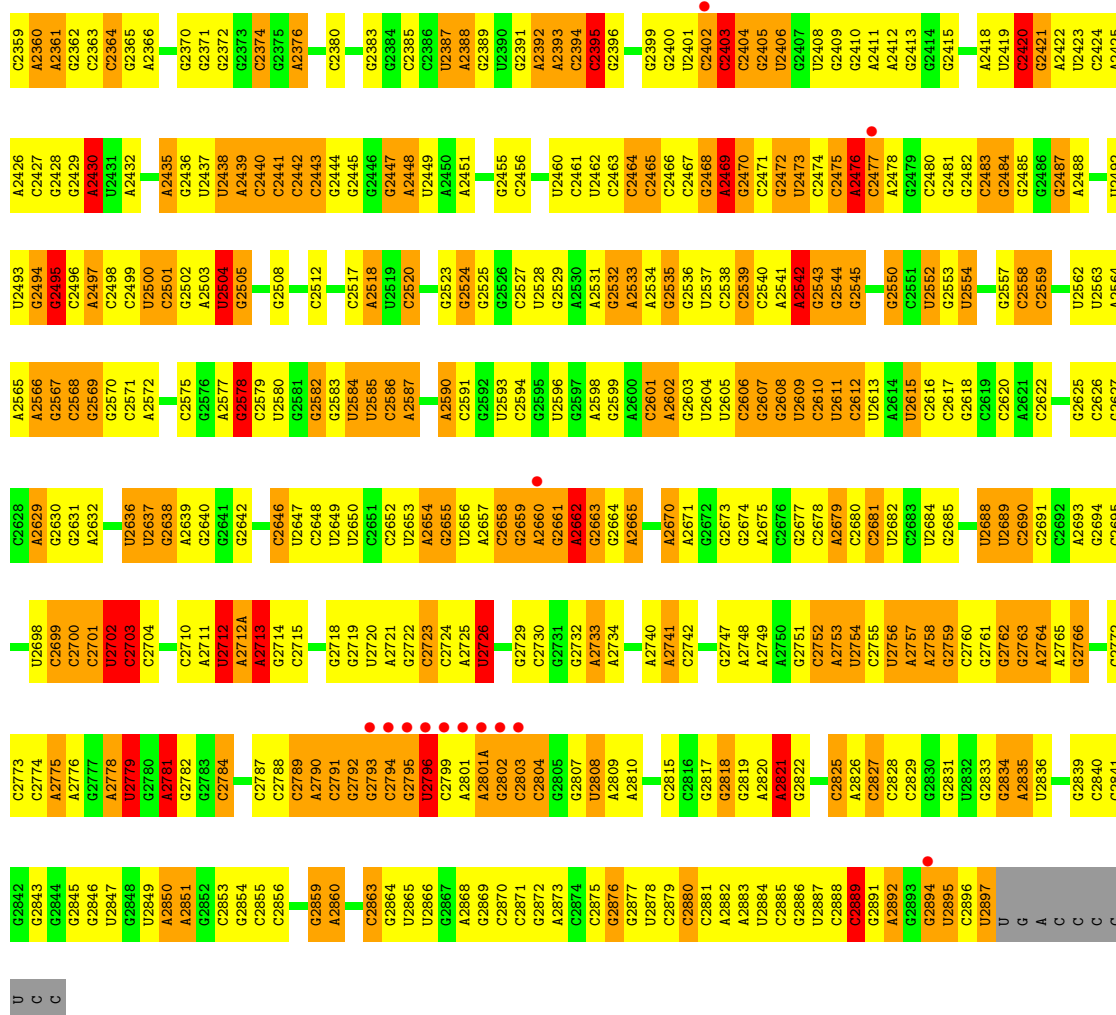
- Molecule 31: 23S ribosomal RNA

Chain BA: 



C1230	U1165	G1044	C982	A917	U847	U779	G717	G642	G582	G512	A447	A371	A310	U271E
G1236	C1166	A1045	A983	A918	G646	G780	A718	A643	G583	A513	U448	G372	A311	C271F
A1237	U1167	A1046	A984	G919	A849	A781	C719	A644	C594	A514	U449	U373	G312	C271G
G1238	C1168	G1047	C985	G920	C850	A782	C720	C645	G585	A515	U450	A374	G313	G271H
G1239	A1169	A1048	C986	G921	U851	A783	C721	A646	A596	C516	C451	C375	G314	G271I
G1240	G1170	G1049	G987	U922	G854	A784	A722	G647	G587	C517	U452	C376	G315	G271J
A1241	G1171	A1050	A988	C923	G855	G785	G723	G648	U588	G518	C453	C377	C316	U271K
A1242	G1172	G1051	G989	C924	G856	C786	U724	G651	C589	U519	C455	C378	C319	U271L
G1245	U1173	C1052	A990	C925	C856	G787	G725	C652	A590	G520	C456	G379	G319	U271M
A1246	U1174	C1053	C991	A926	C857	U788	G726	G656	C591	G521	A457	U380	A320	U271N
G1250	U1175	A1106	C992	G927	U858	A789	A727	U657	G592	G522	U458	G384	G321	G271O
A1255	C1176	G1107	G993	G928	G859	C790	G728	C658	G593	C523	U459	U385	A322	G271P
C1257	A1177	U1108	C994	U930	U860	C791	G729	C659	U594	U524	A460	C385	G323	G271Q
C1258	C1178	C1109	C995	G931	A861	G792	C730	G660	C595	U525	C461	G386	A324	G271R
G1259	G1179	G1110	A996	G932	G862	A793	C731	C661	A526	A527	C462	U387	G325	G271S
A1264	C1180	A1111	C997	A933	A863	G794	G732	G662	U597	G528	U464	G388	G326	G271T
U1255	U1181	G1112	C998	G934	G864	C795	G733	G663	G598	A529	U465	G389	G327	G271U
G1266	A1182	U1113	U999	C935	C865	A734	C664	C665	G600	G530	A466	A394	G328	G271V
C1267	C1185	G1114	A1000	C936	A866	G797	A735	G736	C601	C531	U467	U395	A399	G271X
G1268	G1186	G1115	G1002	U937	C867	C798	C737	G668	G602	A532	U468	G396	A391	U271Y
A1269	U1187	C1116	C999	A945	U868	A800	C738	G669	A603	G533	U469	G397	A332	C271Z
C1270	C1188	G1117	G1003	G947	G869	A802	G739	A670	G604	U534	C470	G398	G333	G272B
G1271	A1189	C1118	C1004	A941	A870	A803	G740	C671	G605	C535	A471	A401	C334	G272C
C1272	G1190	G1119	C1005	U942	U871	U803	G741	C672	U606	A536	G472	C335	C335	G272D
G1273	U1191	C1120	C1006	U943	A872	A804	G742	C673	U607	C537	G473	U405	C336	C272G
C1274	C1192	G1121	A1009	G944	G873	G805	G743	A674	A608	C540	U474	G406	C337	G272H
G1275	U1193	G1122	A1010	A946	G874	C806	G744	A675	A609	C541	U475	C340	A340	U272I
A1276	C1194	C1123	C1007	G947	C875	U807	G745	A676	G610	C542	U476	C341	G341	C272J
C1277	U1195	G1124	A1011	G948	C876	G808	G746	A677	C611	G543	U477	C342	G342	G274
G1278	C1196	A1125	G1012	U949	U877	G809	A747	C678	C612	A547	U478	C343	G343	C275
A1279	G1201	U1126	C1013	C949	A878	U810	G748	C679	G613	A548	U479	C344	G344	C280
C1280	C1202	G1127	U1014	G950	G879	U811	G749	G680	U614	G549	U480	C345	A346	G281
G1281	G1203	A1128	G1015	G951	G880	C812	C750	G681	U614A	G551	U481	C346	A347	A282
C1282	U1204	U1130	G1016	G952	G881	C813	A751	G682	G614B	U554	U482	C348	A348	A283
A1283	G1205	G1131	G1017	A953	G882	C814	A752	G683	A614C	G554	U483	C349	C349	U284
C1284	C1206	U1132	C1018	G954	G883	C815	A753	G684	G615	G559	U484	U350	C285	C286
G1285	U1207	G1133	U1019	C955	C884	C817	G754	G685	G619	U562	U489	C351	C287	C287
C1286	C1208	C1135	A1020	G956	G882	G818	C755	G686	G620	U563	U491	C352	C288	C288
A1287	U1209	G1136	G1021	A957	C893	A819	C756	G687	A621	G562	U492	C353	C292	U293
C1288	C1210	U1137	C1022	U958	C894	A820	U757	G688	G623	C564	U493	C354	U296	C296
G1289	G1211	G1138	U1023	A959	U895	A824	G760	G689	G624	C565	U494	C355	C297	C297
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G1292	A1214	U1141	U1026	C964	C899	U828	G763	C693	A627	U568	U500	U358	G303	U303
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A1294	U1216	A1143	C1028	C968	C902	G830	G765	G700	G629	A571	U505	U362	U363	U363
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A1297	A1220	G1154	G1034	C971	U907	G836	G769	A706	C634	C574	U508	U365	U365	U365
C1298	C1221	A1155	U1035	G972	C908	C837	G770	A707	G635	A575	U509	U366	G366	G366
G1299	U1222	U1156	G1036	G973	A909	C838	U773	C708	G636	U576	U510	U367	G370	G370
C1300	G1223	G1157	G1037	G974	A910	U839	A774	C709	A637	G577	U511	U368	G371	G371
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G1302	G1225	G1159	G1039	G976	C912	G845	G776	G711	U639	G579	U513	U370	G373	G373
C1303	A1226	C1161	C1040	G977	C913	G846	G777	G712	U640	C580	U514	U371	G374	G374
G1304	U1227	U1162	G1041	A980	C914	G847	G778	G713	C641	C581	U515	U372	G375	G375
A1305	G1228	G1163	G1042	A981	C915	G848	G779	G714	C642	C582	U516	U373	G376	G376
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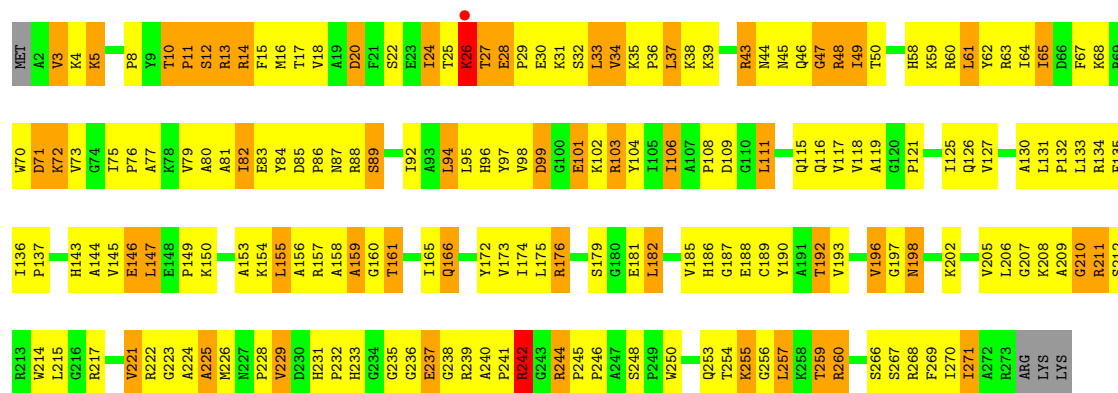
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G2302	G2239	U2011	U1863	C1711	U1578	C1501	G1440	G1371	C1305
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A2291	A2247	A2013	A1937	U1713	A1580	U1503	G1442	A1373	
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A2309	G2246	G2018	C1879	U1720	A1586	C1509	G1448	A1378	U1313
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A2311	C2248	A2020	C1881	A1722	A1588	A1509A	G1450	G1380	C1315
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G2315	G2252		A1885	G1742	C1592	C1513	A1451	A1384	G1319
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C2324	G2261	G2037	C1894	G1750	G1601	G1524	A1462	C1398	U1329
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C2326	G2263	G2039	G1896	G1752	A1603	G1526	G1465	G1400	A1331
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G2331	A2268	A2042	A1900	G1756	A1609	G1529	C1469	U1405	U1406
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	U2267	G2067	U1925	A1784	A1700	A1634	G1494	G1433	G1364
U2291	G2230	C2068	C1926	A1851	A1852	G1568	U1495	U1434	
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A1287	G1225	C1161	G1039	C975	U839	G775	C708	G642	G582	A514	G450	A371	A311
U1288	A1226	G1162	C1040	G975A	C840	G776	U709	A643	G583	A515	C451	G372	G312
C1289	G1227	G1163	C1041	C976	A841	A777	G710	A644	C584	C316	C452	U373	C313
G1290	G1228	G1164	G1042	G977	G842	G778	G711	C545	G585	C517	C453	A374	A314
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C1293	U1234	U1167	A1045	A980	A849	A781	A718	G648	U588	G520	C456	C377	C319
U1294	G1235	G1168	A1046	A983	C850	A782	A719	G649	C589	G521	A457	C378	A320
G1296	G1236	G1170	A1048	A983	G919	A783	C719	G650	A590	G522	C458	G379	A319
C1297	A1237	G1171	G920	G987	U851	A784	C720	G651	C591	G523	U459	U380	G321
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C1299	G1239	A1174	G1051	G989	G855	U787	G723	U657	U594	A526	C461	G323	G323
U1300	U1240	U1175	C1052	A990	C856	A788	U724	C583	C595	C527	G463	G386	G325
A1301	A1241	G1176	C1053	C991	C857	A789	G725	C589	G596	C529	U464	G387	G326
A1302	G1242	A1177	A1106	C992	U858	C790	G726	G660	U597	A529	U465	G388	G327
G1303	G1243	C1178	G1107	G993	G859	C791	A727	C661	G598	A466	A467	G389	U328
C1304	G1244	C1179	U1108	C994	U860	G792	G728	G662	G599	C531	G467	G390	G329
C1305	G1245	C1180	C1109	C995	A861	A793	G729	G663	G600	A532	G468	A394	A390
C1306	A1246	C1181	G1110	A996	G862	G794	C730	C664	C601	G533	C469	U395	A331
A1307	A1247	A1111	G1111	G997	A863	C795	C731	C665	C602	U534	A470	U396	A332
A1308	G1248	G1112	G1112	C998	G864	C796	C732	G666	A603	C535	A471	G397	A333
G1309	U1249	U1113	U1113	U999	C865	C797	G733	U667	G804	A536	A472	G398	C334
C1310	G1250	G1114	G1114	A1000	A866	C797	A734	G668	C605	C537	G473	A401	C335
U1313	C1251	G1115	G1115	A1001	C867	A795	A735	G669	U606	C540	G474	G401	C336
C1314	G1252	U1183	C1116	G1002	U868	G801	C736	A670	U607	C541	U475	U405	C337
C1315	A1253	A1189	G1117	G1003	G869	A802	C737	C571	A608	C542	G476	U406	G338
U1316	U1255	G1190	C1118	C1004	A870	U803	G738	C572	A609	C543	A477	G406	U339
A1317	G1256	G1191	G1118	C1005	U871	A804	G739	C573	G610	C544	A478	A409	G341
C1318	C1257	G1192	G1122	C1006	A872	G805	U740	G674	G611	C545	A479	G410	G342
G1319	G1258	U1195	G1123	C1007	G873	C812	G741	A675	A480	G548	A480	G411	G343
C1320	C1259	C1196	G1124	A1010	G874	U807	G742	A676	G549	G549	C481	G412	G344
A1321	G1260	U1197	G1125	G1011	A945	G808	G743	A677	G551	G551	A482	C413	A345
A1322	C1261	U1198	A1126	G1012	G875	U809	G744	C578	G552	C546	A483	C414	G346
U1323	G1262	U1199	U1130	U1013	U877	U810	G745	C579	G553	C547	C484	A415	G347
G1324	U1263	G1200	G1131	U1014	A878	U811	A746	G680	G615	U557	C485	C416	G348
G1325	G1264	C1201	A1132	G1015	G879	C812	U747	G681	G616	G558	C486	C417	U350
U1326	A1265	U1195	U1133	G1016	G880	U813	U750	G682	C618	G559	G489	G418	G351
C1327	G1266	C1196	C1135	G1017	G881	C814	A751	C683	G619	G560	G491	C419	G352
G1328	U1267	U1205	G1136	C1018	G882	C817	A752	G684	G620	C561	A492	G353	G353
U1329	A1268	G1206	G1137	A953	G883	G818	C753	A685	G621	G562	C493	A423	G354
C1330	A1269	C1207	U1138	G954	C884	G819	C754	G686	G622	U569	G500	G355	G355
A1331	C1270	C1208	G1139	C955	G892	A820	C755	U688	G623	G563	G494	U427	G356
G1332	G1271	G1209	C1140	U853	C894	A824	C756	A689	G624	U566	G495	A428	A357
C1333	A1272	A1210	U1141	A959	U895	A824	U757	G690	G625	A567	G498	A429	U358
G1334	U1273	U1211	U1142	A896	U896	A896	C691	C591	A627	U568	U499	G430	A359
U1335	A1274	G1212	A1142A	C961	C897	U826	G760	C592	G628	U569	G500	U431	G360
A1336	A1275	A1213	A1143	U1026	C898	U827	A761	C693	G629	G570	A501	A432	G361
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G1340	G1279	G1219	C1153	G967	C902	G831	U767	A699	C635	C574	G506	A443	G363B
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C1345	U1281	A1221	A1155	U969	C904	U833	G769	G701	A637	G508	C509	C445	A363F
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G1348	G1285	G1223	C1158	G972	U907	G836	U774	A706	U640	G579	U511	A448	G366
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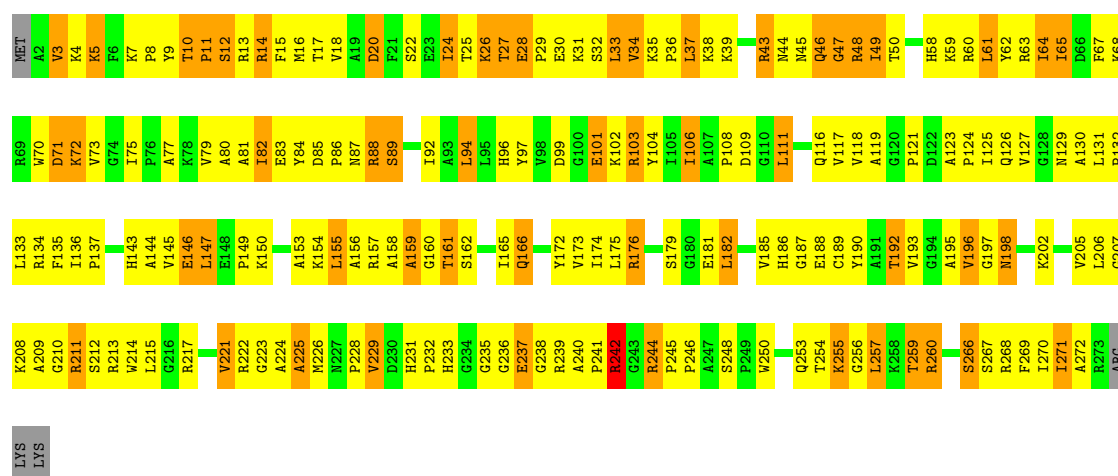
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G2324	U2262	G2190	G2101	C2040	G1973	G1905	C1832	U1768	C1686	G1621	G1555	A1486	G1421	A1354
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A2326	C2264	G2192	C2103	A2042	A1978	C1909	U1834	G1770	U1688	G1625	C1557	G1488	A1427	G1356
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C2363	C2303	A2241	U	U2079	G2018	U1953	G1883	A1809	C1745A	C1662	C1599	G1527	C1463	C1399
G2364	G2304	G2242	A	G2080	A2019	G1954	A1884	G1810	G1746	A1665	G1600	G1528	G1464	G1400
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A2366	C2306	U2244	A	A2082	C2021	U1955	C1886	A1812	A1749	G1667	U1602	A1529	G1466	C1404
G2370	G2307	U2245	U	G2083	U2022	U1956	C1887	G1813	G1750	A1668	G1603	G1529	C1467	A1404
U2371	C2308	G2246	C	C2084	G2023	C1957	G1888	G1814	G1751	A1669	C1604	C1530	C1468	U1405
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G2373	C	U2086	C	U2087	C2025	G1959	A1890	G1752	G1752	C1670	C1507	C1532	G1470	U1407
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G2381	G2316	G2255	C	G2094	A2033	C1967	G1899	G1826	A1762	U1680	C1615	C1549	G1479	G1416
U2382	U2317	G2256	C	G2095	A2034	G1968	A1900	G1827	G1763	G1681	C1616	C1550	G1480	G1417
G2383	G2318	U2257	C	U2096	C2036	A1969	A1901	G1828	G1764	G1682	C1617	C1551	U1481	G1418
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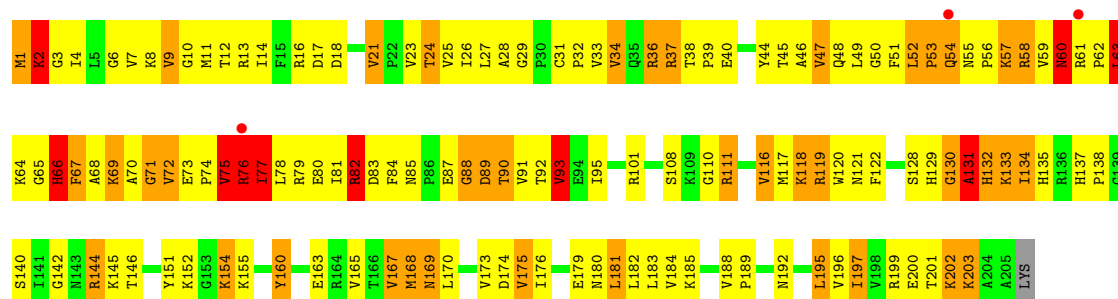
• Molecule 33: 50S ribosomal protein L2

