



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 08:23 PM BST

PDB ID : 4V7Z
Title : Structure of the *Thermus thermophilus* 70S ribosome complexed with telithromycin.
Authors : Bulkley, D.P.; Innis, C.A.; Blaha, G.; Steitz, T.A.
Deposited on : 2010-08-18
Resolution : 3.10 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>

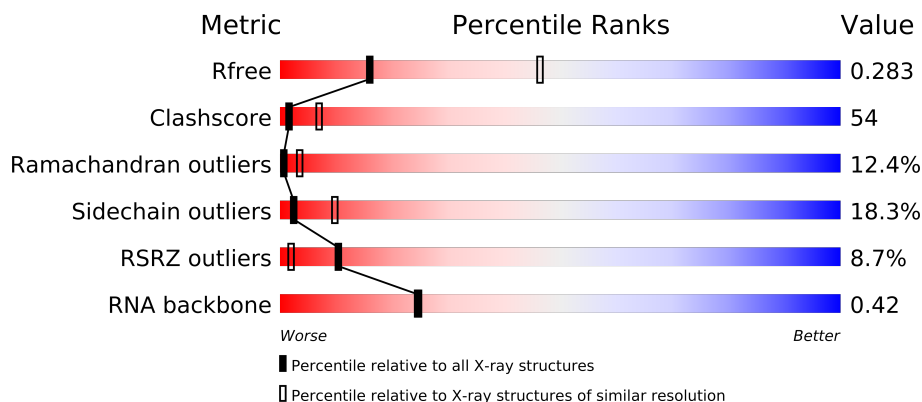
The following versions of software and data (see [references](#)) were used in the production of this report:

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

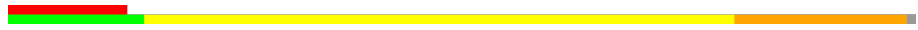
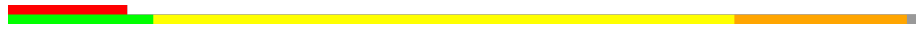
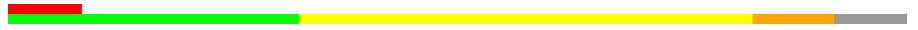
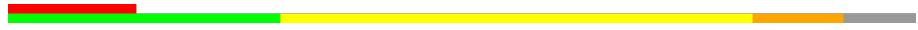
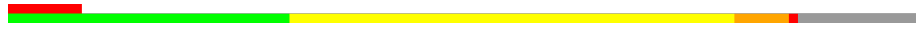
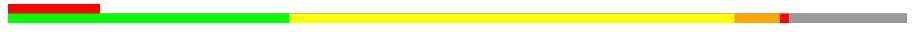
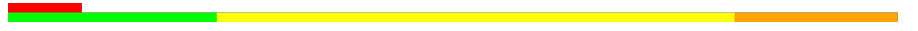





The reported resolution of this entry is 3.10 Å.

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	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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	

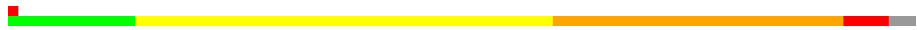
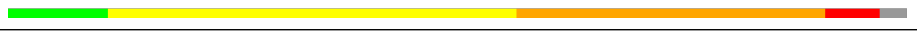
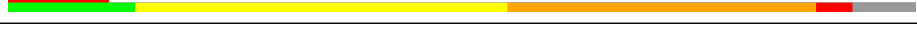