Chain DD:



• Molecule 34: 50S ribosomal protein L3

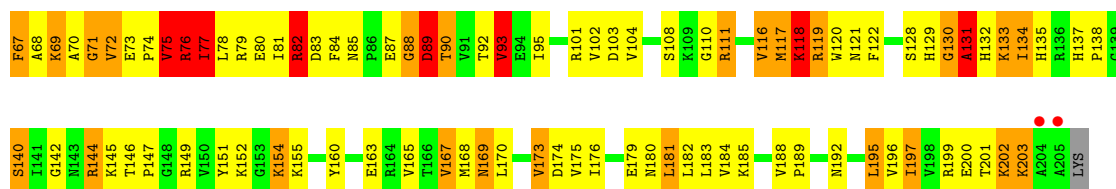
Chain BE:



• Molecule 34: 50S ribosomal protein L3

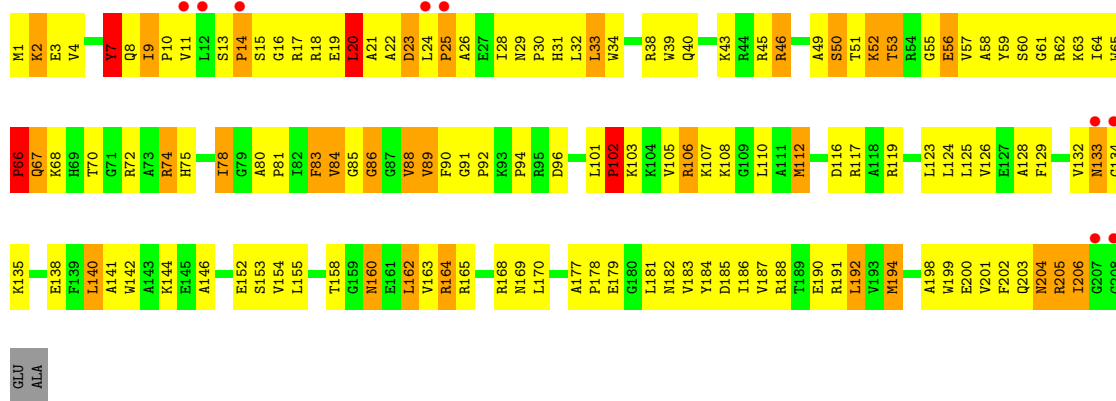
Chain DE:





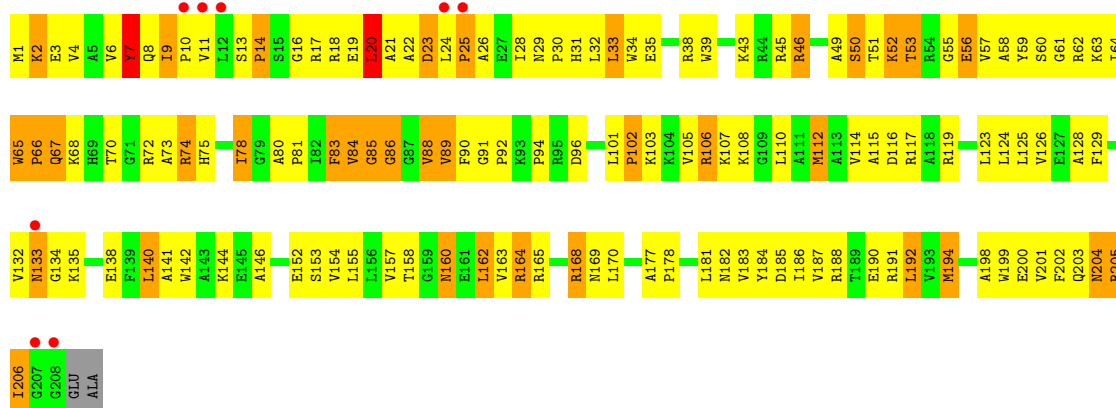
• Molecule 35: 50S ribosomal protein L4

Chain BF:



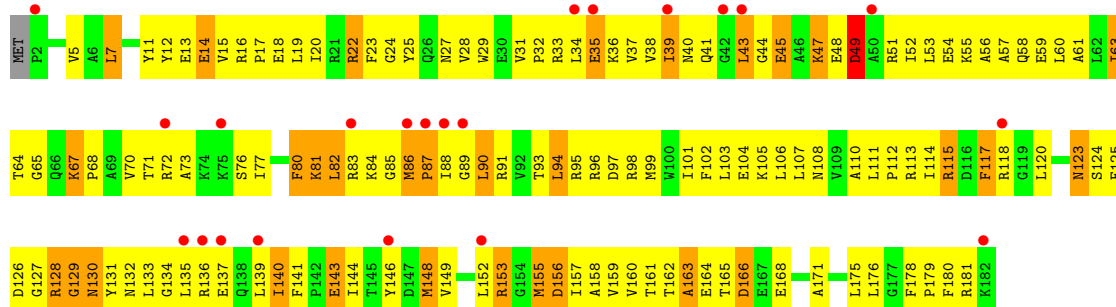
• Molecule 35: 50S ribosomal protein L4

Chain DF:



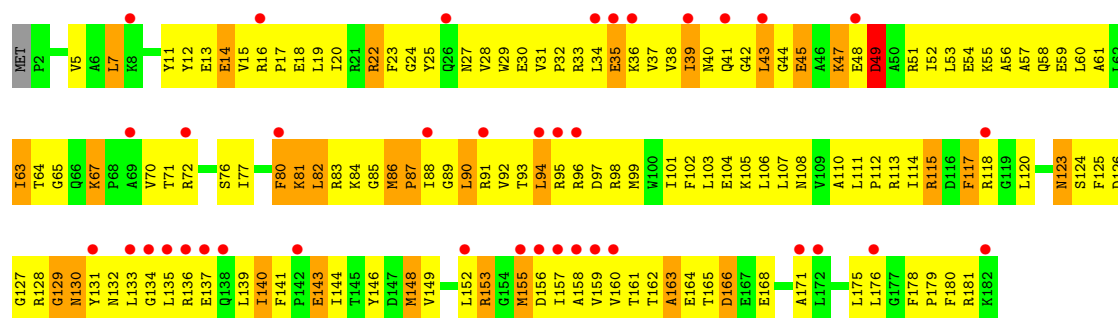
• Molecule 36: 50S ribosomal protein L5

Chain BG:



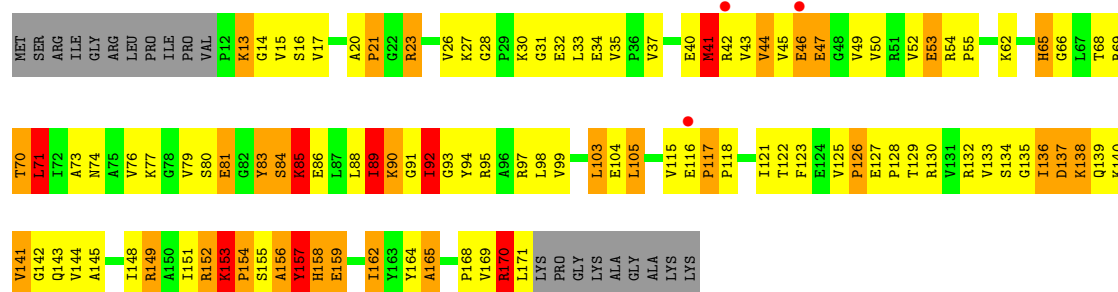
- Molecule 36: 50S ribosomal protein L5

Chain DG:



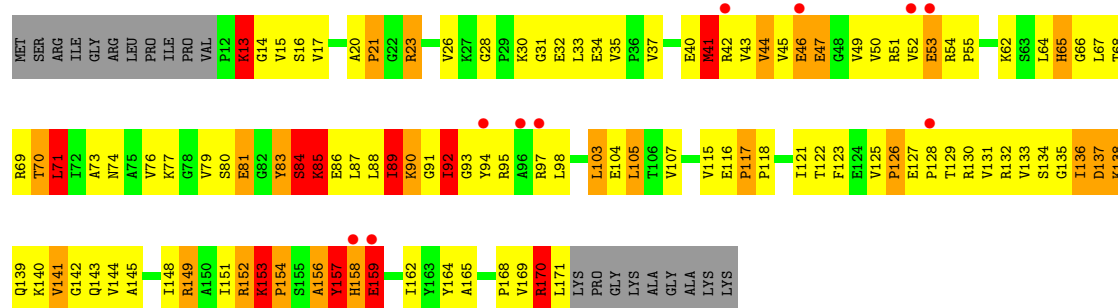
- Molecule 37: 50S ribosomal protein L6

Chain BH:



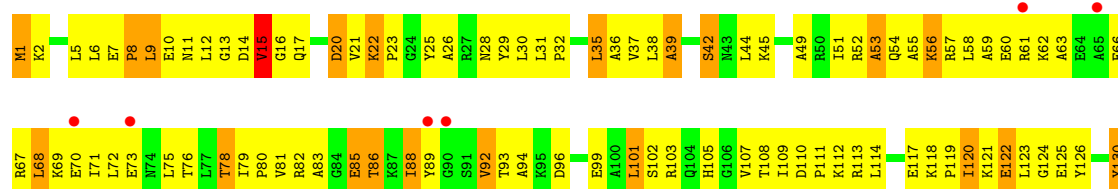
- Molecule 37: 50S ribosomal protein L6

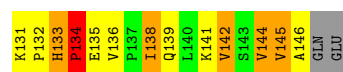
Chain DH:



- Molecule 38: 50S ribosomal protein L9

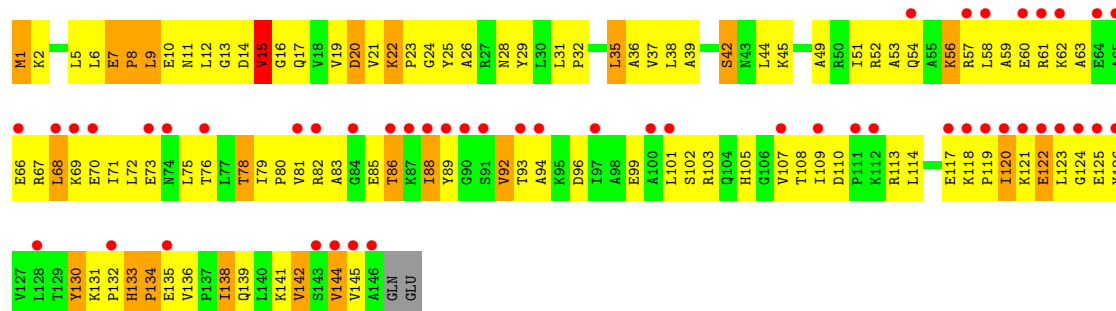
Chain BI:





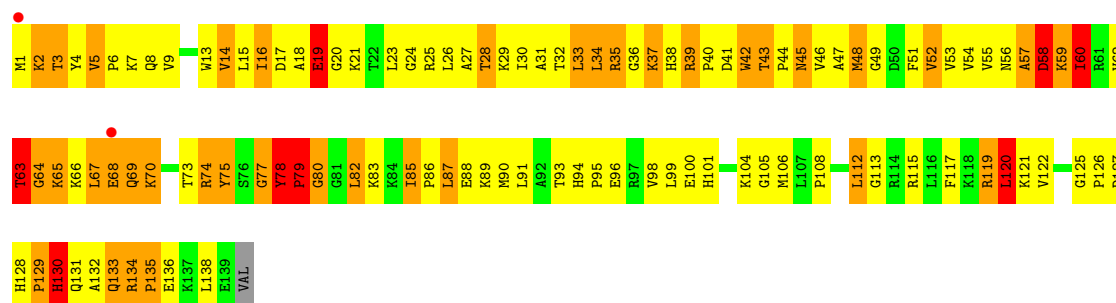
• Molecule 38: 50S ribosomal protein L9

Chain DI:



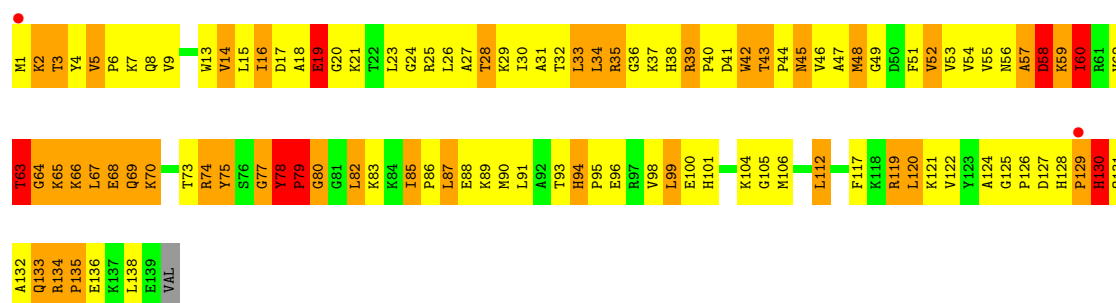
• Molecule 39: 50S ribosomal protein L13

Chain BN:



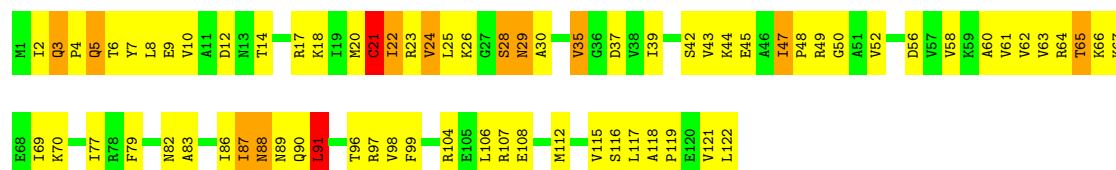
• Molecule 39: 50S ribosomal protein L13

Chain DN:



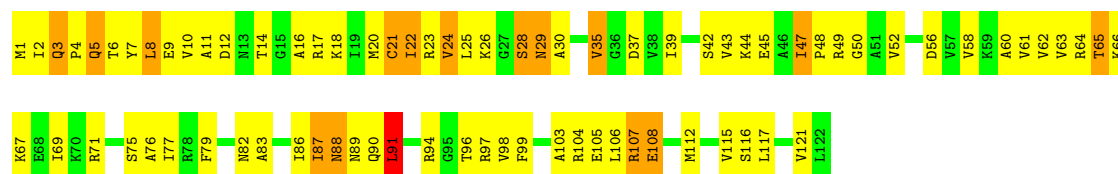
• Molecule 40: 50S ribosomal protein L14

Chain BO:



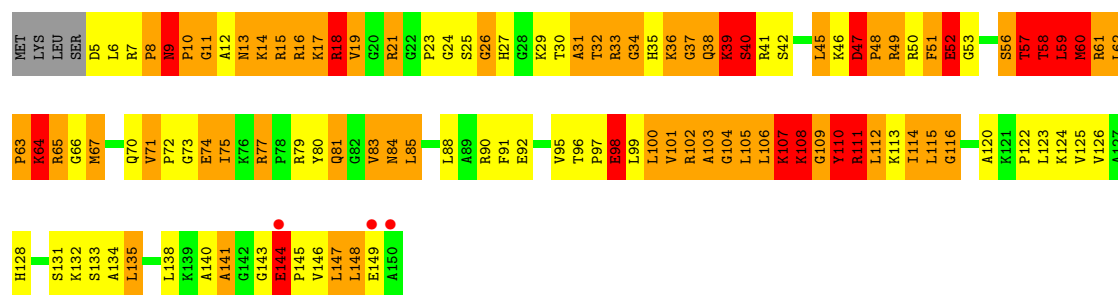
- Molecule 40: 50S ribosomal protein L14

Chain DO:



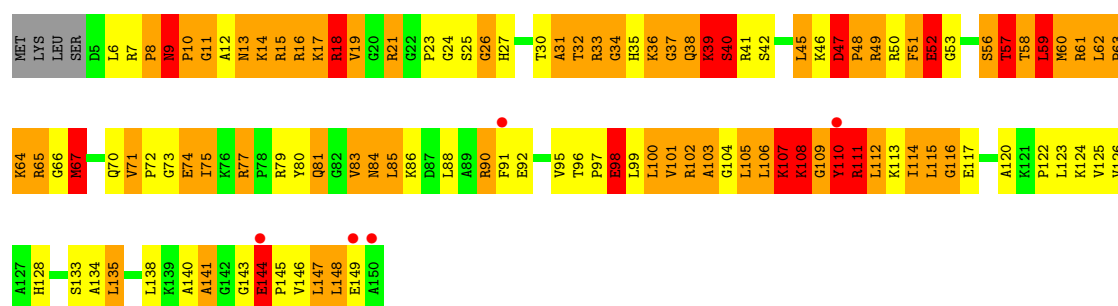
- Molecule 41: 50S ribosomal protein L15