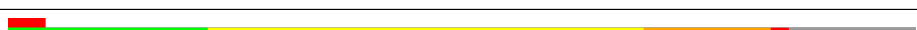

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Mol	Chain	Length	Quality of chain
28	B6	54	
28	D6	54	
29	B7	49	
29	D7	49	
30	B8	65	
30	D8	65	
31	BA	2787	
31	DA	2787	
32	BB	122	
32	DB	122	
33	BD	276	
33	DD	276	
34	BE	206	
34	DE	206	
35	BF	210	
35	DF	210	
36	BG	182	
36	DG	182	
37	BH	180	
37	DH	180	
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 278037 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	9	0	0
			459	288	90	76	5			
27	D5	59	Total	C	N	O	S	9	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	360	Total	Mg	0	0
			360	360		
52	CA	50	Total	Mg	0	0
			50	50		
52	DQ	1	Total	Mg	0	0
			1	1		
52	DF	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	3	Total	Mg	0	0
			3	3		
52	DR	2	Total	Mg	0	0
			2	2		
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	D8	1	Total	Mg	0	0
			1	1		
52	AA	52	Total	Mg	0	0
			52	52		
52	BQ	2	Total	Mg	0	0
			2	2		
52	D7	1	Total	Mg	0	0
			1	1		
52	BU	1	Total	Mg	0	0
			1	1		
52	DD	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	BR	1	Total 1	Mg 1	0	0
52	DA	318	Total 318	Mg 318	0	0
52	B7	1	Total 1	Mg 1	0	0
52	DE	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	1	Total 1	Mg 1	0	0
52	BD	2	Total 2	Mg 2	0	0
52	B0	1	Total 1	Mg 1	0	0
52	DB	3	Total 3	Mg 3	0	0

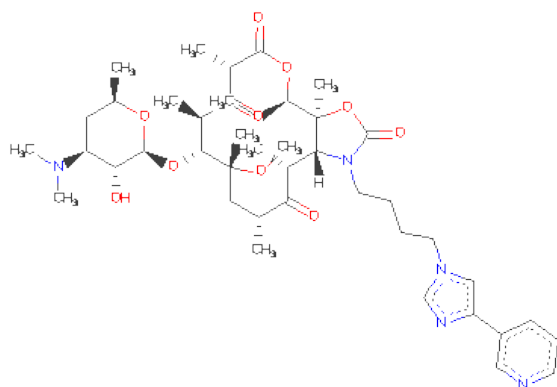
- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

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 TELITHROMYCIN (three-letter code: TEL) (formula: C₄₃H₆₅N₅O₁₀).

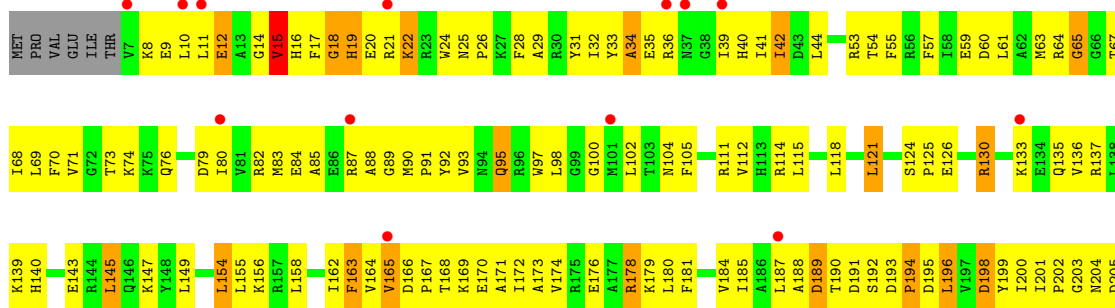


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	BA	1	Total	C	N	O	0	0
			58	43	5	10		
55	DA	1	Total	C	N	O	0	0
			58	43	5	10		