Chain BP:



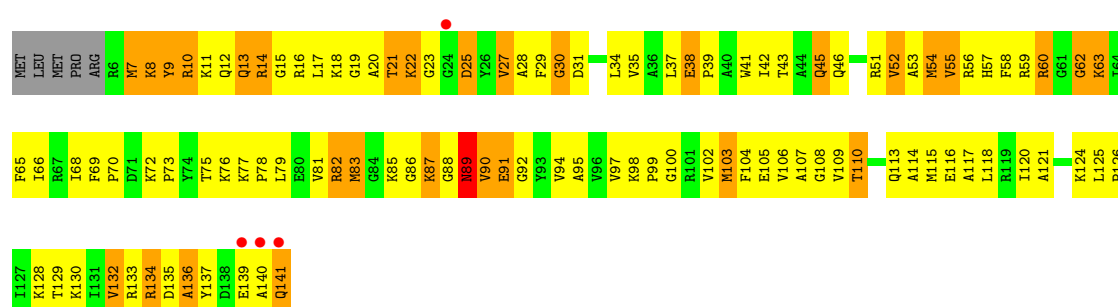
- Molecule 41: 50S ribosomal protein L15

Chain DP:



- Molecule 42: 50S ribosomal protein L16

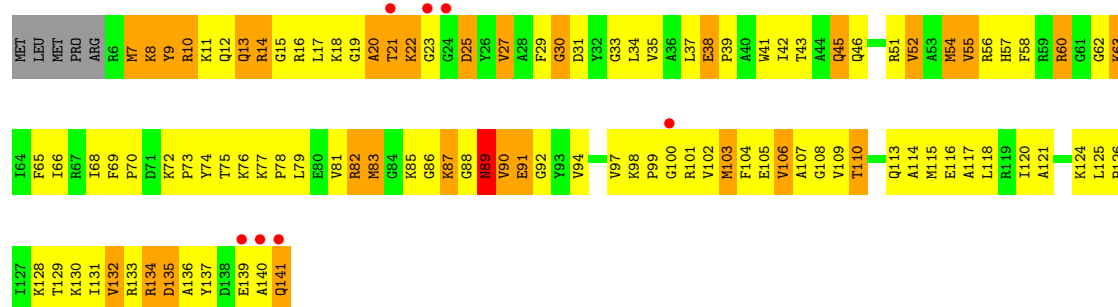
Chain BQ:



- Molecule 42: 50S ribosomal protein L16

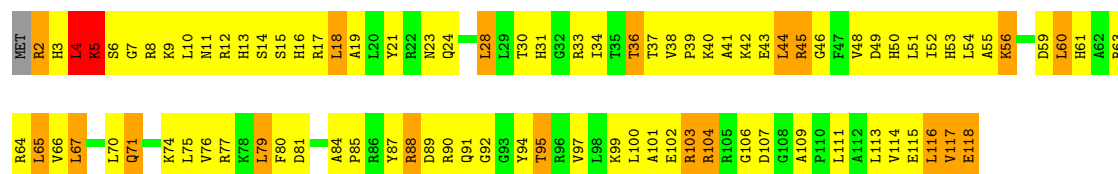
Chain DQ:





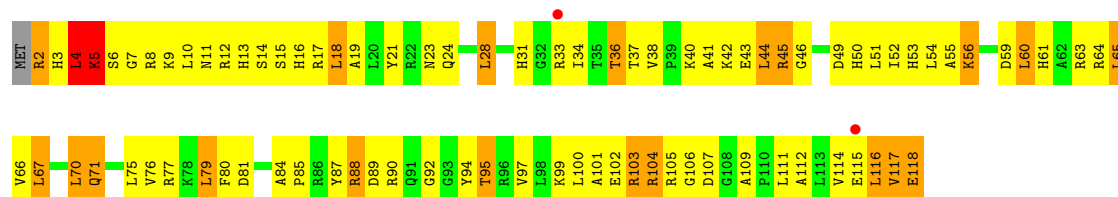
- Molecule 43: 50S ribosomal protein L17

Chain BR:



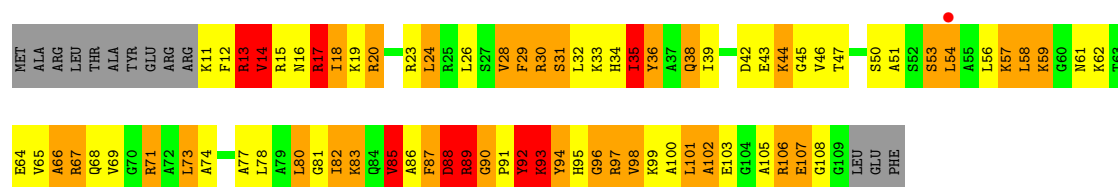
- Molecule 43: 50S ribosomal protein L17

Chain DR:



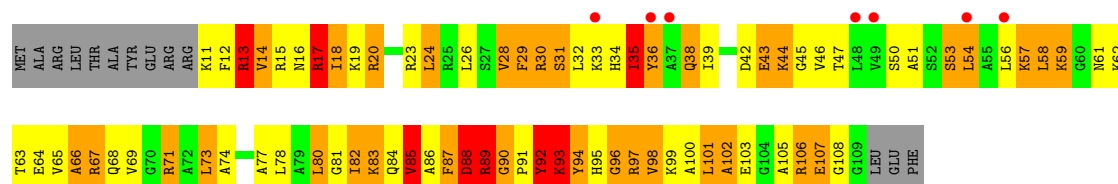
- Molecule 44: 50S ribosomal protein L18

Chain BS:



- Molecule 44: 50S ribosomal protein L18

Chain DS:

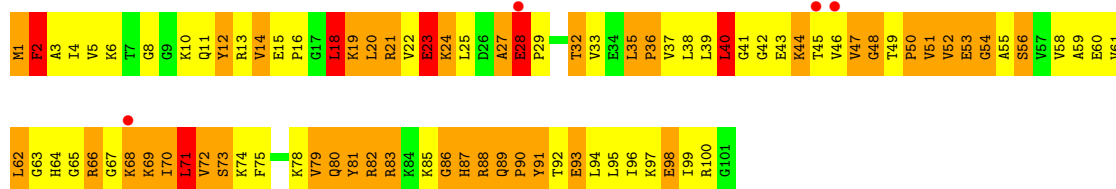


- Molecule 45: 50S ribosomal protein L19

Chain BT:

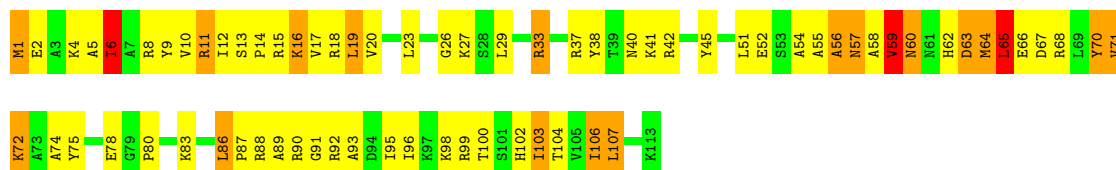
- Molecule 47: 50S ribosomal protein L21

Chain DV:



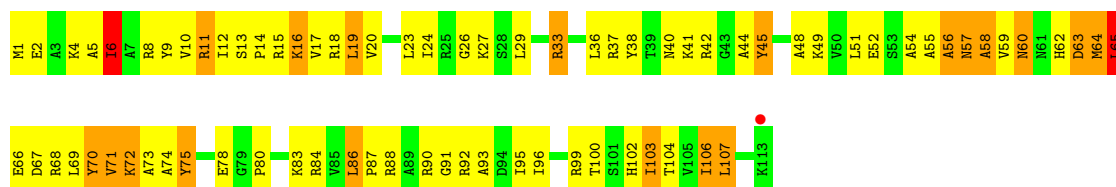
- Molecule 48: 50S ribosomal protein L22

Chain BW:



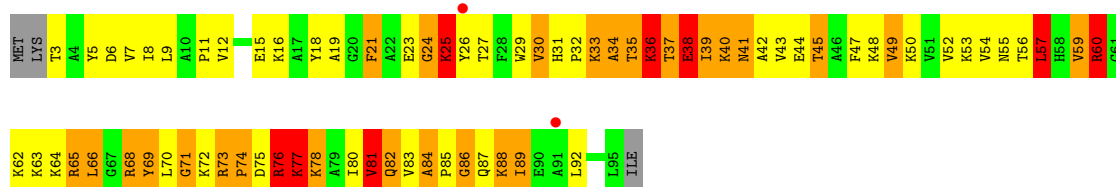
- Molecule 48: 50S ribosomal protein L22

Chain DW:



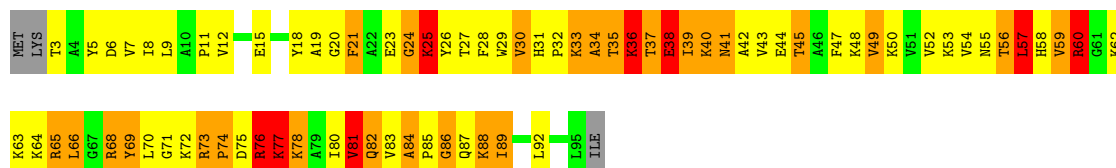
- Molecule 49: 50S ribosomal protein L23

Chain BX:



- Molecule 49: 50S ribosomal protein L23

Chain DX:



- Molecule 50: 50S ribosomal protein L24

Chain BY:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.18Å 448.40Å 621.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 3.00 49.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.57-3.00) 98.6 (49.57-3.00)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.01Å)	Xtriage
Refinement program	Phenix	Depositor
R, R_{free}	0.244 , 0.281 0.249 , 0.281	Depositor DCC
R_{free} test set	57089 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 1140008 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	277987	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: K, CLM, MG, ZN

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	0.54	0/36190	0.92	37/56486 (0.1%)
1	CA	0.53	0/36190	0.93	55/56486 (0.1%)
2	AB	0.29	0/1936	0.51	0/2611
2	CB	0.29	0/1936	0.50	0/2611
3	AC	0.27	0/1637	0.44	0/2207
3	CC	0.26	0/1637	0.44	0/2207
4	AD	0.36	0/1733	0.54	0/2318
4	CD	0.38	1/1733 (0.1%)	0.55	0/2318
5	AE	0.38	0/1163	0.58	0/1566
5	CE	0.37	0/1163	0.59	0/1566
6	AF	0.38	0/856	0.58	0/1154
6	CF	0.36	0/856	0.58	0/1154
7	AG	0.25	0/1276	0.44	0/1709
7	CG	0.25	0/1276	0.44	0/1709
8	AH	0.34	0/1136	0.56	0/1527
8	CH	0.34	0/1136	0.55	0/1527
9	AI	0.25	0/1028	0.44	0/1375
9	CI	0.25	0/1028	0.44	0/1375
10	AJ	0.27	0/808	0.48	0/1087
10	CJ	0.26	0/808	0.49	0/1087
11	AK	0.33	0/900	0.55	0/1213
11	CK	0.35	0/900	0.54	0/1213
12	AL	0.42	0/987	0.65	0/1322
12	CL	0.42	0/987	0.65	0/1322
13	AM	0.26	0/928	0.47	0/1238
13	CM	0.26	0/928	0.46	0/1238
14	AN	0.26	0/501	0.42	0/664
14	CN	0.26	0/501	0.42	0/664
15	AO	0.36	0/745	0.59	0/992
15	CO	0.35	0/745	0.58	0/992
16	AP	0.34	0/717	0.59	0/965
16	CP	0.35	0/717	0.60	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.36	0/837	0.58	0/1119
17	CQ	0.37	0/837	0.59	0/1119
18	AR	0.35	0/579	0.58	0/768
18	CR	0.36	0/579	0.57	0/768
19	AS	0.26	0/643	0.43	0/867
19	CS	0.26	0/643	0.44	0/867
20	AT	0.36	0/765	0.57	0/1007
20	CT	0.35	0/765	0.56	0/1007
21	AU	0.26	0/213	0.43	0/279
21	CU	0.26	0/213	0.43	0/279
22	B0	0.53	0/658	0.70	0/878
22	D0	0.49	0/658	0.70	0/878
23	B1	0.78	0/700	0.99	2/931 (0.2%)
23	D1	0.67	0/700	0.95	1/931 (0.1%)
24	B2	0.66	0/423	0.94	0/560
24	D2	0.55	0/423	0.89	0/560
25	B3	0.61	0/473	0.69	0/636
25	D3	0.49	0/473	0.67	0/636
26	B4	0.30	0/156	0.68	0/215
26	D4	0.30	0/156	0.65	0/215
27	B5	0.84	1/473 (0.2%)	1.02	2/639 (0.3%)
27	D5	0.77	0/473	0.97	1/639 (0.2%)
28	B6	0.89	0/387	1.07	0/517
28	D6	0.71	0/387	1.01	0/517
29	B7	0.64	0/427	0.79	0/563
29	D7	0.67	0/427	0.76	0/563
30	B8	0.72	0/516	1.09	2/681 (0.3%)
30	D8	0.64	0/516	1.04	0/681
31	BA	1.06	84/65745 (0.1%)	1.42	971/102639 (0.9%)
31	DA	0.85	35/65745 (0.1%)	1.41	1008/102639 (1.0%)
32	BB	0.83	0/2853	1.18	23/4451 (0.5%)
32	DB	0.66	0/2853	1.13	19/4451 (0.4%)
33	BD	0.63	0/2155	0.85	2/2907 (0.1%)
33	DD	0.59	0/2155	0.83	1/2907 (0.0%)
34	BE	0.63	0/1597	0.82	0/2155
34	DE	0.56	0/1597	0.81	0/2155
35	BF	0.60	0/1659	0.76	0/2246
35	DF	0.52	1/1659 (0.1%)	0.74	0/2246
36	BG	0.34	0/1498	0.55	0/2013
36	DG	0.30	0/1498	0.54	0/2013
37	BH	0.60	0/1246	0.74	0/1684
37	DH	0.44	0/1246	0.69	0/1684
38	BI	0.38	0/1147	0.61	0/1553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DI	0.40	0/1147	0.61	0/1553
39	BN	0.71	0/1132	0.93	2/1527 (0.1%)
39	DN	0.59	0/1132	0.87	1/1527 (0.1%)
40	BO	0.59	1/943 (0.1%)	0.73	0/1269
40	DO	0.52	0/943	0.73	1/1269 (0.1%)
41	BP	0.69	0/1131	1.03	8/1504 (0.5%)
41	DP	0.60	0/1131	0.98	6/1504 (0.4%)
42	BQ	0.70	0/1100	0.85	1/1470 (0.1%)
42	DQ	0.60	0/1100	0.83	0/1470
43	BR	0.63	0/974	0.82	1/1302 (0.1%)
43	DR	0.56	0/974	0.80	1/1302 (0.1%)
44	BS	0.50	0/779	0.77	0/1038
44	DS	0.43	0/779	0.73	0/1038
45	BT	0.59	0/1114	0.85	2/1488 (0.1%)
45	DT	0.52	0/1114	0.83	1/1488 (0.1%)
46	BU	0.69	0/975	0.76	0/1297
46	DU	0.56	0/975	0.72	0/1297
47	BV	0.72	0/789	0.95	1/1054 (0.1%)
47	DV	0.58	0/789	0.89	1/1054 (0.1%)
48	BW	0.68	0/907	0.84	2/1216 (0.2%)
48	DW	0.58	0/907	0.81	2/1216 (0.2%)
49	BX	0.70	0/740	0.96	2/995 (0.2%)
49	DX	0.63	0/740	0.94	2/995 (0.2%)
50	BY	0.70	1/789 (0.1%)	0.91	0/1053
50	DY	0.60	0/789	0.87	1/1053 (0.1%)
51	BZ	0.47	0/1436	0.67	2/1951 (0.1%)
51	DZ	0.41	0/1436	0.66	1/1951 (0.1%)
All	All	0.75	124/301000 (0.0%)	1.13	2162/449812 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	B1	0	1
23	D1	0	1
24	B2	0	1
24	D2	0	1
27	B5	0	1
27	D5	0	1
28	B6	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	BA	19	0
31	DA	19	0
33	BD	0	3
33	DD	0	3
34	BE	0	2
34	DE	0	2
37	BH	0	1
37	DH	0	1
41	BP	0	5
41	DP	0	4
42	BQ	0	1
42	DQ	0	1
43	BR	0	2
43	DR	0	2
44	BS	0	1
44	DS	0	1
45	BT	0	2
45	DT	0	2
46	BU	0	1
47	BV	0	3
47	DV	0	3
49	BX	0	4
49	DX	0	4
All	All	38	55

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BA	669	G	C4'-C3'	-11.30	1.40	1.53
31	DA	669	G	C4'-C3'	-10.33	1.41	1.53
31	BA	1300	U	C4'-C3'	-9.89	1.42	1.53
31	BA	1332	G	N9-C4	-9.70	1.30	1.38
31	DA	783	A	N9-C4	-9.28	1.32	1.37

The worst 5 of 2162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	BA	1332	G	N3-C4-C5	18.18	137.69	128.60
31	DA	1779	U	C5-C6-N1	-17.02	114.19	122.70
31	BA	1779	U	C5-C6-N1	-16.17	114.61	122.70
31	BA	1332	G	N3-C4-N9	-15.97	116.42	126.00
31	BA	1332	G	C2-N3-C4	-15.30	104.25	111.90

5 of 38 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	BA	100	G	C1'
31	BA	472	A	C3'
31	BA	669	G	C4',C3',C1'
31	BA	945	A	C1'
31	BA	1300	U	C4',C3',C1'

5 of 55 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	B1	30	VAL	Peptide
24	B2	55	ARG	Peptide
27	B5	51	TYR	Peptide
28	B6	47	THR	Peptide
33	BD	47	GLY	Peptide

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	32329	0	16318	1597	0
1	CA	32329	0	16318	1553	0
2	AB	1901	0	1951	215	0
2	CB	1901	0	1951	207	0
3	AC	1613	0	1677	116	0
3	CC	1613	0	1677	116	0
4	AD	1703	0	1765	190	0
4	CD	1703	0	1764	192	0
5	AE	1147	0	1207	101	0
5	CE	1147	0	1207	100	0
6	AF	843	0	857	96	0
6	CF	843	0	857	98	0
7	AG	1257	0	1296	75	0
7	CG	1257	0	1296	75	0
8	AH	1116	0	1177	101	0
8	CH	1116	0	1177	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AI	1011	0	1042	101	0
9	CI	1011	0	1042	104	0
10	AJ	795	0	840	105	0
10	CJ	795	0	840	102	0
11	AK	885	0	904	63	0
11	CK	885	0	904	68	0
12	AL	971	0	1057	100	0
12	CL	971	0	1057	103	0
13	AM	921	0	976	88	0
13	CM	921	0	976	91	0
14	AN	492	0	530	47	0
14	CN	492	0	529	46	0
15	AO	734	0	771	76	0
15	CO	734	0	771	78	0
16	AP	701	0	720	91	0
16	CP	701	0	720	97	0
17	AQ	824	0	891	66	0
17	CQ	824	0	891	55	0
18	AR	574	0	644	76	0
18	CR	574	0	644	78	0
19	AS	630	0	652	51	0
19	CS	630	0	652	52	0
20	AT	763	0	861	82	0
20	CT	763	0	861	73	0
21	AU	209	0	221	9	0
21	CU	209	0	221	9	0
22	B0	650	0	654	55	0
22	D0	650	0	654	57	0
23	B1	693	0	764	146	0
23	D1	693	0	764	143	0
24	B2	421	0	461	119	0
24	D2	421	0	461	123	0
25	B3	468	0	523	32	0
25	D3	468	0	523	41	0
26	B4	157	0	69	20	0
26	D4	157	0	69	21	0
27	B5	459	0	480	94	0
27	D5	459	0	480	86	0
28	B6	381	0	390	102	0
28	D6	381	0	390	97	0
29	B7	419	0	467	37	0
29	D7	419	0	467	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B8	508	0	576	158	0
30	D8	508	0	576	154	0
31	BA	58698	0	29590	2607	0
31	DA	58698	0	29591	2784	0
32	BB	2551	0	1295	145	0
32	DB	2551	0	1295	156	0
33	BD	2105	0	2182	325	0
33	DD	2105	0	2182	333	0
34	BE	1564	0	1629	240	0
34	DE	1564	0	1629	249	0
35	BF	1624	0	1677	182	0
35	DF	1624	0	1677	185	0
36	BG	1474	0	1534	190	0
36	DG	1474	0	1534	187	0
37	BH	1223	0	1282	162	0
37	DH	1223	0	1282	157	0
38	BI	1132	0	1218	120	0
38	DI	1132	0	1218	125	0
39	BN	1105	0	1180	218	0
39	DN	1105	0	1180	229	0
40	BO	933	0	996	77	0
40	DO	933	0	996	86	0
41	BP	1114	0	1187	302	0
41	DP	1114	0	1187	289	0
42	BQ	1080	0	1127	165	0
42	DQ	1080	0	1127	176	0
43	BR	960	0	1021	135	0
43	DR	960	0	1021	132	0
44	BS	771	0	832	149	0
44	DS	771	0	832	139	0
45	BT	1100	0	1164	210	0
45	DT	1100	0	1164	201	0
46	BU	958	0	1015	145	0
46	DU	958	0	1015	151	0
47	BV	779	0	851	224	0
47	DV	779	0	851	225	0
48	BW	896	0	953	76	0
48	DW	896	0	953	84	0
49	BX	726	0	778	168	0
49	DX	726	0	778	164	0
50	BY	776	0	870	177	0
50	DY	776	0	870	178	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	BZ	1404	0	1432	153	0
51	DZ	1404	0	1432	149	0
52	AA	56	0	0	0	0
52	B1	1	0	0	0	0
52	B5	2	0	0	0	0
52	BA	368	0	0	0	0
52	BB	7	0	0	0	0
52	BD	1	0	0	0	0
52	BE	1	0	0	0	0
52	BF	1	0	0	0	0
52	BP	2	0	0	0	0
52	BQ	2	0	0	0	0
52	BR	2	0	0	0	0
52	BU	1	0	0	0	0
52	BX	1	0	0	0	0
52	CA	53	0	0	0	0
52	D1	1	0	0	0	0
52	D5	2	0	0	0	0
52	DA	332	0	0	0	0
52	DB	4	0	0	0	0
52	DD	1	0	0	0	0
52	DE	1	0	0	0	0
52	DF	1	0	0	0	0
52	DP	1	0	0	0	0
52	DQ	1	0	0	0	0
52	DR	1	0	0	0	0
52	DU	1	0	0	0	0
52	DX	1	0	0	0	0
53	AD	1	0	0	0	0
53	AN	1	0	0	0	0
53	CD	1	0	0	2	0
53	CN	1	0	0	0	0
54	BA	1	0	0	0	0
54	DA	1	0	0	0	0
55	BA	20	0	10	0	0
55	DA	20	0	10	0	0
All	All	277987	0	189127	18994	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

The worst 5 of 18994 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:B5:46:CYS:SG	27:B5:47:PRO:HD2	1.78	1.22
31:BA:1899:G:H22	31:BA:1902:C:N4	1.41	1.18
30:B8:32:LEU:CB	30:B8:35:GLN:H	1.57	1.17
32:DB:20:C:H2'	32:DB:21:G:H5''	1.25	1.17
1:CA:1442:G:O2'	1:CA:1442(A):G:H5''	1.43	1.16

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	155 (66%)	61 (26%)	17 (7%)	2	8
2	CB	233/256 (91%)	155 (66%)	60 (26%)	18 (8%)	1	7
3	AC	205/239 (86%)	148 (72%)	46 (22%)	11 (5%)	3	17
3	CC	205/239 (86%)	148 (72%)	45 (22%)	12 (6%)	2	14
4	AD	206/209 (99%)	129 (63%)	57 (28%)	20 (10%)	1	4
4	CD	206/209 (99%)	131 (64%)	55 (27%)	20 (10%)	1	4
5	AE	149/162 (92%)	103 (69%)	36 (24%)	10 (7%)	2	10
5	CE	149/162 (92%)	104 (70%)	36 (24%)	9 (6%)	2	14
6	AF	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	3	18
6	CF	99/101 (98%)	78 (79%)	16 (16%)	5 (5%)	3	18
7	AG	153/156 (98%)	123 (80%)	28 (18%)	2 (1%)	18	62
7	CG	153/156 (98%)	124 (81%)	27 (18%)	2 (1%)	18	62
8	AH	136/138 (99%)	98 (72%)	25 (18%)	13 (10%)	1	4
8	CH	136/138 (99%)	97 (71%)	27 (20%)	12 (9%)	1	5
9	AI	123/128 (96%)	89 (72%)	26 (21%)	8 (6%)	2	11
9	CI	123/128 (96%)	91 (74%)	24 (20%)	8 (6%)	2	11
10	AJ	97/105 (92%)	78 (80%)	15 (16%)	4 (4%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CJ	97/105 (92%)	78 (80%)	14 (14%)	5 (5%)	3	18
11	AK	117/129 (91%)	92 (79%)	23 (20%)	2 (2%)	14	54
11	CK	117/129 (91%)	90 (77%)	25 (21%)	2 (2%)	14	54
12	AL	123/135 (91%)	85 (69%)	25 (20%)	13 (11%)	1	3
12	CL	123/135 (91%)	82 (67%)	27 (22%)	14 (11%)	1	3
13	AM	107/126 (85%)	80 (75%)	21 (20%)	6 (6%)	3	16
13	CM	107/126 (85%)	81 (76%)	19 (18%)	7 (6%)	2	11
14	AN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	14	54
14	CN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	14	54
15	AO	86/89 (97%)	65 (76%)	14 (16%)	7 (8%)	1	7
15	CO	86/89 (97%)	64 (74%)	16 (19%)	6 (7%)	2	9
16	AP	82/88 (93%)	51 (62%)	18 (22%)	13 (16%)	0	1
16	CP	82/88 (93%)	52 (63%)	18 (22%)	12 (15%)	0	1
17	AQ	98/105 (93%)	79 (81%)	11 (11%)	8 (8%)	1	6
17	CQ	98/105 (93%)	78 (80%)	13 (13%)	7 (7%)	2	9
18	AR	68/88 (77%)	49 (72%)	14 (21%)	5 (7%)	2	8
18	CR	68/88 (77%)	46 (68%)	16 (24%)	6 (9%)	1	5
19	AS	77/93 (83%)	59 (77%)	11 (14%)	7 (9%)	1	5
19	CS	77/93 (83%)	59 (77%)	11 (14%)	7 (9%)	1	5
20	AT	97/106 (92%)	70 (72%)	18 (19%)	9 (9%)	1	5
20	CT	97/106 (92%)	68 (70%)	20 (21%)	9 (9%)	1	5
21	AU	23/27 (85%)	17 (74%)	5 (22%)	1 (4%)	4	23
21	CU	23/27 (85%)	17 (74%)	4 (17%)	2 (9%)	1	5
22	B0	83/85 (98%)	69 (83%)	10 (12%)	4 (5%)	4	20
22	D0	83/85 (98%)	68 (82%)	11 (13%)	4 (5%)	4	20
23	B1	87/98 (89%)	47 (54%)	24 (28%)	16 (18%)	0	1
23	D1	87/98 (89%)	46 (53%)	24 (28%)	17 (20%)	0	0
24	B2	49/72 (68%)	23 (47%)	14 (29%)	12 (24%)	0	0
24	D2	49/72 (68%)	22 (45%)	15 (31%)	12 (24%)	0	0
25	B3	58/60 (97%)	50 (86%)	8 (14%)	0	100	100
25	D3	58/60 (97%)	48 (83%)	10 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	B4	30/71 (42%)	4 (13%)	14 (47%)	12 (40%)	0	0
26	D4	30/71 (42%)	3 (10%)	15 (50%)	12 (40%)	0	0
27	B5	57/60 (95%)	43 (75%)	4 (7%)	10 (18%)	0	1
27	D5	57/60 (95%)	42 (74%)	6 (10%)	9 (16%)	0	1
28	B6	41/54 (76%)	21 (51%)	6 (15%)	14 (34%)	0	0
28	D6	41/54 (76%)	21 (51%)	7 (17%)	13 (32%)	0	0
29	B7	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
29	D7	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
30	B8	62/65 (95%)	41 (66%)	12 (19%)	9 (14%)	0	1
30	D8	62/65 (95%)	42 (68%)	12 (19%)	8 (13%)	0	2
33	BD	270/276 (98%)	211 (78%)	44 (16%)	15 (6%)	3	16
33	DD	270/276 (98%)	208 (77%)	46 (17%)	16 (6%)	2	14
34	BE	203/206 (98%)	147 (72%)	31 (15%)	25 (12%)	1	2
34	DE	203/206 (98%)	144 (71%)	37 (18%)	22 (11%)	1	3
35	BF	206/210 (98%)	158 (77%)	34 (16%)	14 (7%)	2	10
35	DF	206/210 (98%)	154 (75%)	36 (18%)	16 (8%)	1	7
36	BG	177/182 (97%)	125 (71%)	35 (20%)	17 (10%)	1	4
36	DG	177/182 (97%)	126 (71%)	34 (19%)	17 (10%)	1	4
37	BH	158/180 (88%)	102 (65%)	31 (20%)	25 (16%)	0	1
37	DH	158/180 (88%)	101 (64%)	31 (20%)	26 (16%)	0	1
38	BI	144/148 (97%)	98 (68%)	30 (21%)	16 (11%)	1	3
38	DI	144/148 (97%)	99 (69%)	33 (23%)	12 (8%)	1	6
39	BN	137/140 (98%)	89 (65%)	28 (20%)	20 (15%)	0	1
39	DN	137/140 (98%)	92 (67%)	25 (18%)	20 (15%)	0	1
40	BO	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	14	54
40	DO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	9	40
41	BP	144/150 (96%)	71 (49%)	33 (23%)	40 (28%)	0	0
41	DP	144/150 (96%)	70 (49%)	33 (23%)	41 (28%)	0	0
42	BQ	134/141 (95%)	97 (72%)	21 (16%)	16 (12%)	1	2
42	DQ	134/141 (95%)	92 (69%)	25 (19%)	17 (13%)	0	2
43	BR	115/118 (98%)	86 (75%)	22 (19%)	7 (6%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	DR	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	2	14
44	BS	97/112 (87%)	45 (46%)	22 (23%)	30 (31%)	0	0
44	DS	97/112 (87%)	44 (45%)	22 (23%)	31 (32%)	0	0
45	BT	130/146 (89%)	91 (70%)	21 (16%)	18 (14%)	0	2
45	DT	130/146 (89%)	91 (70%)	21 (16%)	18 (14%)	0	2
46	BU	115/118 (98%)	89 (77%)	18 (16%)	8 (7%)	2	9
46	DU	115/118 (98%)	86 (75%)	21 (18%)	8 (7%)	2	9
47	BV	97/101 (96%)	54 (56%)	18 (19%)	25 (26%)	0	0
47	DV	97/101 (96%)	53 (55%)	19 (20%)	25 (26%)	0	0
48	BW	111/113 (98%)	85 (77%)	17 (15%)	9 (8%)	1	7
48	DW	111/113 (98%)	83 (75%)	19 (17%)	9 (8%)	1	7
49	BX	91/96 (95%)	47 (52%)	23 (25%)	21 (23%)	0	0
49	DX	91/96 (95%)	48 (53%)	23 (25%)	20 (22%)	0	0
50	BY	99/110 (90%)	47 (48%)	22 (22%)	30 (30%)	0	0
50	DY	99/110 (90%)	44 (44%)	25 (25%)	30 (30%)	0	0
51	BZ	175/206 (85%)	123 (70%)	32 (18%)	20 (11%)	1	3
51	DZ	175/206 (85%)	121 (69%)	36 (21%)	18 (10%)	1	4
All	All	11148/12060 (92%)	7786 (70%)	2170 (20%)	1192 (11%)	1	3

5 of 1192 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	18	GLY
2	AB	20	GLU
2	AB	106	LYS
2	AB	165	VAL
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%)	170 (84%)	32 (16%)	4	18
2	CB	202/220 (92%)	168 (83%)	34 (17%)	3	15
3	AC	160/188 (85%)	153 (96%)	7 (4%)	39	82
3	CC	160/188 (85%)	153 (96%)	7 (4%)	39	82
4	AD	180/181 (99%)	156 (87%)	24 (13%)	6	25
4	CD	180/181 (99%)	156 (87%)	24 (13%)	6	25
5	AE	115/123 (94%)	95 (83%)	20 (17%)	3	14
5	CE	115/123 (94%)	95 (83%)	20 (17%)	3	14
6	AF	90/90 (100%)	79 (88%)	11 (12%)	7	29
6	CF	90/90 (100%)	78 (87%)	12 (13%)	6	25
7	AG	126/127 (99%)	122 (97%)	4 (3%)	51	89
7	CG	126/127 (99%)	122 (97%)	4 (3%)	51	89
8	AH	119/119 (100%)	106 (89%)	13 (11%)	9	35
8	CH	119/119 (100%)	106 (89%)	13 (11%)	9	35
9	AI	98/99 (99%)	90 (92%)	8 (8%)	17	52
9	CI	98/99 (99%)	90 (92%)	8 (8%)	17	52
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	8	33
10	CJ	88/92 (96%)	78 (89%)	10 (11%)	8	33
11	AK	90/99 (91%)	82 (91%)	8 (9%)	14	48
11	CK	90/99 (91%)	83 (92%)	7 (8%)	18	55
12	AL	104/111 (94%)	92 (88%)	12 (12%)	8	32
12	CL	104/111 (94%)	91 (88%)	13 (12%)	7	28
13	AM	93/101 (92%)	87 (94%)	6 (6%)	24	65
13	CM	93/101 (92%)	87 (94%)	6 (6%)	24	65
14	AN	49/50 (98%)	45 (92%)	4 (8%)	17	52
14	CN	49/50 (98%)	45 (92%)	4 (8%)	17	52
15	AO	79/80 (99%)	68 (86%)	11 (14%)	5	23
15	CO	79/80 (99%)	68 (86%)	11 (14%)	5	23
16	AP	72/74 (97%)	58 (81%)	14 (19%)	2	11
16	CP	72/74 (97%)	59 (82%)	13 (18%)	2	13
17	AQ	94/97 (97%)	82 (87%)	12 (13%)	6	27
17	CQ	94/97 (97%)	82 (87%)	12 (13%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	61/77 (79%)	55 (90%)	6 (10%)	12	41
18	CR	61/77 (79%)	55 (90%)	6 (10%)	12	41
19	AS	69/80 (86%)	62 (90%)	7 (10%)	11	39
19	CS	69/80 (86%)	62 (90%)	7 (10%)	11	39
20	AT	76/82 (93%)	68 (90%)	8 (10%)	10	37
20	CT	76/82 (93%)	68 (90%)	8 (10%)	10	37
21	AU	19/22 (86%)	19 (100%)	0	100	100
21	CU	19/22 (86%)	19 (100%)	0	100	100
22	B0	61/67 (91%)	53 (87%)	8 (13%)	6	25
22	D0	61/67 (91%)	53 (87%)	8 (13%)	6	25
23	B1	73/83 (88%)	53 (73%)	20 (27%)	0	3
23	D1	73/83 (88%)	55 (75%)	18 (25%)	1	4
24	B2	46/67 (69%)	33 (72%)	13 (28%)	0	3
24	D2	46/67 (69%)	33 (72%)	13 (28%)	0	3
25	B3	51/52 (98%)	45 (88%)	6 (12%)	8	30
25	D3	51/52 (98%)	44 (86%)	7 (14%)	5	24
27	B5	51/52 (98%)	40 (78%)	11 (22%)	1	8
27	D5	51/52 (98%)	38 (74%)	13 (26%)	1	4
28	B6	43/52 (83%)	27 (63%)	16 (37%)	0	1
28	D6	43/52 (83%)	28 (65%)	15 (35%)	0	1
29	B7	41/42 (98%)	33 (80%)	8 (20%)	2	11
29	D7	41/42 (98%)	32 (78%)	9 (22%)	1	7
30	B8	53/55 (96%)	40 (76%)	13 (24%)	1	5
30	D8	53/55 (96%)	41 (77%)	12 (23%)	1	6
33	BD	213/218 (98%)	166 (78%)	47 (22%)	1	7
33	DD	213/218 (98%)	165 (78%)	48 (22%)	1	7
34	BE	165/166 (99%)	122 (74%)	43 (26%)	1	4
34	DE	165/166 (99%)	122 (74%)	43 (26%)	1	4
35	BF	165/166 (99%)	134 (81%)	31 (19%)	2	12
35	DF	165/166 (99%)	137 (83%)	28 (17%)	3	15
36	BG	155/156 (99%)	134 (86%)	21 (14%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	DG	155/156 (99%)	134 (86%)	21 (14%)	6	24
37	BH	132/148 (89%)	105 (80%)	27 (20%)	2	9
37	DH	132/148 (89%)	105 (80%)	27 (20%)	2	9
38	BI	122/124 (98%)	104 (85%)	18 (15%)	4	21
38	DI	122/124 (98%)	104 (85%)	18 (15%)	4	21
39	BN	117/119 (98%)	79 (68%)	38 (32%)	0	2
39	DN	117/119 (98%)	79 (68%)	38 (32%)	0	2
40	BO	100/100 (100%)	81 (81%)	19 (19%)	2	12
40	DO	100/100 (100%)	81 (81%)	19 (19%)	2	12
41	BP	112/116 (97%)	72 (64%)	40 (36%)	0	1
41	DP	112/116 (97%)	72 (64%)	40 (36%)	0	1
42	BQ	106/111 (96%)	86 (81%)	20 (19%)	2	12
42	DQ	106/111 (96%)	85 (80%)	21 (20%)	2	11
43	BR	100/101 (99%)	81 (81%)	19 (19%)	2	12
43	DR	100/101 (99%)	80 (80%)	20 (20%)	2	10
44	BS	77/88 (88%)	53 (69%)	24 (31%)	0	2
44	DS	77/88 (88%)	54 (70%)	23 (30%)	0	2
45	BT	116/127 (91%)	81 (70%)	35 (30%)	0	2
45	DT	116/127 (91%)	81 (70%)	35 (30%)	0	2
46	BU	92/94 (98%)	79 (86%)	13 (14%)	5	23
46	DU	92/94 (98%)	79 (86%)	13 (14%)	5	23
47	BV	82/82 (100%)	53 (65%)	29 (35%)	0	1
47	DV	82/82 (100%)	53 (65%)	29 (35%)	0	1
48	BW	91/92 (99%)	70 (77%)	21 (23%)	1	6
48	DW	91/92 (99%)	71 (78%)	20 (22%)	1	7
49	BX	74/78 (95%)	54 (73%)	20 (27%)	1	3
49	DX	74/78 (95%)	53 (72%)	21 (28%)	0	3
50	BY	84/91 (92%)	60 (71%)	24 (29%)	0	3
50	DY	84/91 (92%)	61 (73%)	23 (27%)	0	3
51	BZ	155/179 (87%)	130 (84%)	25 (16%)	3	17
51	DZ	155/179 (87%)	130 (84%)	25 (16%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9322/9876 (94%)	7670 (82%)	1652 (18%)	3 14