G1505	G1437	A1377	C1317	U1196	C1128	G1068	C1006	G947	C882	A814	A753	U692
U1506	G1438	C1378	C1320	G1197	C1129	C1069	U1012	C948	C883	A815	C754	G693
A1507	C1439	U1379	C1321	G1198	A1130	U1070	G1013	A949	U884	A816	G755	A694
G1508	C1440	U1380	C1322	U1199	G1131	C1071	A1014	U950	C885	C817	G756	A695
C1509	G1441	U1381	C1323	C1200	C1132	G1072	A1015	G951	G889	A819	U757	A696
U1510	G1442	C1382	C1324	A1201	G1133	U1073	A1016	U952	G890	U820	G758	U697
G1511	G1442A	C1383	A1324	C1202	G1134	G1074	G1017	G953	U891	G821	G759	G698
A1512	A1442B	C1384	C1325	C1203	U1135	C1075	G1018	G954	G892	C822	G760	C699
U1513	G1443	G1385	G1326	A1204	U1136	C1076	C1019	U955	A894	C823	G761	G700
C1514	G1444	G1386	C1327	U1205	C1137	G1077	U1020	U956	G893	C824	G762	C701
G1515	U1446	G1387	C1328	G1206	G1138	U1078	U1020	U957	G894	G825	G763	A702
C1516	A1447	C1388	A1329	C1207	G1139	G1079	G1023	A958	G895	G826	G764	G703
U1517	G1452	U1330	U1330	C1208	G1140	A1080	G1024	A959	G896	C827	G765	A704
A1518	G1456	G1331	G1331	G1209	G1142	G1081	U1025	U960	C897	U827	A766	U705
U1519	G1457	A1332	A1332	G1210	G1143	U1082	G1026	U961	A900	A828	A767	A706
G1520	U1460	C1333	C1333	U1211	G1146	U1083	U1027	U962	A901	G829	A768	C707
U1521	G1461	G1334	G1334	U1212	A1147	U1084	C1028	G963	A902	G830	A769	G708
U1522	G1462	C1335	C1335	A1213	G1147	U1085	C1029	A964	G903	U831	C770	G709
G1523	G1463	A1336	C1336	C1214	U1148	U1086	C1030	A965	G906	C832	G771	G710
C1524	A1396	G1337	G1337	G1215	G1149	U1087	G1030A	G966	G907	U833	U772	G711
U1527	C1464	U1338	A1339	G1216	U1150	G1088	C1030B	A967	A907	C834	G773	A712
U1528	C1465	A1339	A1339	C1217	A1151	G1089	G1030C	A968	A908	U835	G774	G713
G1529	C1466	C1340	A1340	C1218	A1152	U1090	A1030D	A969	A909	G836	G775	G714
U1530	G1467	U1341	U1341	U1219	G1153	U1091	G1031	A970	A910	G837	G776	A715
A1531	A1468	C1342	C1342	G1220	G1154	A1092	G1032	G971	C910	G838	A777	A716
U	G1469	G1343	G1343	G1221	G1155	A1093	G1033	C972	U911	U839	G778	C717
C	G1470	C1344	C1344	G1222	G1156	U1094	U1034	G973	C912	C840	C779	G718
C	G1471	U1345	U1345	C1223	A1157	U1095	G1035	A974	A913	G841	A780	C719
A	U1472	A1346	A1346	G1224	C1158	C1096	A1036	A975	A914	C842	A781	C720
C	A1473	G1347	A1347	A1225	U1159	C1097	G1036	G976	A915	U843	A782	G721
C	G1474	U1348	U1348	C1226	G1160	U1098	C1037	A977	G916	G851	C783	A722
U	U1408	A1349	A1349	A1227	C1161	G1099	C1038	A978	G917	G852	C784	U723
C	C1409	A1350	A1350	C1228	C1162	C1100	U1039	C979	A918	G853	G785	G724
C	G1478	U1351	U1351	G1229	C1163	A1101	A1040	C980	A919	G854	G786	G725
U	C1479	C1352	C1352	A1230	G1164	A1102	A1041	U981	U920	G855	A787	C726
U	G1480	G1353	G1353	G1231	C1165	C1103	U1044	U982	U921	C856	U788	G727
U	U1481	C1354	C1354	U1232	G1166	G1104	A1045	A983	G922	C857	U789	A728
C	G1482	G1355	G1355	G1233	A1168	A1105	C1046	C984	A923	G858	A790	A729
C	A1483	G1356	G1356	C1234	A1169	G1106	A1047	C985	C924	A859	G791	G730
U	U1484	A1357	A1357	U1235	A1170	C1107	G1048	A986	G925	A860	U792	G731
U	G1485	U1358	U1358	C1236	G1171	G1108	U1049	G987	G926	C861	U793	C732
U	G1486	C1359	C1359	G1237	C1172	C1109	U1050	G988	G927	C862	A794	A733
U	G1487	A1360	A1360	A1238	G1173	A1110	G1051	C989	C930	U863	G734	G734
U	G1488	G1361	G1361	U1239	G1174	A1111	C1052	C990	C931	A864	C735	C735
U	G1489	C1362	C1362	U1240	G1175	C1112	U1053	U991	C932	A865	C736	C736
U	C1490	A1363	A1363	G1241	A1176	C1113	G1054	U992	G933	C868	G799	C737
U	G1491	U1364	U1364	C1242	C1179	C1114	A1055	A993	C934	G869	G800	C738
U	A1492	G1365	G1365	C1243	A1180	C1115	U1056	A994	C935	U870	U801	C739
U	U1425	A1366	A1366	A1244	G1181	C1116	G1057	C995	A936	A802	U802	U740
U	G1494	C1367	C1367	C1245	G1182	C1117	G1058	A996	C937	U871	G803	G741
U	U1495	U1368	U1368	U1246	G1183	C1118	C1059	U997	A938	A872	U804	G742
U	G1496	A1369	A1369	U1247	A1184	C1119	G1060	G998	A939	A873	C805	C745
U	G1497	C1370	C1370	C1249	G1185	U1120	G1061	C999	G939	G874	C806	A746
U	U1498	G1371	G1371	A1250	G1186	U1121	U1062	U1000	C940	C875	A807	A746
U	A1499	A1372	A1372	A1251	C1189	U1122	U1063	G941	C941	G876	C808	C747
U	C1500	G1373	G1373	A1252	G1190	A1123	G1064	A1001	G942	C877	G809	C748
U	A1501	A1374	A1374	C1253	G1191	U1125	U1065	G943	U943	G878	C810	C749
U	A1502	A1375	A1375	U1254	G1192	U1126	C1066	G944	G944	C879	C811	G750
U	G1504	U1376	U1376	G1255	A1191	G1127	A1067	A1005	A946	C880	C812	U751