5 of 1652 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BW	60	ASN
7	CG	36	LYS
46	DU	66	ASN
49	BX	49	VAL
2	CB	90	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 277 such sidechains are listed below:

Mol	Chain	Res	Type
48	BW	40	ASN
6	CF	18	GLN
45	DT	90	GLN
48	BW	62	HIS
2	CB	204	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	280 (18%)	31 (2%)
1	CA	1503/1522 (98%)	283 (18%)	31 (2%)
31	BA	2723/2787 (97%)	712 (26%)	70 (2%)
31	DA	2723/2787 (97%)	706 (25%)	69 (2%)
32	BB	118/122 (96%)	34 (28%)	1 (0%)
32	DB	118/122 (96%)	35 (29%)	1 (0%)
All	All	8688/8862 (98%)	2050 (23%)	203 (2%)

5 of 2050 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	41	G

5 of 203 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	BA	2439	A
1	CA	429	U
31	DA	1934	C
31	BA	2689	U
1	CA	60	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 853 ligands modelled in this entry, 851 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	$\# Z > 2$
55	CLM	BA	3370	54	20,20,20	1.80	1 (5%)	27,27,27	1.13	2 (7%)
55	CLM	DA	3334	54	20,20,20	1.80	1 (5%)	27,27,27	1.13	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	CLM	BA	3370	54	-	0/22/22/22	0/1/1/1
55	CLM	DA	3334	54	-	0/22/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	3334	CLM	C9-N9	-7.20	1.34	1.46
55	BA	3370	CLM	C9-N9	-7.17	1.34	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	3334	CLM	O9A-N9-C9	2.71	119.99	114.58
55	BA	3370	CLM	O9A-N9-C9	2.71	119.98	114.58
55	BA	3370	CLM	C1-C2-N2	2.13	120.01	115.49
55	DA	3334	CLM	C1-C2-N2	2.13	120.01	115.49

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	3
13	AM	3
47	DV	1
36	DG	1
36	BG	1
9	AI	1
9	CI	1
47	BV	1
28	D6	1
28	B6	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CM	69:GLU	C	70:LEU	N	5.35

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AM	69:GLU	C	70:LEU	N	5.34
1	BG	112:PRO	C	113:ARG	N	4.53
1	DG	112:PRO	C	113:ARG	N	4.53
1	CM	112:GLY	C	113:PRO	N	4.49

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%)	0.79	222 (14%) 3 1	42, 106, 199, 201	0
1	CA	1504/1522 (98%)	0.63	189 (12%) 4 1	46, 105, 198, 201	0
2	AB	235/256 (91%)	0.35	13 (5%) 24 5	83, 146, 188, 195	0
2	CB	235/256 (91%)	0.56	22 (9%) 9 2	84, 149, 187, 196	0
3	AC	207/239 (86%)	0.61	22 (10%) 7 2	97, 158, 187, 194	0
3	CC	207/239 (86%)	0.70	25 (12%) 5 1	98, 160, 187, 194	0
4	AD	208/209 (99%)	0.13	2 (0%) 79 22	72, 112, 165, 186	0
4	CD	208/209 (99%)	0.05	2 (0%) 79 22	70, 111, 164, 185	0
5	AE	151/162 (93%)	0.13	3 (1%) 62 12	59, 97, 151, 194	0
5	CE	151/162 (93%)	0.19	1 (0%) 84 28	64, 98, 153, 194	0
6	AF	101/101 (100%)	0.04	0 100 100	66, 111, 160, 183	0
6	CF	101/101 (100%)	0.05	1 (0%) 79 22	67, 113, 160, 188	0
7	AG	155/156 (99%)	0.92	31 (20%) 2 1	124, 172, 192, 197	0
7	CG	155/156 (99%)	1.08	30 (19%) 2 1	125, 172, 192, 198	0
8	AH	138/138 (100%)	-0.06	1 (0%) 84 28	67, 102, 147, 162	0
8	CH	138/138 (100%)	-0.01	0 100 100	66, 102, 147, 163	0
9	AI	127/128 (99%)	1.42	31 (24%) 1 1	125, 179, 196, 199	0
9	CI	127/128 (99%)	1.74	42 (33%) 1 0	126, 180, 197, 199	0
10	AJ	99/105 (94%)	1.76	36 (36%) 1 0	122, 175, 196, 198	0
10	CJ	99/105 (94%)	1.87	37 (37%) 1 0	121, 176, 197, 199	0
11	AK	119/129 (92%)	0.30	7 (5%) 22 5	63, 105, 164, 188	0
11	CK	119/129 (92%)	0.34	6 (5%) 28 6	65, 104, 168, 191	0
12	AL	125/135 (92%)	0.09	4 (3%) 45 9	57, 89, 154, 198	0
12	CL	125/135 (92%)	0.27	5 (4%) 36 7	55, 89, 158, 198	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	115/126 (91%)	1.40	34 (29%) 1 0	136, 190, 198, 200	0
13	CM	115/126 (91%)	1.45	36 (31%) 1 0	136, 188, 197, 199	0
14	AN	60/61 (98%)	1.05	7 (11%) 5 2	113, 167, 193, 196	0
14	CN	60/61 (98%)	0.73	6 (10%) 8 2	112, 168, 191, 196	0
15	AO	88/89 (98%)	0.02	1 (1%) 77 21	59, 91, 149, 155	0
15	CO	88/89 (98%)	0.02	0 100 100	63, 92, 150, 157	0
16	AP	84/88 (95%)	0.51	6 (7%) 16 4	77, 101, 161, 188	0
16	CP	84/88 (95%)	0.30	1 (1%) 75 20	78, 100, 154, 186	0
17	AQ	100/105 (95%)	-0.06	1 (1%) 79 22	62, 93, 138, 158	0
17	CQ	100/105 (95%)	0.04	2 (2%) 62 12	59, 92, 140, 157	0
18	AR	70/88 (79%)	0.28	2 (2%) 49 9	73, 98, 167, 197	0
18	CR	70/88 (79%)	0.80	5 (7%) 16 4	74, 100, 167, 196	0
19	AS	79/93 (84%)	2.00	31 (39%) 1 0	142, 191, 198, 199	0
19	CS	79/93 (84%)	1.88	28 (35%) 1 0	142, 190, 198, 199	0
20	AT	99/106 (93%)	0.03	1 (1%) 79 22	73, 110, 157, 186	0
20	CT	99/106 (93%)	0.26	5 (5%) 27 6	74, 108, 156, 189	0
21	AU	25/27 (92%)	2.78	15 (60%) 0 0	138, 175, 193, 196	0
21	CU	25/27 (92%)	2.53	16 (64%) 0 0	135, 172, 193, 195	0
22	B0	85/85 (100%)	0.48	8 (9%) 9 2	34, 59, 182, 197	0
22	D0	85/85 (100%)	0.31	8 (9%) 9 2	40, 64, 178, 197	0
23	B1	89/98 (90%)	0.12	1 (1%) 77 21	37, 64, 141, 187	0
23	D1	89/98 (90%)	0.06	0 100 100	40, 66, 142, 191	0
24	B2	51/72 (70%)	0.48	3 (5%) 22 5	49, 87, 184, 193	0
24	D2	51/72 (70%)	0.29	4 (7%) 13 3	50, 91, 183, 195	0
25	B3	60/60 (100%)	-0.06	1 (1%) 67 15	36, 56, 132, 180	0
25	D3	60/60 (100%)	0.15	2 (3%) 44 8	42, 61, 138, 178	0
26	B4	32/71 (45%)	-0.08	0 100 100	109, 156, 186, 191	0
26	D4	32/71 (45%)	0.03	0 100 100	112, 161, 188, 195	0
27	B5	59/60 (98%)	0.25	4 (6%) 17 4	25, 47, 180, 195	0
27	D5	59/60 (98%)	0.10	4 (6%) 17 4	28, 50, 184, 195	0
28	B6	45/54 (83%)	0.34	2 (4%) 33 7	36, 70, 133, 185	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/54 (83%)	0.53	2 (4%) 33 7	42, 74, 138, 184	0
29	B7	49/49 (100%)	0.14	1 (2%) 62 12	26, 33, 117, 170	0
29	D7	49/49 (100%)	0.19	1 (2%) 62 12	27, 37, 118, 170	0
30	B8	64/65 (98%)	0.12	0 100 100	34, 57, 138, 181	0
30	D8	64/65 (98%)	0.03	0 100 100	38, 59, 139, 183	0
31	BA	2725/2787 (97%)	0.02	53 (1%) 64 13	26, 46, 145, 201	0
31	DA	2725/2787 (97%)	-0.09	86 (3%) 45 9	27, 51, 149, 201	0
32	BB	119/122 (97%)	0.21	4 (3%) 43 8	39, 91, 140, 185	0
32	DB	119/122 (97%)	0.46	12 (10%) 7 2	48, 95, 154, 190	0
33	BD	272/276 (98%)	-0.18	1 (0%) 90 41	27, 47, 100, 177	0
33	DD	272/276 (98%)	-0.18	0 100 100	29, 50, 104, 181	0
34	BE	205/206 (99%)	0.01	3 (1%) 70 16	25, 52, 145, 189	0
34	DE	205/206 (99%)	-0.10	3 (1%) 70 16	29, 56, 142, 189	0
35	BF	208/210 (99%)	0.17	9 (4%) 34 7	24, 58, 180, 197	0
35	DF	208/210 (99%)	0.19	8 (3%) 38 7	27, 63, 178, 197	0
36	BG	181/182 (99%)	0.70	22 (12%) 5 1	87, 145, 189, 199	0
36	DG	181/182 (99%)	1.19	38 (20%) 1 1	91, 153, 193, 199	0
37	BH	160/180 (88%)	0.15	3 (1%) 64 13	62, 102, 150, 193	0
37	DH	160/180 (88%)	0.60	10 (6%) 19 5	70, 110, 157, 195	0
38	BI	146/148 (98%)	0.19	6 (4%) 35 7	52, 143, 185, 195	0
38	DI	146/148 (98%)	1.71	50 (34%) 1 0	56, 156, 188, 198	0
39	BN	139/140 (99%)	-0.02	2 (1%) 72 18	32, 60, 140, 187	0
39	DN	139/140 (99%)	-0.16	2 (1%) 72 18	38, 65, 142, 188	0
40	BO	122/122 (100%)	-0.27	0 100 100	32, 52, 105, 141	0
40	DO	122/122 (100%)	-0.39	0 100 100	35, 55, 111, 146	0
41	BP	146/150 (97%)	0.29	3 (2%) 60 12	22, 79, 148, 199	0
41	DP	146/150 (97%)	0.17	5 (3%) 43 8	27, 81, 150, 198	0
42	BQ	136/141 (96%)	0.18	4 (2%) 49 9	39, 64, 150, 189	0
42	DQ	136/141 (96%)	0.22	7 (5%) 27 6	43, 69, 149, 190	0
43	BR	117/118 (99%)	-0.17	0 100 100	28, 44, 113, 143	0
43	DR	117/118 (99%)	-0.11	2 (1%) 67 15	30, 49, 115, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BS	99/112 (88%)	0.20	1 (1%) 79 22	53, 98, 141, 178	0
44	DS	99/112 (88%)	0.56	7 (7%) 16 4	63, 103, 146, 180	0
45	BT	132/146 (90%)	0.10	3 (2%) 57 12	42, 73, 157, 191	0
45	DT	132/146 (90%)	0.02	5 (3%) 38 7	46, 77, 159, 194	0
46	BU	117/118 (99%)	0.05	2 (1%) 67 15	23, 50, 114, 190	0
46	DU	117/118 (99%)	-0.01	1 (0%) 81 24	32, 56, 119, 193	0
47	BV	101/101 (100%)	0.30	4 (3%) 36 7	32, 91, 171, 194	0
47	DV	101/101 (100%)	0.33	4 (3%) 36 7	35, 97, 169, 195	0
48	BW	113/113 (100%)	-0.27	0 100 100	28, 40, 101, 168	0
48	DW	113/113 (100%)	-0.23	1 (0%) 81 24	31, 43, 106, 175	0
49	BX	93/96 (96%)	0.14	2 (2%) 59 12	36, 65, 142, 184	0
49	DX	93/96 (96%)	-0.05	0 100 100	42, 69, 147, 185	0
50	BY	101/110 (91%)	0.48	9 (8%) 10 3	39, 91, 191, 199	0
50	DY	101/110 (91%)	0.44	11 (10%) 6 2	40, 96, 191, 199	0
51	BZ	177/206 (85%)	0.02	1 (0%) 86 32	56, 100, 150, 175	0
51	DZ	177/206 (85%)	0.14	3 (1%) 67 15	63, 103, 153, 179	0
All	All	20064/20922 (95%)	0.30	1357 (6%) 17 4	22, 84, 190, 201	0

The worst 5 of 1357 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	DA	652	C	15.4
35	BF	208	GLY	14.2
1	AA	88	A	13.7
1	AA	1026	G	12.7
31	DA	2802	G	12.4

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
52	MG	BA	3035	1/1	0.26	-	18,18,18,18	0
52	MG	DA	3179	1/1	0.22	-	29,29,29,29	0
52	MG	BA	3161	1/1	0.19	-	32,32,32,32	0
52	MG	BA	3092	1/1	0.40	-	19,19,19,19	0
52	MG	DA	3071	1/1	0.41	-	31,31,31,31	0
52	MG	DA	3154	1/1	0.41	-	51,51,51,51	0
52	MG	DA	3302	1/1	0.26	-	39,39,39,39	0
52	MG	BA	3310	1/1	0.42	-	31,31,31,31	0
52	MG	DA	3109	1/1	0.26	-	48,48,48,48	0
52	MG	BA	3008	1/1	0.43	-	27,27,27,27	0
52	MG	BA	3362	1/1	0.33	-	50,50,50,50	0
52	MG	CA	1638	1/1	1.12	-	64,64,64,64	0
52	MG	DR	201	1/1	0.23	-	34,34,34,34	0
52	MG	AA	1642	1/1	0.29	-	46,46,46,46	0
52	MG	BA	3071	1/1	0.31	-	22,22,22,22	0
52	MG	DA	3159	1/1	0.18	-	40,40,40,40	0
52	MG	AA	1627	1/1	0.18	-	60,60,60,60	0
52	MG	BA	3047	1/1	0.45	-	22,22,22,22	0
52	MG	BA	3297	1/1	0.24	-	31,31,31,31	0
52	MG	DA	3261	1/1	0.12	-	51,51,51,51	0
52	MG	BF	301	1/1	0.34	-	43,43,43,43	0
52	MG	DA	3178	1/1	0.36	-	30,30,30,30	0
52	MG	DA	3041	1/1	0.31	-	29,29,29,29	0
52	MG	AA	1613	1/1	0.21	-	62,62,62,62	0
52	MG	DA	3259	1/1	0.47	-	79,79,79,79	0
52	MG	DA	3254	1/1	0.13	-	46,46,46,46	0
52	MG	BA	3201	1/1	0.57	-	31,31,31,31	0
52	MG	DA	3026	1/1	0.25	-	55,55,55,55	0
52	MG	DA	3043	1/1	0.24	-	49,49,49,49	0
52	MG	CA	1607	1/1	0.34	-	46,46,46,46	0
52	MG	DA	3230	1/1	0.24	-	25,25,25,25	0
52	MG	BA	3080	1/1	0.57	-	14,14,14,14	0
52	MG	BA	3065	1/1	0.22	-	28,28,28,28	0
52	MG	DA	3079	1/1	0.18	-	36,36,36,36	0
52	MG	DA	3152	1/1	0.32	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3207	1/1	0.59	-	32,32,32,32	0
52	MG	BA	3075	1/1	0.42	-	38,38,38,38	0
52	MG	BA	3107	1/1	0.20	-	7,7,7,7	0
52	MG	DA	3146	1/1	0.27	-	37,37,37,37	0
52	MG	DA	3207	1/1	0.40	-	54,54,54,54	0
52	MG	AA	1602	1/1	0.47	-	32,32,32,32	0
52	MG	BA	3231	1/1	0.07	-	26,26,26,26	0
52	MG	DA	3250	1/1	0.28	-	56,56,56,56	0
52	MG	BA	3135	1/1	0.20	-	30,30,30,30	0
52	MG	DA	3033	1/1	0.20	-	31,31,31,31	0
52	MG	BA	3284	1/1	0.28	-	39,39,39,39	0
52	MG	BA	3247	1/1	0.52	-	35,35,35,35	0
52	MG	AA	1649	1/1	0.25	-	76,76,76,76	0
52	MG	DA	3095	1/1	0.23	-	47,47,47,47	0
52	MG	BA	3143	1/1	0.57	-	29,29,29,29	0
52	MG	DA	3051	1/1	0.46	-	29,29,29,29	0
52	MG	BA	3175	1/1	0.61	-	43,43,43,43	0
52	MG	BA	3093	1/1	0.81	-	50,50,50,50	0
52	MG	BA	3227	1/1	0.54	-	22,22,22,22	0
52	MG	CA	1625	1/1	0.49	-	59,59,59,59	0
52	MG	DA	3028	1/1	0.20	-	34,34,34,34	0
52	MG	BA	3234	1/1	0.16	-	16,16,16,16	0
52	MG	DA	3224	1/1	0.47	-	41,41,41,41	0
52	MG	BA	3013	1/1	0.35	-	7,7,7,7	0
52	MG	DA	3173	1/1	0.67	-	57,57,57,57	0
52	MG	CA	1620	1/1	0.25	-	45,45,45,45	0
52	MG	BA	3334	1/1	0.30	-	39,39,39,39	0
52	MG	BA	3313	1/1	0.60	-	56,56,56,56	0
52	MG	AA	1635	1/1	0.12	-	53,53,53,53	0
52	MG	DA	3307	1/1	0.17	-	42,42,42,42	0
52	MG	DA	3223	1/1	0.59	-	37,37,37,37	0
52	MG	BA	3286	1/1	0.41	-	44,44,44,44	0
52	MG	BA	3344	1/1	0.09	-	56,56,56,56	0
52	MG	BA	3321	1/1	0.22	-	33,33,33,33	0
52	MG	DA	3185	1/1	0.42	-	49,49,49,49	0
52	MG	CA	1606	1/1	0.72	-	52,52,52,52	0
52	MG	BA	3271	1/1	0.12	-	53,53,53,53	0
52	MG	BA	3034	1/1	0.15	-	45,45,45,45	0
52	MG	DA	3331	1/1	0.12	-	67,67,67,67	0
52	MG	BA	3356	1/1	0.09	-	60,60,60,60	0
52	MG	DA	3321	1/1	0.03	-	41,41,41,41	0
52	MG	DA	3227	1/1	0.22	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3161	1/1	0.12	-	44,44,44,44	0
52	MG	DA	3017	1/1	0.40	-	37,37,37,37	0
52	MG	DA	3038	1/1	0.48	-	25,25,25,25	0
52	MG	BA	3109	1/1	0.65	-	40,40,40,40	0
52	MG	DA	3272	1/1	0.41	-	47,47,47,47	0
52	MG	DA	3119	1/1	0.36	-	36,36,36,36	0
52	MG	AA	1640	1/1	0.34	-	60,60,60,60	0
52	MG	DA	3064	1/1	0.47	-	44,44,44,44	0
52	MG	BA	3263	1/1	0.17	-	29,29,29,29	0
52	MG	BA	3350	1/1	0.30	-	54,54,54,54	0
52	MG	BA	3260	1/1	0.20	-	13,13,13,13	0
52	MG	BA	3085	1/1	0.18	-	9,9,9,9	0
52	MG	DA	3100	1/1	0.44	-	35,35,35,35	0
52	MG	BA	3129	1/1	0.12	-	33,33,33,33	0
52	MG	DA	3050	1/1	0.26	-	33,33,33,33	0
52	MG	BA	3153	1/1	0.35	-	34,34,34,34	0
52	MG	DA	3015	1/1	0.35	-	52,52,52,52	0
52	MG	DA	3193	1/1	0.62	-	40,40,40,40	0
52	MG	DA	3024	1/1	0.36	-	47,47,47,47	0
52	MG	DA	3140	1/1	0.43	-	42,42,42,42	0
52	MG	BA	3059	1/1	0.32	-	25,25,25,25	0
52	MG	BA	3078	1/1	0.37	-	22,22,22,22	0
52	MG	DA	3311	1/1	0.20	-	29,29,29,29	0
52	MG	DA	3172	1/1	0.31	-	48,48,48,48	0
52	MG	BA	3241	1/1	0.15	-	44,44,44,44	0
52	MG	AA	1603	1/1	0.30	-	43,43,43,43	0
52	MG	BA	3269	1/1	0.31	-	34,34,34,34	0
52	MG	BA	3272	1/1	0.40	-	36,36,36,36	0
52	MG	BA	3216	1/1	0.47	-	35,35,35,35	0
52	MG	BA	3197	1/1	0.17	-	27,27,27,27	0
52	MG	CA	1633	1/1	0.73	-	50,50,50,50	0
52	MG	DA	3134	1/1	0.48	-	28,28,28,28	0
52	MG	BA	3259	1/1	0.34	-	40,40,40,40	0
53	ZN	AD	301	1/1	0.28	-	109,109,109,109	0
52	MG	DA	3032	1/1	0.35	-	31,31,31,31	0
52	MG	BA	3322	1/1	0.37	-	41,41,41,41	0
52	MG	BA	3299	1/1	0.24	-	37,37,37,37	0
52	MG	BA	3124	1/1	0.40	-	39,39,39,39	0
52	MG	B1	101	1/1	0.31	-	25,25,25,25	0
52	MG	CA	1636	1/1	0.19	-	77,77,77,77	0
52	MG	DA	3052	1/1	0.45	-	36,36,36,36	0
52	MG	DA	3221	1/1	0.61	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3248	1/1	0.27	-	33,33,33,33	0
52	MG	DA	3325	1/1	0.48	-	46,46,46,46	0
52	MG	DA	3257	1/1	0.34	-	46,46,46,46	0
52	MG	BA	3292	1/1	0.10	-	41,41,41,41	0
52	MG	BA	3254	1/1	0.60	-	34,34,34,34	0
52	MG	DA	3099	1/1	0.56	-	34,34,34,34	0
52	MG	BA	3012	1/1	0.42	-	38,38,38,38	0
52	MG	BA	3094	1/1	0.52	-	30,30,30,30	0
52	MG	DA	3294	1/1	0.11	-	46,46,46,46	0
52	MG	DA	3241	1/1	0.10	-	54,54,54,54	0
52	MG	DA	3029	1/1	0.19	-	43,43,43,43	0
52	MG	AA	1614	1/1	0.33	-	47,47,47,47	0
52	MG	BA	3166	1/1	0.16	-	27,27,27,27	0
52	MG	DA	3200	1/1	0.17	-	37,37,37,37	0
52	MG	DA	3105	1/1	0.15	-	39,39,39,39	0
52	MG	BA	3343	1/1	0.52	-	40,40,40,40	0
52	MG	CA	1604	1/1	0.31	-	67,67,67,67	0
52	MG	DA	3164	1/1	0.51	-	41,41,41,41	0
52	MG	BA	3083	1/1	0.47	-	34,34,34,34	0
52	MG	DA	3277	1/1	0.11	-	38,38,38,38	0
52	MG	BA	3206	1/1	0.47	-	29,29,29,29	0
52	MG	BA	3183	1/1	0.34	-	43,43,43,43	0
52	MG	BA	3270	1/1	0.40	-	26,26,26,26	0
52	MG	BA	3130	1/1	0.10	-	36,36,36,36	0
52	MG	BA	3188	1/1	0.48	-	36,36,36,36	0
52	MG	BA	3200	1/1	0.28	-	12,12,12,12	0
52	MG	BA	3112	1/1	0.19	-	14,14,14,14	0
52	MG	DA	3126	1/1	0.13	-	36,36,36,36	0
52	MG	AA	1634	1/1	0.58	-	51,51,51,51	0
52	MG	DA	3208	1/1	0.43	-	34,34,34,34	0
52	MG	DA	3005	1/1	0.15	-	49,49,49,49	0
52	MG	AA	1650	1/1	0.42	-	49,49,49,49	0
52	MG	BA	3328	1/1	0.30	-	27,27,27,27	0
52	MG	CA	1605	1/1	0.29	-	68,68,68,68	0
52	MG	BA	3222	1/1	0.49	-	20,20,20,20	0
52	MG	DA	3106	1/1	0.74	-	53,53,53,53	0
52	MG	DA	3236	1/1	0.56	-	71,71,71,71	0
52	MG	BA	3139	1/1	0.59	-	30,30,30,30	0
52	MG	BA	3171	1/1	0.66	-	35,35,35,35	0
52	MG	DA	3235	1/1	0.19	-	48,48,48,48	0
52	MG	BA	3298	1/1	0.35	-	41,41,41,41	0
52	MG	BA	3224	1/1	0.28	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3230	1/1	0.63	-	37,37,37,37	0
52	MG	DA	3131	1/1	0.24	-	55,55,55,55	0
52	MG	DA	3318	1/1	0.27	-	43,43,43,43	0
52	MG	BA	3054	1/1	0.27	-	48,48,48,48	0
52	MG	BA	3274	1/1	0.43	-	33,33,33,33	0
52	MG	CA	1629	1/1	0.15	-	57,57,57,57	0
52	MG	BA	3021	1/1	0.38	-	19,19,19,19	0
52	MG	DA	3267	1/1	0.35	-	46,46,46,46	0
52	MG	BA	3062	1/1	0.15	-	30,30,30,30	0
52	MG	BA	3255	1/1	0.39	-	54,54,54,54	0
52	MG	DA	3084	1/1	0.31	-	31,31,31,31	0
52	MG	DA	3034	1/1	0.32	-	38,38,38,38	0
52	MG	BA	3063	1/1	0.42	-	45,45,45,45	0
52	MG	CA	1617	1/1	0.48	-	48,48,48,48	0
52	MG	BA	3023	1/1	0.27	-	13,13,13,13	0
52	MG	AA	1612	1/1	0.51	-	56,56,56,56	0
52	MG	CA	1624	1/1	0.32	-	50,50,50,50	0
52	MG	DA	3175	1/1	0.40	-	51,51,51,51	0
52	MG	BA	3150	1/1	0.37	-	40,40,40,40	0
52	MG	BA	3038	1/1	0.40	-	17,17,17,17	0
52	MG	DA	3136	1/1	0.26	-	48,48,48,48	0
52	MG	BA	3186	1/1	0.37	-	38,38,38,38	0
52	MG	BA	3363	1/1	0.16	-	54,54,54,54	0
52	MG	AA	1625	1/1	0.51	-	40,40,40,40	0
52	MG	BA	3302	1/1	0.62	-	31,31,31,31	0
52	MG	DA	3165	1/1	0.23	-	38,38,38,38	0
52	MG	DA	3220	1/1	0.15	-	40,40,40,40	0
52	MG	DA	3118	1/1	0.28	-	43,43,43,43	0
52	MG	DA	3123	1/1	0.17	-	38,38,38,38	0
52	MG	DA	3097	1/1	0.29	-	30,30,30,30	0
52	MG	BA	3184	1/1	0.48	-	40,40,40,40	0
52	MG	DD	301	1/1	0.25	-	32,32,32,32	0
52	MG	DA	3271	1/1	0.47	-	56,56,56,56	0
52	MG	DA	3268	1/1	0.69	-	63,63,63,63	0
52	MG	DA	3124	1/1	0.23	-	49,49,49,49	0
52	MG	DA	3187	1/1	0.51	-	44,44,44,44	0
52	MG	DA	3039	1/1	0.49	-	48,48,48,48	0
52	MG	DA	3169	1/1	0.44	-	45,45,45,45	0
52	MG	BA	3156	1/1	0.44	-	12,12,12,12	0
52	MG	BA	3014	1/1	0.51	-	30,30,30,30	0
52	MG	DA	3170	1/1	0.12	-	42,42,42,42	0
52	MG	DA	3248	1/1	0.29	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3222	1/1	0.43	-	41,41,41,41	0
52	MG	BB	204	1/1	0.32	-	41,41,41,41	0
52	MG	BB	201	1/1	0.45	-	35,35,35,35	0
52	MG	DA	3107	1/1	0.35	-	15,15,15,15	0
52	MG	BA	3266	1/1	0.37	-	37,37,37,37	0
52	MG	DA	3056	1/1	0.31	-	24,24,24,24	0
52	MG	CA	1609	1/1	0.27	-	41,41,41,41	0
55	CLM	DA	3334	20/20	0.48	-	90,90,90,90	0
52	MG	DA	3094	1/1	0.61	-	38,38,38,38	0
52	MG	DA	3255	1/1	0.36	-	49,49,49,49	0
52	MG	DA	3195	1/1	0.37	-	36,36,36,36	0
52	MG	AA	1645	1/1	0.43	-	61,61,61,61	0
52	MG	AA	1610	1/1	0.14	-	33,33,33,33	0
52	MG	CA	1621	1/1	0.40	-	50,50,50,50	0
52	MG	BA	3228	1/1	0.35	-	27,27,27,27	0
52	MG	DA	3157	1/1	0.27	-	48,48,48,48	0
52	MG	BA	3339	1/1	0.25	-	31,31,31,31	0
52	MG	BA	3076	1/1	0.22	-	21,21,21,21	0
52	MG	BR	201	1/1	0.33	-	7,7,7,7	0
52	MG	BA	3268	1/1	0.46	-	38,38,38,38	0
52	MG	BA	3007	1/1	0.58	-	40,40,40,40	0
52	MG	BA	3240	1/1	0.30	-	50,50,50,50	0
52	MG	BA	3332	1/1	0.41	-	35,35,35,35	0
52	MG	DA	3054	1/1	0.23	-	55,55,55,55	0
52	MG	CA	1641	1/1	0.20	-	45,45,45,45	0
52	MG	BA	3049	1/1	0.49	-	23,23,23,23	0
52	MG	DA	3081	1/1	0.47	-	24,24,24,24	0
52	MG	DA	3226	1/1	0.48	-	55,55,55,55	0
52	MG	DA	3319	1/1	0.51	-	55,55,55,55	0
52	MG	BA	3327	1/1	0.23	-	48,48,48,48	0
52	MG	BA	3117	1/1	0.29	-	50,50,50,50	0
52	MG	BA	3073	1/1	0.24	-	7,7,7,7	0
52	MG	DA	3150	1/1	0.44	-	32,32,32,32	0
52	MG	DA	3289	1/1	0.28	-	53,53,53,53	0
52	MG	BE	301	1/1	0.42	-	16,16,16,16	0
52	MG	DA	3203	1/1	0.29	-	38,38,38,38	0
52	MG	BA	3290	1/1	0.26	-	40,40,40,40	0
52	MG	BA	3025	1/1	0.18	-	29,29,29,29	0
52	MG	DA	3031	1/1	0.17	-	51,51,51,51	0
54	K	BA	3369	1/1	0.15	-	41,41,41,41	0
52	MG	BA	3265	1/1	0.24	-	43,43,43,43	0
52	MG	BA	3176	1/1	0.37	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	CA	1603	1/1	0.34	-	32,32,32,32	0
53	ZN	CN	101	1/1	0.17	-	136,136,136,136	0
52	MG	DA	3201	1/1	0.20	-	43,43,43,43	0
52	MG	BA	3304	1/1	0.45	-	49,49,49,49	0
52	MG	DA	3088	1/1	0.34	-	40,40,40,40	0
52	MG	AA	1626	1/1	0.33	-	46,46,46,46	0
52	MG	DA	3021	1/1	0.25	-	38,38,38,38	0
52	MG	BA	3040	1/1	0.50	-	37,37,37,37	0
52	MG	BA	3341	1/1	0.70	-	66,66,66,66	0
52	MG	BA	3134	1/1	0.26	-	36,36,36,36	0
52	MG	DA	3142	1/1	0.50	-	32,32,32,32	0
52	MG	DA	3177	1/1	0.31	-	37,37,37,37	0
52	MG	BA	3333	1/1	0.36	-	50,50,50,50	0
52	MG	BA	3177	1/1	0.72	-	67,67,67,67	0
52	MG	BA	3288	1/1	0.36	-	46,46,46,46	0
52	MG	BA	3122	1/1	0.47	-	37,37,37,37	0
52	MG	BA	3314	1/1	0.40	-	41,41,41,41	0
52	MG	DA	3045	1/1	0.31	-	30,30,30,30	0
52	MG	DA	3083	1/1	0.36	-	37,37,37,37	0
52	MG	BA	3368	1/1	0.07	-	60,60,60,60	0
52	MG	BA	3084	1/1	0.27	-	5,5,5,5	0
52	MG	CA	1653	1/1	0.12	-	47,47,47,47	0
52	MG	DE	301	1/1	0.34	-	31,31,31,31	0
52	MG	DA	3121	1/1	0.20	-	49,49,49,49	0
52	MG	CA	1650	1/1	0.32	-	45,45,45,45	0
52	MG	DA	3171	1/1	0.33	-	26,26,26,26	0
52	MG	DA	3320	1/1	0.24	-	31,31,31,31	0
52	MG	CA	1616	1/1	0.40	-	45,45,45,45	0
52	MG	BA	3039	1/1	0.66	-	37,37,37,37	0
52	MG	BA	3337	1/1	0.41	-	32,32,32,32	0
52	MG	DA	3234	1/1	0.64	-	60,60,60,60	0
52	MG	DA	3314	1/1	0.15	-	40,40,40,40	0
52	MG	DA	3077	1/1	0.25	-	38,38,38,38	0
52	MG	DA	3149	1/1	0.52	-	54,54,54,54	0
52	MG	BA	3145	1/1	0.47	-	33,33,33,33	0
52	MG	BA	3277	1/1	0.22	-	10,10,10,10	0
52	MG	BX	101	1/1	0.21	-	21,21,21,21	0
52	MG	AA	1615	1/1	0.18	-	35,35,35,35	0
52	MG	DA	3278	1/1	0.40	-	54,54,54,54	0