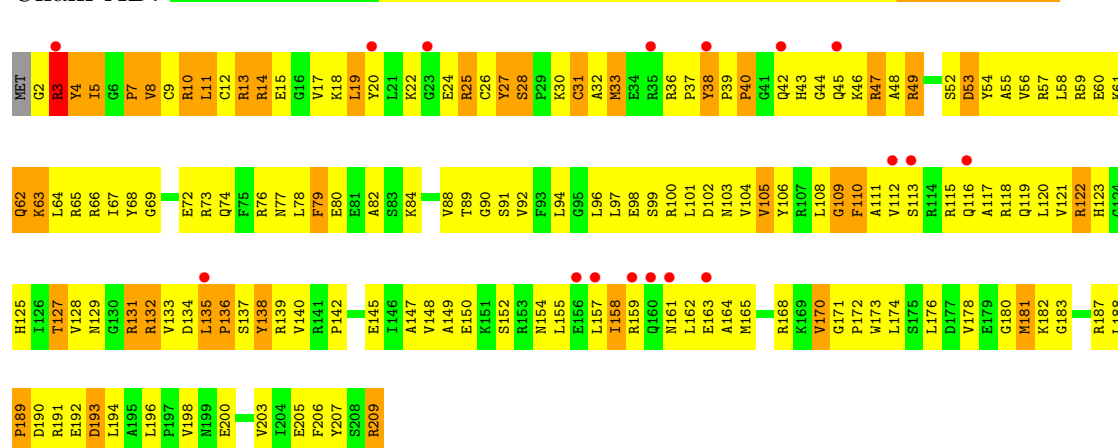
• Molecule 1: 16S rRNA

C882	C883	A814	U751	C889	C829	G568	G505	A431	C370	C307	A246	C187	A60
C883	U884	A815	G752	G890	G630	C569	A509	A432	G371	C308	G247	C188	G61
C885	U889	A816	G755	U692	A632	G570	A510	C433	C372	G309	U129	C189	U62
A889	U889	C817	C754	G693	A633	A571	C511	U434	A373		A250	C189A	C63
		G818	G756	A694	C534	A573	C513	C435	A374	C312	U252	C190	G64
A892	C893	A819	U757	A895	G635	A574	C514	C436	U375	A313	U253	C190C	U65
C892	C894	U820	G758	A896	U636	G575	C514	U437	G376	C314	U254	C190E	G66
G895	G895	G821	A759		G576	G577	G515	A439	G377	A315	G255	U189E	G67
		C822	G760	G638	U516	A441	U516	A441	C378	G316	U256	G189F	G68
C896	C897	G825	G761	G700	G639	C578	C518	C442	G380	C320	G257	G189H	G69
C897		C826	G762	A701	A640	G579	C518	C443	C381	A321	G258	G189I	G70
		U827	G763	A702	U641	U580	C519	C444	A382	C322	G259	G189J	G71
A900	A901	A828	G764	G703	A642	G581	A520	G445	A383	U323	G260	G189K	G72
A902	G903	A829	A766	A704	G644	U582	G521	G446	G384	G324	U261	U190	G73
C904	C904	U831	A767	A706	C645	A584	C522	G447	C385	A325	A262	G191	G74
U905	U905	C832	G768	C707	U646	G585	G524	C449	U387	A327	U264	U192	G75
		U833	G769	G647	C586	G525	G524	G450	G388	C328	G265	C193	G76
C906	C907	U834	C770	G709	A648	G587	C526	A451	A389	A329	G266	C194	G77