52	MG	DA	3066	1/1	0.40	-	29,29,29,29	0
52	MG	BA	3276	1/1	0.33	-	35,35,35,35	0
52	MG	BA	3068	1/1	0.54	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3100	1/1	0.30	-	23,23,23,23	0
52	MG	DA	3037	1/1	0.63	-	33,33,33,33	0
52	MG	DQ	201	1/1	0.25	-	42,42,42,42	0
52	MG	BA	3163	1/1	0.48	-	53,53,53,53	0
52	MG	BA	3203	1/1	0.12	-	47,47,47,47	0
52	MG	DA	3306	1/1	0.42	-	54,54,54,54	0
52	MG	BA	3125	1/1	0.43	-	18,18,18,18	0
52	MG	AA	1633	1/1	0.11	-	42,42,42,42	0
52	MG	CA	1615	1/1	0.29	-	64,64,64,64	0
52	MG	BA	3366	1/1	0.12	-	52,52,52,52	0
52	MG	BA	3148	1/1	0.36	-	23,23,23,23	0
52	MG	BA	3018	1/1	0.25	-	27,27,27,27	0
52	MG	DA	3304	1/1	0.75	-	63,63,63,63	0
52	MG	DA	3160	1/1	0.52	-	51,51,51,51	0
52	MG	AA	1631	1/1	0.57	-	52,52,52,52	0
52	MG	BA	3296	1/1	0.08	-	36,36,36,36	0
52	MG	DA	3291	1/1	0.20	-	36,36,36,36	0
52	MG	BA	3189	1/1	0.17	-	46,46,46,46	0
52	MG	BA	3194	1/1	0.43	-	30,30,30,30	0
52	MG	DA	3147	1/1	0.28	-	43,43,43,43	0
52	MG	DA	3198	1/1	0.28	-	37,37,37,37	0
52	MG	BA	3223	1/1	0.40	-	25,25,25,25	0
52	MG	BA	3121	1/1	0.24	-	34,34,34,34	0
52	MG	DA	3003	1/1	0.61	-	39,39,39,39	0
52	MG	DA	3158	1/1	0.27	-	33,33,33,33	0
52	MG	DA	3087	1/1	0.10	-	24,24,24,24	0
52	MG	DA	3089	1/1	0.53	-	31,31,31,31	0
52	MG	DA	3264	1/1	0.18	-	58,58,58,58	0
52	MG	BA	3319	1/1	0.33	-	46,46,46,46	0
52	MG	BA	3055	1/1	0.28	-	19,19,19,19	0
52	MG	BA	3174	1/1	0.35	-	29,29,29,29	0
52	MG	CA	1634	1/1	0.12	-	47,47,47,47	0
52	MG	BA	3236	1/1	0.19	-	31,31,31,31	0
52	MG	BA	3090	1/1	0.32	-	14,14,14,14	0
52	MG	CA	1608	1/1	0.28	-	68,68,68,68	0
52	MG	BB	202	1/1	0.26	-	27,27,27,27	0
52	MG	DA	3213	1/1	0.36	-	26,26,26,26	0
52	MG	DA	3035	1/1	0.39	-	31,31,31,31	0
52	MG	BA	3046	1/1	0.32	-	24,24,24,24	0
52	MG	CA	1647	1/1	0.29	-	49,49,49,49	0
52	MG	BA	3002	1/1	0.43	-	23,23,23,23	0
52	MG	BA	3285	1/1	0.36	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3174	1/1	0.26	-	54,54,54,54	0
52	MG	BA	3133	1/1	0.26	-	25,25,25,25	0
52	MG	DA	3167	1/1	0.16	-	63,63,63,63	0
52	MG	BA	3213	1/1	0.40	-	17,17,17,17	0
52	MG	BA	3089	1/1	0.30	-	15,15,15,15	0
52	MG	DA	3117	1/1	0.12	-	54,54,54,54	0
52	MG	CA	1637	1/1	0.32	-	65,65,65,65	0
52	MG	CA	1630	1/1	0.55	-	66,66,66,66	0
52	MG	BA	3136	1/1	0.45	-	22,22,22,22	0
52	MG	BA	3020	1/1	0.24	-	8,8,8,8	0
52	MG	BA	3106	1/1	0.42	-	37,37,37,37	0
52	MG	BA	3205	1/1	0.45	-	34,34,34,34	0
52	MG	CA	1613	1/1	0.30	-	58,58,58,58	0
52	MG	DA	3327	1/1	0.13	-	41,41,41,41	0
52	MG	BA	3167	1/1	0.37	-	51,51,51,51	0
52	MG	AA	1652	1/1	0.67	-	44,44,44,44	0
52	MG	BA	3245	1/1	0.42	-	52,52,52,52	0
52	MG	AA	1606	1/1	0.47	-	86,86,86,86	0
52	MG	DA	3093	1/1	0.46	-	44,44,44,44	0
52	MG	BQ	201	1/1	0.16	-	18,18,18,18	0
52	MG	BA	3338	1/1	0.44	-	50,50,50,50	0
52	MG	BA	3170	1/1	0.62	-	36,36,36,36	0
52	MG	BA	3053	1/1	0.37	-	6,6,6,6	0
52	MG	DA	3009	1/1	0.37	-	47,47,47,47	0
52	MG	BA	3060	1/1	0.31	-	31,31,31,31	0
52	MG	DA	3078	1/1	0.38	-	31,31,31,31	0
52	MG	DA	3316	1/1	0.17	-	62,62,62,62	0
52	MG	AA	1620	1/1	0.54	-	52,52,52,52	0
52	MG	BA	3010	1/1	0.34	-	37,37,37,37	0
52	MG	AA	1629	1/1	0.36	-	49,49,49,49	0
52	MG	AA	1623	1/1	0.40	-	31,31,31,31	0
52	MG	DA	3013	1/1	0.38	-	10,10,10,10	0
52	MG	BA	3202	1/1	0.55	-	35,35,35,35	0
52	MG	BA	3099	1/1	0.27	-	34,34,34,34	0
52	MG	CA	1645	1/1	0.33	-	45,45,45,45	0
52	MG	DA	3197	1/1	0.42	-	46,46,46,46	0
52	MG	BA	3155	1/1	0.26	-	39,39,39,39	0
52	MG	BA	3187	1/1	0.51	-	33,33,33,33	0
52	MG	BA	3232	1/1	0.26	-	27,27,27,27	0
52	MG	DA	3329	1/1	0.23	-	51,51,51,51	0
52	MG	DA	3058	1/1	0.28	-	42,42,42,42	0
52	MG	BA	3114	1/1	0.39	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3232	1/1	0.63	-	63,63,63,63	0
52	MG	BA	3235	1/1	0.49	-	38,38,38,38	0
52	MG	DA	3030	1/1	0.19	-	37,37,37,37	0
52	MG	DA	3273	1/1	0.26	-	39,39,39,39	0
52	MG	DA	3180	1/1	0.32	-	38,38,38,38	0
52	MG	DA	3135	1/1	0.60	-	39,39,39,39	0
52	MG	DA	3151	1/1	0.32	-	40,40,40,40	0
52	MG	DA	3153	1/1	0.65	-	73,73,73,73	0
52	MG	DA	3010	1/1	0.34	-	35,35,35,35	0
52	MG	BA	3120	1/1	0.33	-	25,25,25,25	0
52	MG	AA	1630	1/1	0.47	-	49,49,49,49	0
52	MG	BA	3131	1/1	0.45	-	45,45,45,45	0
52	MG	BA	3123	1/1	0.30	-	40,40,40,40	0
55	CLM	BA	3370	20/20	0.45	-	90,90,90,90	0
52	MG	BA	3316	1/1	0.33	-	41,41,41,41	0
52	MG	DA	3067	1/1	0.18	-	35,35,35,35	0
52	MG	DA	3004	1/1	0.19	-	19,19,19,19	0
52	MG	DA	3129	1/1	0.25	-	36,36,36,36	0
52	MG	DA	3309	1/1	0.18	-	66,66,66,66	0
52	MG	CA	1631	1/1	0.09	-	71,71,71,71	0
52	MG	DA	3310	1/1	0.35	-	56,56,56,56	0
52	MG	BA	3357	1/1	0.31	-	44,44,44,44	0
52	MG	BA	3354	1/1	0.28	-	40,40,40,40	0
52	MG	DA	3322	1/1	0.34	-	45,45,45,45	0
52	MG	BA	3031	1/1	0.20	-	39,39,39,39	0
52	MG	DA	3023	1/1	0.40	-	27,27,27,27	0
52	MG	DA	3317	1/1	0.06	-	48,48,48,48	0
52	MG	BA	3198	1/1	0.76	-	62,62,62,62	0
52	MG	DA	3096	1/1	0.46	-	61,61,61,61	0
52	MG	BA	3158	1/1	0.31	-	9,9,9,9	0
52	MG	BA	3221	1/1	0.21	-	31,31,31,31	0
52	MG	BA	3104	1/1	0.10	-	22,22,22,22	0
52	MG	BA	3138	1/1	0.33	-	4,4,4,4	0
52	MG	DA	3275	1/1	0.52	-	51,51,51,51	0
52	MG	CA	1626	1/1	0.47	-	68,68,68,68	0
52	MG	BA	3033	1/1	0.23	-	18,18,18,18	0
52	MG	DA	3252	1/1	0.31	-	57,57,57,57	0
52	MG	DA	3176	1/1	0.19	-	66,66,66,66	0
52	MG	BA	3315	1/1	0.23	-	43,43,43,43	0
52	MG	BA	3067	1/1	0.47	-	28,28,28,28	0
52	MG	BA	3242	1/1	0.27	-	33,33,33,33	0
52	MG	BA	3128	1/1	0.79	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3293	1/1	0.28	-	47,47,47,47	0
52	MG	BA	3336	1/1	0.32	-	49,49,49,49	0
52	MG	DA	3212	1/1	0.20	-	33,33,33,33	0
52	MG	BP	202	1/1	0.18	-	0,0,0,0	0
52	MG	DA	3138	1/1	0.32	-	31,31,31,31	0
52	MG	DA	3205	1/1	0.64	-	39,39,39,39	0
52	MG	DA	3266	1/1	0.52	-	45,45,45,45	0
52	MG	AA	1617	1/1	0.42	-	57,57,57,57	0
52	MG	BB	203	1/1	0.09	-	55,55,55,55	0
52	MG	DA	3237	1/1	0.17	-	57,57,57,57	0
52	MG	BA	3325	1/1	0.52	-	53,53,53,53	0
52	MG	DA	3076	1/1	0.19	-	23,23,23,23	0
52	MG	BA	3048	1/1	0.45	-	22,22,22,22	0
52	MG	DA	3258	1/1	0.12	-	38,38,38,38	0
52	MG	BA	3022	1/1	0.27	-	37,37,37,37	0
52	MG	DA	3016	1/1	0.55	-	29,29,29,29	0
52	MG	AA	1601	1/1	0.17	-	50,50,50,50	0
52	MG	BA	3165	1/1	0.16	-	26,26,26,26	0
52	MG	BA	3360	1/1	0.43	-	48,48,48,48	0
52	MG	BA	3098	1/1	0.26	-	59,59,59,59	0
52	MG	BA	3303	1/1	0.14	-	37,37,37,37	0
52	MG	BA	3103	1/1	0.28	-	27,27,27,27	0
52	MG	DA	3279	1/1	0.46	-	44,44,44,44	0
52	MG	B5	102	1/1	0.47	-	44,44,44,44	0
52	MG	AA	1643	1/1	0.91	-	66,66,66,66	0
52	MG	DA	3068	1/1	0.31	-	57,57,57,57	0
52	MG	BA	3041	1/1	0.41	-	24,24,24,24	0
52	MG	DA	3293	1/1	0.65	-	54,54,54,54	0
52	MG	BA	3211	1/1	0.22	-	30,30,30,30	0
52	MG	DA	3324	1/1	0.23	-	38,38,38,38	0
52	MG	DA	3062	1/1	0.14	-	24,24,24,24	0
52	MG	DA	3168	1/1	0.47	-	32,32,32,32	0
52	MG	DA	3002	1/1	0.40	-	22,22,22,22	0
52	MG	DA	3286	1/1	0.26	-	43,43,43,43	0
52	MG	BA	3137	1/1	0.26	-	34,34,34,34	0
52	MG	BA	3209	1/1	0.32	-	36,36,36,36	0
52	MG	BA	3239	1/1	0.15	-	32,32,32,32	0
52	MG	DA	3270	1/1	0.39	-	55,55,55,55	0
52	MG	AA	1656	1/1	0.12	-	62,62,62,62	0
52	MG	CA	1622	1/1	0.37	-	46,46,46,46	0
52	MG	DU	201	1/1	0.38	-	60,60,60,60	0
52	MG	BA	3017	1/1	0.40	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3179	1/1	0.39	-	25,25,25,25	0
52	MG	BU	201	1/1	0.30	-	25,25,25,25	0
52	MG	DA	3122	1/1	0.56	-	40,40,40,40	0
52	MG	DA	3244	1/1	0.41	-	36,36,36,36	0
52	MG	BA	3172	1/1	0.47	-	18,18,18,18	0
52	MG	BA	3030	1/1	0.23	-	17,17,17,17	0
52	MG	DA	3253	1/1	0.42	-	32,32,32,32	0
52	MG	DA	3049	1/1	0.48	-	42,42,42,42	0
52	MG	BA	3275	1/1	0.36	-	29,29,29,29	0
52	MG	BA	3210	1/1	0.38	-	29,29,29,29	0
52	MG	DA	3085	1/1	0.15	-	19,19,19,19	0
52	MG	BA	3015	1/1	0.31	-	29,29,29,29	0
52	MG	DA	3025	1/1	0.38	-	46,46,46,46	0
52	MG	CA	1628	1/1	0.52	-	50,50,50,50	0
52	MG	BA	3283	1/1	0.30	-	50,50,50,50	0
52	MG	BA	3115	1/1	0.41	-	34,34,34,34	0
52	MG	DA	3022	1/1	0.21	-	38,38,38,38	0
52	MG	DA	3116	1/1	0.22	-	45,45,45,45	0
52	MG	BA	3324	1/1	0.37	-	53,53,53,53	0
52	MG	DA	3181	1/1	0.63	-	29,29,29,29	0
52	MG	DA	3285	1/1	0.19	-	33,33,33,33	0
52	MG	DA	3074	1/1	0.57	-	54,54,54,54	0
52	MG	AA	1622	1/1	0.43	-	40,40,40,40	0
52	MG	BA	3095	1/1	0.39	-	38,38,38,38	0
52	MG	DA	3111	1/1	0.55	-	39,39,39,39	0
52	MG	BA	3079	1/1	0.21	-	36,36,36,36	0
52	MG	BA	3061	1/1	0.33	-	35,35,35,35	0
52	MG	AA	1647	1/1	0.27	-	46,46,46,46	0
52	MG	BA	3358	1/1	0.46	-	59,59,59,59	0
52	MG	CA	1601	1/1	0.17	-	61,61,61,61	0
52	MG	DA	3162	1/1	0.47	-	50,50,50,50	0
52	MG	DA	3263	1/1	0.25	-	65,65,65,65	0
52	MG	BA	3361	1/1	0.22	-	52,52,52,52	0
52	MG	DA	3300	1/1	0.40	-	54,54,54,54	0
52	MG	AA	1641	1/1	0.23	-	64,64,64,64	0
52	MG	AA	1611	1/1	0.16	-	72,72,72,72	0
52	MG	BA	3300	1/1	0.35	-	45,45,45,45	0
52	MG	BA	3346	1/1	0.10	-	63,63,63,63	0
52	MG	BA	3147	1/1	0.41	-	28,28,28,28	0
52	MG	BA	3243	1/1	0.24	-	30,30,30,30	0
52	MG	DA	3137	1/1	0.10	-	69,69,69,69	0
52	MG	BA	3335	1/1	0.39	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3073	1/1	0.25	-	27,27,27,27	0
52	MG	DA	3148	1/1	0.25	-	51,51,51,51	0
52	MG	DA	3115	1/1	0.22	-	47,47,47,47	0
52	MG	BA	3088	1/1	0.30	-	33,33,33,33	0
52	MG	DA	3229	1/1	0.53	-	36,36,36,36	0
52	MG	DA	3328	1/1	0.45	-	61,61,61,61	0
52	MG	DA	3182	1/1	0.42	-	41,41,41,41	0
52	MG	DA	3042	1/1	0.18	-	29,29,29,29	0
52	MG	BA	3306	1/1	0.47	-	35,35,35,35	0
52	MG	BA	3119	1/1	0.33	-	34,34,34,34	0
52	MG	AA	1607	1/1	0.57	-	47,47,47,47	0
52	MG	BA	3051	1/1	0.45	-	19,19,19,19	0
52	MG	BA	3237	1/1	0.45	-	42,42,42,42	0
52	MG	DA	3144	1/1	0.51	-	43,43,43,43	0
52	MG	DB	203	1/1	0.07	-	73,73,73,73	0
52	MG	DA	3128	1/1	0.17	-	29,29,29,29	0
52	MG	DA	3057	1/1	0.27	-	32,32,32,32	0
52	MG	BA	3149	1/1	0.14	-	8,8,8,8	0
52	MG	BA	3151	1/1	0.36	-	47,47,47,47	0
52	MG	DA	3299	1/1	0.20	-	41,41,41,41	0
52	MG	BA	3152	1/1	0.11	-	49,49,49,49	0
52	MG	AA	1637	1/1	0.52	-	51,51,51,51	0
52	MG	DA	3007	1/1	0.40	-	48,48,48,48	0
52	MG	BA	3320	1/1	0.93	-	52,52,52,52	0
52	MG	DA	3027	1/1	0.54	-	36,36,36,36	0
52	MG	BA	3261	1/1	0.21	-	27,27,27,27	0
52	MG	DA	3196	1/1	0.35	-	33,33,33,33	0
52	MG	DA	3276	1/1	0.72	-	44,44,44,44	0
52	MG	CA	1640	1/1	0.10	-	53,53,53,53	0
52	MG	BA	3208	1/1	0.23	-	17,17,17,17	0
52	MG	BA	3052	1/1	0.48	-	23,23,23,23	0
52	MG	DA	3284	1/1	0.57	-	49,49,49,49	0
52	MG	BA	3036	1/1	0.35	-	8,8,8,8	0
52	MG	DA	3090	1/1	0.28	-	33,33,33,33	0
52	MG	AA	1609	1/1	0.39	-	52,52,52,52	0
52	MG	BA	3144	1/1	0.55	-	29,29,29,29	0
52	MG	DA	3092	1/1	0.65	-	47,47,47,47	0
52	MG	AA	1651	1/1	0.32	-	45,45,45,45	0
52	MG	DA	3245	1/1	0.17	-	65,65,65,65	0
52	MG	BA	3057	1/1	0.22	-	37,37,37,37	0
52	MG	CA	1652	1/1	0.14	-	61,61,61,61	0
52	MG	BA	3256	1/1	0.12	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3133	1/1	0.10	-	55,55,55,55	0
52	MG	BA	3004	1/1	0.28	-	14,14,14,14	0
52	MG	CA	1643	1/1	0.24	-	42,42,42,42	0
52	MG	BA	3101	1/1	0.29	-	24,24,24,24	0
52	MG	DA	3113	1/1	0.09	-	59,59,59,59	0
52	MG	CA	1627	1/1	0.71	-	81,81,81,81	0
52	MG	DA	3125	1/1	0.15	-	33,33,33,33	0
52	MG	BA	3160	1/1	0.45	-	41,41,41,41	0
52	MG	BA	3126	1/1	0.21	-	29,29,29,29	0
52	MG	DA	3011	1/1	0.43	-	27,27,27,27	0
52	MG	CA	1614	1/1	0.57	-	57,57,57,57	0
52	MG	AA	1654	1/1	0.67	-	64,64,64,64	0
52	MG	BD	301	1/1	0.30	-	25,25,25,25	0
52	MG	DA	3166	1/1	0.56	-	64,64,64,64	0
52	MG	DA	3036	1/1	0.37	-	12,12,12,12	0
52	MG	BA	3181	1/1	0.14	-	32,32,32,32	0
52	MG	DA	3215	1/1	0.28	-	27,27,27,27	0
52	MG	BA	3045	1/1	0.34	-	14,14,14,14	0
52	MG	BA	3340	1/1	0.18	-	39,39,39,39	0
52	MG	BA	3294	1/1	0.44	-	40,40,40,40	0
52	MG	BA	3351	1/1	0.29	-	48,48,48,48	0
52	MG	DA	3296	1/1	0.22	-	45,45,45,45	0
52	MG	DX	101	1/1	0.25	-	45,45,45,45	0
52	MG	DA	3001	1/1	0.32	-	45,45,45,45	0
52	MG	DA	3141	1/1	0.48	-	35,35,35,35	0
52	MG	DA	3184	1/1	0.24	-	32,32,32,32	0
52	MG	BA	3146	1/1	0.29	-	33,33,33,33	0
52	MG	DB	202	1/1	0.34	-	60,60,60,60	0
52	MG	AA	1632	1/1	0.55	-	51,51,51,51	0
52	MG	BA	3162	1/1	0.31	-	45,45,45,45	0
52	MG	BA	3178	1/1	0.21	-	32,32,32,32	0
52	MG	CA	1644	1/1	0.16	-	43,43,43,43	0
52	MG	DA	3061	1/1	0.37	-	34,34,34,34	0
52	MG	BA	3220	1/1	0.55	-	22,22,22,22	0
52	MG	CA	1642	1/1	1.13	-	71,71,71,71	0
52	MG	DA	3075	1/1	0.41	-	38,38,38,38	0
52	MG	D1	101	1/1	0.36	-	47,47,47,47	0
52	MG	BA	3087	1/1	0.18	-	10,10,10,10	0
52	MG	BA	3364	1/1	0.25	-	64,64,64,64	0
52	MG	DA	3190	1/1	0.29	-	43,43,43,43	0
52	MG	DA	3323	1/1	0.61	-	62,62,62,62	0
52	MG	BA	3110	1/1	0.43	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3238	1/1	0.13	-	36,36,36,36	0
52	MG	BA	3097	1/1	0.27	-	32,32,32,32	0
52	MG	DA	3108	1/1	0.32	-	39,39,39,39	0
52	MG	AA	1618	1/1	0.15	-	53,53,53,53	0
52	MG	BA	3196	1/1	0.33	-	26,26,26,26	0
52	MG	DA	3101	1/1	0.24	-	34,34,34,34	0
52	MG	BA	3287	1/1	0.27	-	27,27,27,27	0
52	MG	BA	3001	1/1	0.30	-	36,36,36,36	0
52	MG	BA	3116	1/1	0.09	-	41,41,41,41	0
52	MG	BA	3301	1/1	0.58	-	36,36,36,36	0
52	MG	CA	1646	1/1	0.68	-	58,58,58,58	0
52	MG	BA	3352	1/1	0.21	-	51,51,51,51	0
52	MG	BA	3190	1/1	0.46	-	36,36,36,36	0
52	MG	DA	3018	1/1	0.25	-	29,29,29,29	0
52	MG	BP	201	1/1	0.45	-	35,35,35,35	0
52	MG	BA	3142	1/1	0.33	-	26,26,26,26	0
52	MG	DA	3211	1/1	0.74	-	50,50,50,50	0
52	MG	BA	3066	1/1	0.41	-	34,34,34,34	0
52	MG	DA	3155	1/1	0.20	-	41,41,41,41	0
52	MG	CA	1618	1/1	0.45	-	58,58,58,58	0
52	MG	AA	1624	1/1	0.42	-	59,59,59,59	0
52	MG	BA	3127	1/1	0.34	-	44,44,44,44	0
52	MG	BA	3019	1/1	0.50	-	13,13,13,13	0
52	MG	DA	3217	1/1	0.10	-	36,36,36,36	0
52	MG	DA	3243	1/1	0.39	-	56,56,56,56	0
52	MG	CA	1619	1/1	0.45	-	40,40,40,40	0
52	MG	DA	3020	1/1	0.51	-	33,33,33,33	0
52	MG	BA	3305	1/1	0.24	-	54,54,54,54	0
52	MG	DA	3189	1/1	0.13	-	42,42,42,42	0
52	MG	BA	3044	1/1	0.24	-	9,9,9,9	0
52	MG	DA	3283	1/1	0.60	-	52,52,52,52	0
52	MG	BA	3262	1/1	0.14	-	30,30,30,30	0
52	MG	DA	3297	1/1	0.47	-	55,55,55,55	0
52	MG	DA	3112	1/1	0.38	-	28,28,28,28	0
52	MG	CA	1611	1/1	0.57	-	76,76,76,76	0
52	MG	DA	3251	1/1	0.22	-	72,72,72,72	0
52	MG	AA	1653	1/1	0.32	-	46,46,46,46	0
52	MG	BA	3043	1/1	0.16	-	32,32,32,32	0
52	MG	DA	3044	1/1	0.31	-	35,35,35,35	0
52	MG	DA	3216	1/1	0.43	-	45,45,45,45	0
52	MG	DA	3080	1/1	0.69	-	30,30,30,30	0
52	MG	BA	3091	1/1	0.20	-	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3256	1/1	0.18	-	46,46,46,46	0
52	MG	BA	3264	1/1	0.23	-	11,11,11,11	0
52	MG	BA	3359	1/1	0.78	-	39,39,39,39	0
52	MG	BA	3367	1/1	0.07	-	47,47,47,47	0
52	MG	DA	3326	1/1	0.13	-	49,49,49,49	0
52	MG	BA	3217	1/1	0.34	-	34,34,34,34	0
52	MG	BA	3096	1/1	0.35	-	16,16,16,16	0
52	MG	DA	3104	1/1	0.40	-	41,41,41,41	0
52	MG	DA	3110	1/1	0.19	-	50,50,50,50	0
52	MG	BA	3317	1/1	0.29	-	53,53,53,53	0
52	MG	BA	3312	1/1	0.12	-	41,41,41,41	0
52	MG	DA	3239	1/1	0.69	-	41,41,41,41	0
52	MG	BA	3154	1/1	0.33	-	77,77,77,77	0
52	MG	BA	3329	1/1	0.21	-	49,49,49,49	0
52	MG	BA	3323	1/1	0.51	-	42,42,42,42	0
52	MG	BA	3331	1/1	0.45	-	37,37,37,37	0
52	MG	AA	1646	1/1	0.11	-	48,48,48,48	0
52	MG	DA	3127	1/1	0.17	-	33,33,33,33	0
52	MG	BA	3212	1/1	0.36	-	30,30,30,30	0
52	MG	DA	3313	1/1	0.60	-	48,48,48,48	0
52	MG	DA	3265	1/1	0.14	-	38,38,38,38	0
52	MG	AA	1608	1/1	0.41	-	70,70,70,70	0
52	MG	BA	3215	1/1	0.21	-	10,10,10,10	0
52	MG	BA	3289	1/1	0.23	-	44,44,44,44	0
52	MG	DA	3040	1/1	0.86	-	58,58,58,58	0
52	MG	DA	3209	1/1	0.25	-	51,51,51,51	0
52	MG	DA	3091	1/1	0.36	-	11,11,11,11	0
52	MG	CA	1635	1/1	0.69	-	73,73,73,73	0
52	MG	AA	1621	1/1	0.46	-	37,37,37,37	0
52	MG	BA	3258	1/1	0.17	-	21,21,21,21	0
52	MG	BA	3037	1/1	0.40	-	1,1,1,1	0
52	MG	BA	3204	1/1	0.17	-	36,36,36,36	0
52	MG	DA	3047	1/1	0.45	-	33,33,33,33	0
52	MG	DA	3231	1/1	0.50	-	54,54,54,54	0
52	MG	DA	3012	1/1	0.41	-	26,26,26,26	0
52	MG	BA	3082	1/1	0.23	-	6,6,6,6	0
52	MG	BA	3218	1/1	0.27	-	30,30,30,30	0
52	MG	DA	3114	1/1	0.18	-	46,46,46,46	0
52	MG	BA	3225	1/1	0.51	-	32,32,32,32	0
52	MG	BA	3191	1/1	0.37	-	19,19,19,19	0
52	MG	BQ	202	1/1	0.30	-	37,37,37,37	0
52	MG	DA	3262	1/1	0.58	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3345	1/1	0.21	-	43,43,43,43	0
52	MG	DA	3301	1/1	0.18	-	15,15,15,15	0
52	MG	BA	3009	1/1	0.49	-	38,38,38,38	0
52	MG	BA	3185	1/1	0.20	-	45,45,45,45	0
52	MG	DA	3246	1/1	0.11	-	43,43,43,43	0
53	ZN	CD	301	1/1	0.27	-	107,107,107,107	0
52	MG	BA	3157	1/1	0.30	-	13,13,13,13	0
52	MG	BA	3026	1/1	0.24	-	45,45,45,45	0
52	MG	BA	3249	1/1	0.34	-	54,54,54,54	0
52	MG	BA	3280	1/1	0.33	-	41,41,41,41	0
52	MG	D5	101	1/1	0.40	-	30,30,30,30	0
52	MG	DA	3303	1/1	0.19	-	43,43,43,43	0
52	MG	DA	3188	1/1	0.58	-	43,43,43,43	0
52	MG	AA	1655	1/1	0.19	-	45,45,45,45	0
52	MG	DA	3308	1/1	0.13	-	43,43,43,43	0
52	MG	AA	1619	1/1	0.27	-	44,44,44,44	0
52	MG	DA	3274	1/1	0.40	-	71,71,71,71	0
52	MG	DA	3218	1/1	0.26	-	24,24,24,24	0
52	MG	BA	3349	1/1	0.73	-	65,65,65,65	0
52	MG	DA	3281	1/1	0.63	-	63,63,63,63	0
52	MG	DA	3019	1/1	0.54	-	25,25,25,25	0
52	MG	DA	3130	1/1	0.17	-	53,53,53,53	0
52	MG	BA	3281	1/1	0.23	-	41,41,41,41	0
52	MG	BA	3077	1/1	0.25	-	20,20,20,20	0
52	MG	BA	3250	1/1	0.52	-	48,48,48,48	0
52	MG	BB	207	1/1	0.20	-	58,58,58,58	0
52	MG	DA	3006	1/1	0.49	-	38,38,38,38	0
52	MG	BA	3192	1/1	0.27	-	17,17,17,17	0
52	MG	DA	3312	1/1	0.51	-	45,45,45,45	0
52	MG	CA	1632	1/1	0.17	-	56,56,56,56	0
52	MG	CA	1623	1/1	0.13	-	50,50,50,50	0
52	MG	BA	3233	1/1	0.22	-	20,20,20,20	0
52	MG	BA	3159	1/1	0.61	-	52,52,52,52	0
52	MG	DA	3288	1/1	0.18	-	42,42,42,42	0
52	MG	BA	3058	1/1	0.23	-	30,30,30,30	0
52	MG	AA	1639	1/1	0.35	-	48,48,48,48	0
52	MG	BA	3273	1/1	0.10	-	3,3,3,3	0
52	MG	BA	3102	1/1	0.35	-	38,38,38,38	0
52	MG	BA	3011	1/1	0.38	-	17,17,17,17	0
52	MG	BA	3141	1/1	0.14	-	47,47,47,47	0
52	MG	CA	1602	1/1	0.41	-	40,40,40,40	0
52	MG	BA	3028	1/1	0.41	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3086	1/1	0.17	-	34,34,34,34	0
52	MG	BA	3219	1/1	0.52	-	24,24,24,24	0
52	MG	DA	3214	1/1	0.35	-	39,39,39,39	0
52	MG	BA	3140	1/1	0.44	-	44,44,44,44	0
52	MG	DA	3103	1/1	0.46	-	33,33,33,33	0
52	MG	BA	3278	1/1	0.15	-	31,31,31,31	0
52	MG	CA	1612	1/1	0.30	-	48,48,48,48	0
52	MG	DF	301	1/1	0.33	-	53,53,53,53	0
52	MG	DA	3240	1/1	0.08	-	40,40,40,40	0
52	MG	DA	3070	1/1	0.22	-	35,35,35,35	0
52	MG	BA	3309	1/1	0.50	-	49,49,49,49	0
52	MG	BA	3291	1/1	0.13	-	54,54,54,54	0
52	MG	DA	3072	1/1	0.80	-	71,71,71,71	0
52	MG	BA	3257	1/1	0.17	-	35,35,35,35	0
52	MG	DB	201	1/1	0.35	-	57,57,57,57	0
52	MG	BA	3342	1/1	1.21	-	69,69,69,69	0
52	MG	BA	3074	1/1	0.49	-	48,48,48,48	0
52	MG	BA	3365	1/1	0.27	-	43,43,43,43	0
52	MG	DA	3192	1/1	0.58	-	36,36,36,36	0
52	MG	DA	3048	1/1	0.37	-	30,30,30,30	0
52	MG	BA	3164	1/1	0.28	-	33,33,33,33	0
52	MG	DA	3008	1/1	0.36	-	33,33,33,33	0
52	MG	BA	3326	1/1	0.32	-	40,40,40,40	0
52	MG	BA	3307	1/1	0.25	-	38,38,38,38	0
52	MG	DA	3202	1/1	0.46	-	46,46,46,46	0
52	MG	DB	204	1/1	0.39	-	37,37,37,37	0
52	MG	BA	3111	1/1	0.49	-	41,41,41,41	0
52	MG	BA	3253	1/1	0.22	-	17,17,17,17	0
52	MG	BA	3081	1/1	0.35	-	7,7,7,7	0
52	MG	BA	3318	1/1	0.34	-	34,34,34,34	0
52	MG	BA	3003	1/1	0.68	-	44,44,44,44	0
52	MG	AA	1628	1/1	0.60	-	70,70,70,70	0
52	MG	BA	3193	1/1	0.42	-	46,46,46,46	0
52	MG	DA	3204	1/1	0.19	-	42,42,42,42	0
52	MG	DA	3098	1/1	0.44	-	34,34,34,34	0
52	MG	DA	3156	1/1	0.32	-	51,51,51,51	0
52	MG	BA	3050	1/1	0.27	-	21,21,21,21	0
52	MG	BA	3016	1/1	0.29	-	11,11,11,11	0
52	MG	CA	1639	1/1	0.51	-	50,50,50,50	0
52	MG	BA	3027	1/1	0.44	-	25,25,25,25	0
52	MG	BA	3282	1/1	0.50	-	46,46,46,46	0
52	MG	BA	3006	1/1	0.55	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3108	1/1	0.16	-	31,31,31,31	0
52	MG	DA	3060	1/1	0.29	-	46,46,46,46	0
52	MG	DA	3269	1/1	0.14	-	61,61,61,61	0
52	MG	AA	1604	1/1	0.29	-	62,62,62,62	0
52	MG	DA	3210	1/1	0.20	-	46,46,46,46	0
52	MG	DA	3191	1/1	0.35	-	38,38,38,38	0
52	MG	DA	3219	1/1	0.29	-	25,25,25,25	0
52	MG	BA	3311	1/1	0.13	-	38,38,38,38	0
52	MG	DA	3242	1/1	0.19	-	35,35,35,35	0
52	MG	BA	3199	1/1	0.38	-	42,42,42,42	0
52	MG	DA	3332	1/1	0.14	-	69,69,69,69	0
52	MG	AA	1644	1/1	0.31	-	68,68,68,68	0
52	MG	BA	3173	1/1	0.22	-	50,50,50,50	0
52	MG	DA	3282	1/1	0.19	-	61,61,61,61	0
52	MG	DA	3249	1/1	0.17	-	48,48,48,48	0
52	MG	DA	3059	1/1	0.39	-	24,24,24,24	0
52	MG	DA	3295	1/1	0.55	-	73,73,73,73	0
52	MG	DA	3194	1/1	0.24	-	22,22,22,22	0
54	K	DA	3333	1/1	0.30	-	62,62,62,62	0
52	MG	BA	3214	1/1	0.20	-	23,23,23,23	0
53	ZN	AN	101	1/1	0.17	-	144,144,144,144	0
52	MG	BA	3347	1/1	0.37	-	47,47,47,47	0
52	MG	DP	201	1/1	0.12	-	19,19,19,19	0
52	MG	BA	3330	1/1	0.47	-	48,48,48,48	0
52	MG	DA	3082	1/1	0.38	-	44,44,44,44	0
52	MG	DA	3225	1/1	0.17	-	37,37,37,37	0
52	MG	BA	3005	1/1	0.30	-	26,26,26,26	0
52	MG	BA	3042	1/1	0.24	-	7,7,7,7	0
52	MG	BA	3169	1/1	0.31	-	33,33,33,33	0
52	MG	DA	3183	1/1	0.38	-	35,35,35,35	0
52	MG	DA	3315	1/1	0.19	-	43,43,43,43	0
52	MG	BA	3229	1/1	0.34	-	26,26,26,26	0
52	MG	DA	3305	1/1	0.84	-	46,46,46,46	0
52	MG	BA	3238	1/1	0.67	-	43,43,43,43	0
52	MG	DA	3292	1/1	0.23	-	52,52,52,52	0
52	MG	DA	3199	1/1	0.49	-	43,43,43,43	0
52	MG	BA	3105	1/1	0.45	-	19,19,19,19	0
52	MG	CA	1648	1/1	0.74	-	53,53,53,53	0
52	MG	BA	3069	1/1	0.21	-	26,26,26,26	0
52	MG	BA	3308	1/1	0.30	-	45,45,45,45	0
52	MG	DA	3102	1/1	0.47	-	24,24,24,24	0
52	MG	BA	3295	1/1	0.21	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3072	1/1	0.49	-	41,41,41,41	0
52	MG	DA	3228	1/1	0.17	-	38,38,38,38	0
52	MG	BA	3032	1/1	0.31	-	15,15,15,15	0
52	MG	BA	3024	1/1	0.29	-	20,20,20,20	0
52	MG	DA	3065	1/1	0.15	-	30,30,30,30	0
52	MG	BA	3353	1/1	0.10	-	31,31,31,31	0
52	MG	DA	3163	1/1	0.57	-	30,30,30,30	0
52	MG	BA	3070	1/1	0.28	-	24,24,24,24	0
52	MG	AA	1616	1/1	0.06	-	57,57,57,57	0
52	MG	AA	1605	1/1	0.34	-	71,71,71,71	0
52	MG	BA	3132	1/1	0.20	-	15,15,15,15	0
52	MG	DA	3290	1/1	0.35	-	55,55,55,55	0
52	MG	CA	1649	1/1	0.34	-	55,55,55,55	0
52	MG	DA	3287	1/1	1.01	-	61,61,61,61	0
52	MG	DA	3206	1/1	0.44	-	45,45,45,45	0
52	MG	DA	3055	1/1	0.39	-	34,34,34,34	0
52	MG	BA	3029	1/1	0.28	-	25,25,25,25	0
52	MG	DA	3139	1/1	0.68	-	43,43,43,43	0
52	MG	BA	3348	1/1	0.15	-	34,34,34,34	0
52	MG	BA	3279	1/1	0.26	-	39,39,39,39	0
52	MG	DA	3260	1/1	0.34	-	34,34,34,34	0
52	MG	CA	1651	1/1	0.59	-	51,51,51,51	0
52	MG	DA	3053	1/1	0.42	-	21,21,21,21	0
52	MG	DA	3132	1/1	0.74	-	53,53,53,53	0
52	MG	BA	3267	1/1	0.20	-	41,41,41,41	0
52	MG	DA	3014	1/1	0.31	-	71,71,71,71	0
52	MG	B5	101	1/1	0.34	-	28,28,28,28	0
52	MG	BA	3226	1/1	0.15	-	14,14,14,14	0
52	MG	DA	3247	1/1	0.14	-	37,37,37,37	0
52	MG	BA	3180	1/1	0.54	-	46,46,46,46	0
52	MG	DA	3145	1/1	0.47	-	40,40,40,40	0
52	MG	DA	3298	1/1	0.57	-	59,59,59,59	0
52	MG	BA	3064	1/1	0.44	-	41,41,41,41	0
52	MG	DA	3330	1/1	0.20	-	53,53,53,53	0
52	MG	DA	3046	1/1	0.37	-	34,34,34,34	0
52	MG	DA	3233	1/1	0.49	-	51,51,51,51	0
52	MG	BA	3252	1/1	0.19	-	50,50,50,50	0
52	MG	DA	3186	1/1	0.22	-	42,42,42,42	0
52	MG	DA	3120	1/1	0.19	-	36,36,36,36	0
52	MG	BA	3251	1/1	0.15	-	40,40,40,40	0
52	MG	BB	205	1/1	0.17	-	59,59,59,59	0
52	MG	DA	3069	1/1	0.22	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3086	1/1	0.32	-	27,27,27,27	0
52	MG	BA	3168	1/1	0.36	-	21,21,21,21	0
52	MG	CA	1610	1/1	0.24	-	66,66,66,66	0
52	MG	BA	3118	1/1	0.20	-	38,38,38,38	0
52	MG	BA	3246	1/1	0.29	-	40,40,40,40	0
52	MG	BA	3355	1/1	0.60	-	51,51,51,51	0
52	MG	AA	1638	1/1	0.44	-	69,69,69,69	0
52	MG	BA	3113	1/1	0.19	-	26,26,26,26	0
52	MG	DA	3063	1/1	0.29	-	38,38,38,38	0
52	MG	BR	202	1/1	0.55	-	31,31,31,31	0
52	MG	BA	3182	1/1	0.43	-	37,37,37,37	0
52	MG	DA	3143	1/1	0.23	-	40,40,40,40	0
52	MG	BA	3195	1/1	0.33	-	49,49,49,49	0
52	MG	BA	3244	1/1	0.26	-	50,50,50,50	0
52	MG	AA	1648	1/1	1.16	-	80,80,80,80	0
52	MG	DA	3280	1/1	0.38	-	70,70,70,70	0
52	MG	AA	1636	1/1	0.43	-	47,47,47,47	0
52	MG	BB	206	1/1	0.65	-	48,48,48,48	0
52	MG	BA	3056	1/1	0.13	-	20,20,20,20	0
52	MG	D5	102	1/1	0.46	-	58,58,58,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.