A907	A908	C835	G771	G710	G649	U588	G527	A452	C390	C330	C267	U195	G78
A909	A910	U836	U772	G711	G650	C589	C528	A453	G391	G331	C268	U196	G79
C910	C911	C837	G773	A712	C651	C590	G529	G448	G392	G332	C269	U197	G80
U911	U912	G838	G774	G713	U652	U591	G530	A448	A393	G333	A270	U198	G81
C912	C913	U839	G775	G714	A653	G592	U531	C449	G394	C334	C271	G199	G82
A914	A915	C840	G776	A715	G654	G593	A532	A458	C395	C335	C272	U200	G83
G916	G917	U841	U777	A716	A655	G594	A533	C460	G396	C336	C273	G201	G84
C918	C919	C848	C778	G717	G656	C595	U534	A461	A397	C337	A274	U202	G85
C920	C921	U851	G779	U718	G657	C596	A535	C470	C398	A338	G275	U203	G86
C922	C923	A852	A780	C720	U659	G597	C536	A472	G400	C339	G276	U204	G87
C924	C925	C853	U781	G721	G660	U598	G537	C473	C401	C341	G278	G216	G88
C926	C927	U854	A782	A722	G661	C599	G538	G474	G402	C342	A279	C217	G89
C928	C929	C854	C783	U723	G662	C601	A539	G475	C403	U343	C280	C218	G90
C930	C931	C855	G784	A663	G663	A602	G540	G476	U404	A344	G281	G219	G91
C932	C933	U857	G785	G725	G664	U603	G542	A477	U405	C345	A282	G220	G92
C934	C935	C857	C856	C726	A665	G604	C543	C479	G406	G346	C283	U222	G93
C936	C937	U858	U788	G727	G666	U605	G544	U480	G407	C347	G284	U223	G94
C938	C939	A859	U789										



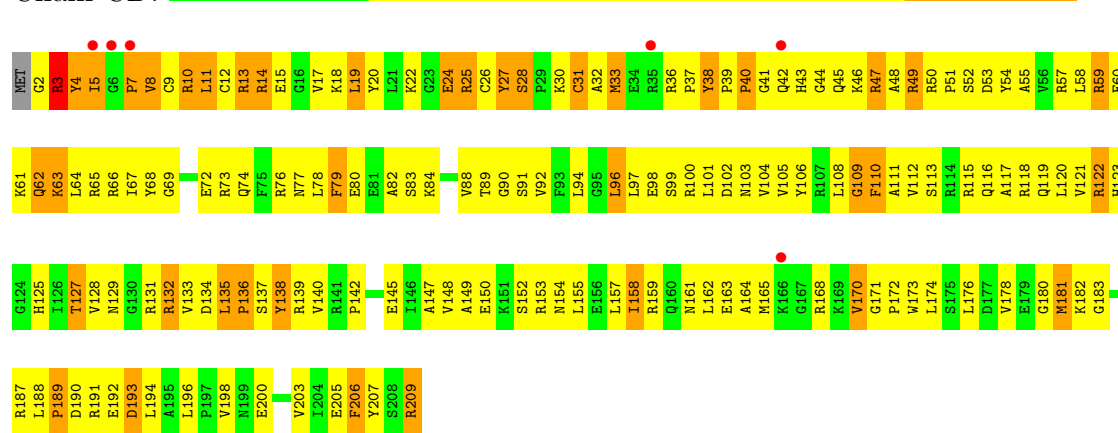
- Molecule 4: 30S ribosomal protein S4

Chain AD:



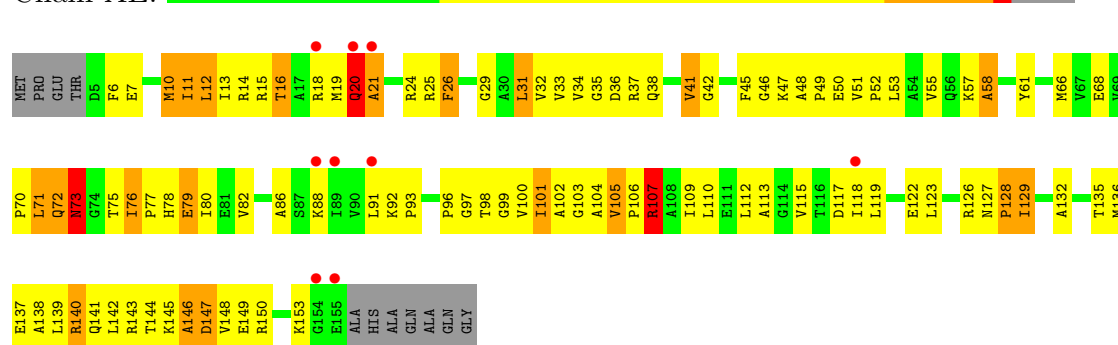
- Molecule 4: 30S ribosomal protein S4

Chain CD:



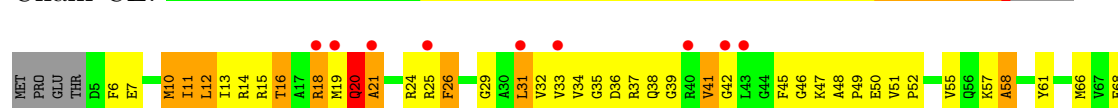
- Molecule 5: 30S ribosomal protein S5

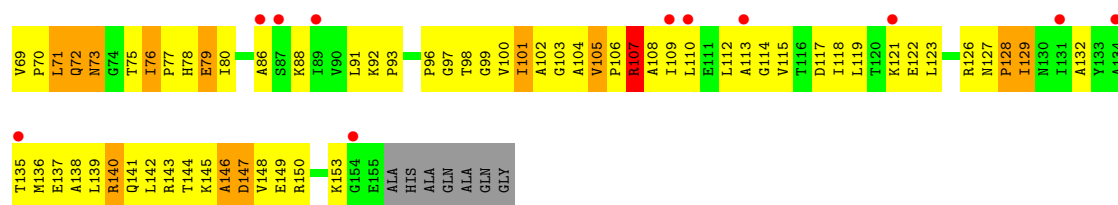
Chain AE:



- Molecule 5: 30S ribosomal protein S5

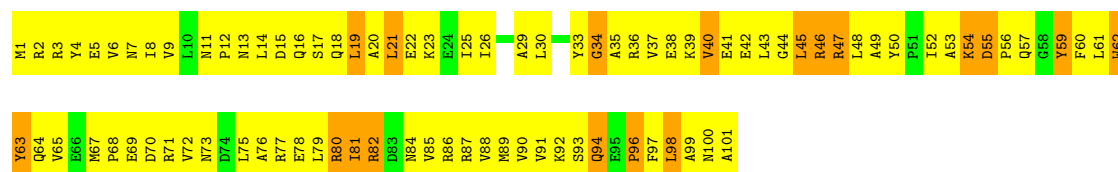
Chain CE:





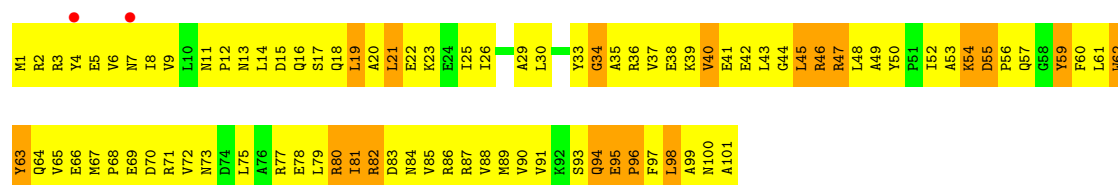
• Molecule 6: 30S ribosomal protein S6

Chain AF:



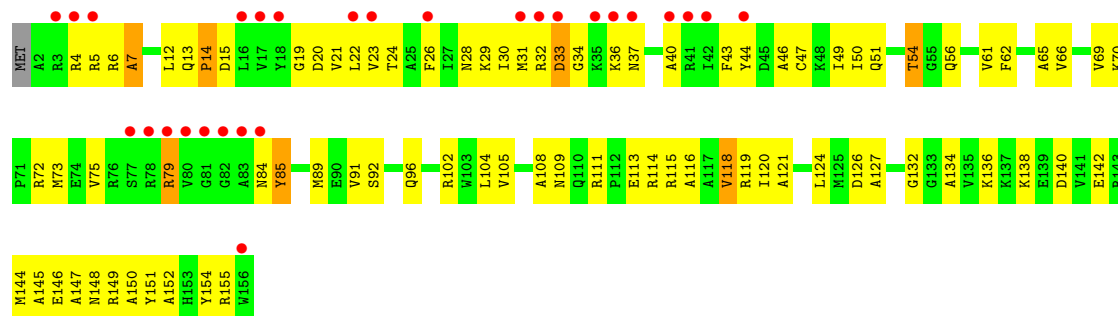
• Molecule 6: 30S ribosomal protein S6

Chain CF:



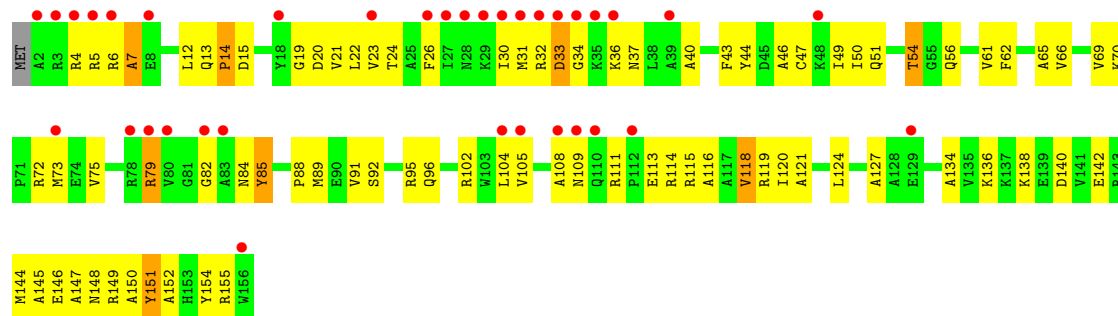
• Molecule 7: 30S ribosomal protein S7

Chain AG:



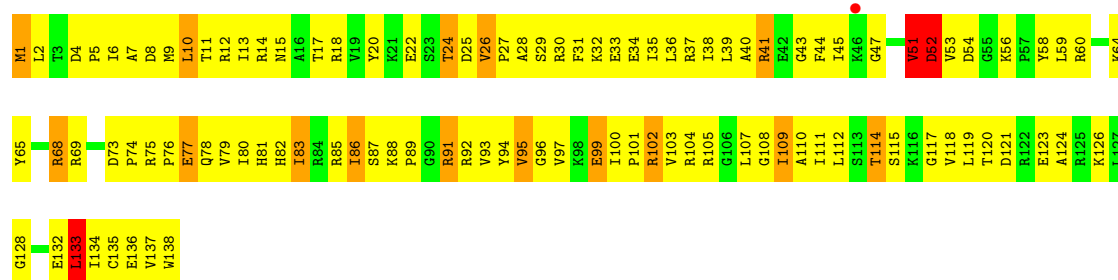
• Molecule 7: 30S ribosomal protein S7

Chain CG:



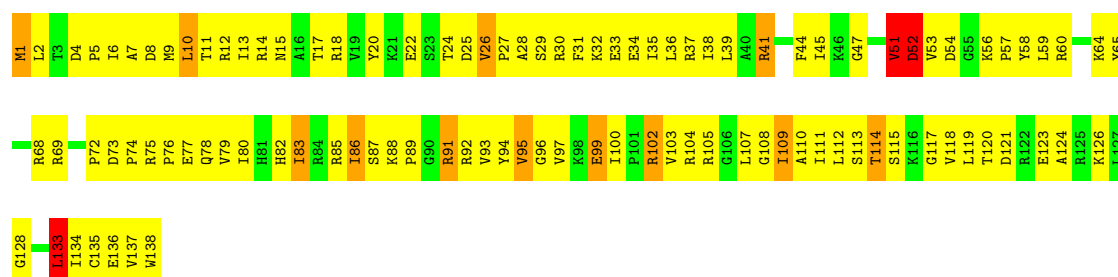
- Molecule 8: 30S ribosomal protein S8

Chain AH:



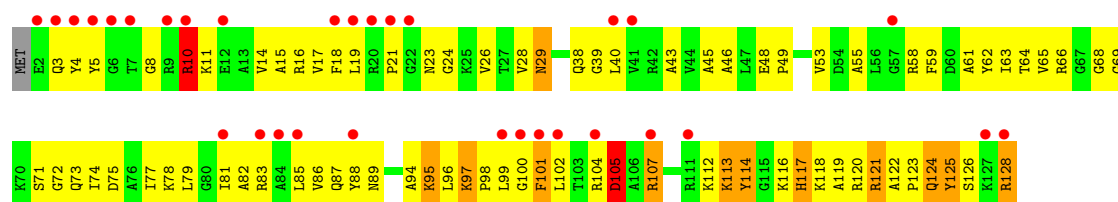
- Molecule 8: 30S ribosomal protein S8

Chain CH:



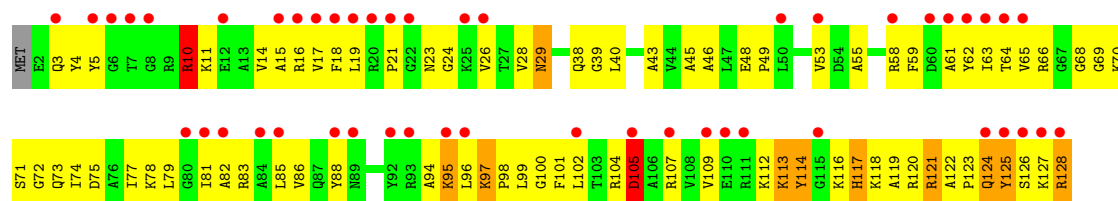
- Molecule 9: 30S ribosomal protein S9

Chain AI:



- Molecule 9: 30S ribosomal protein S9

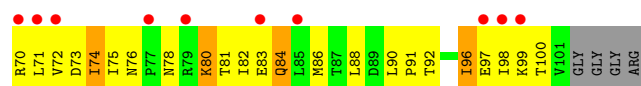
Chain CI:



- Molecule 10: 30S ribosomal protein S10

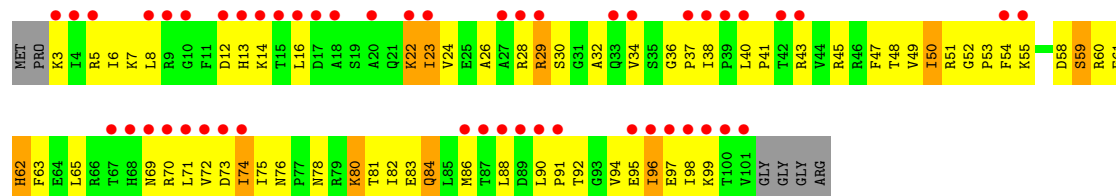
Chain AJ:





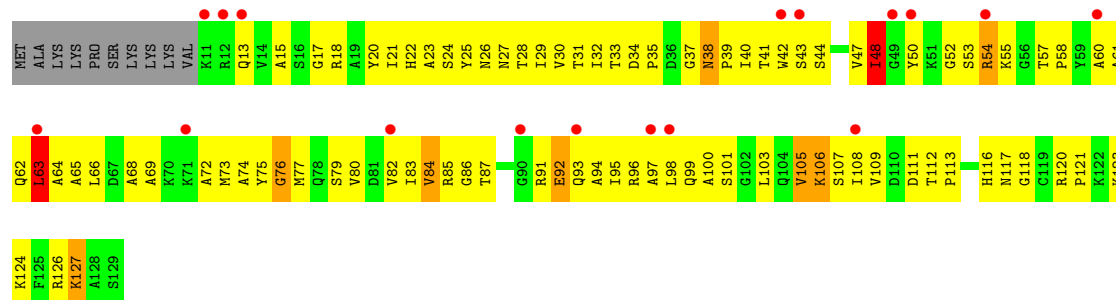
- Molecule 10: 30S ribosomal protein S10

Chain CJ:



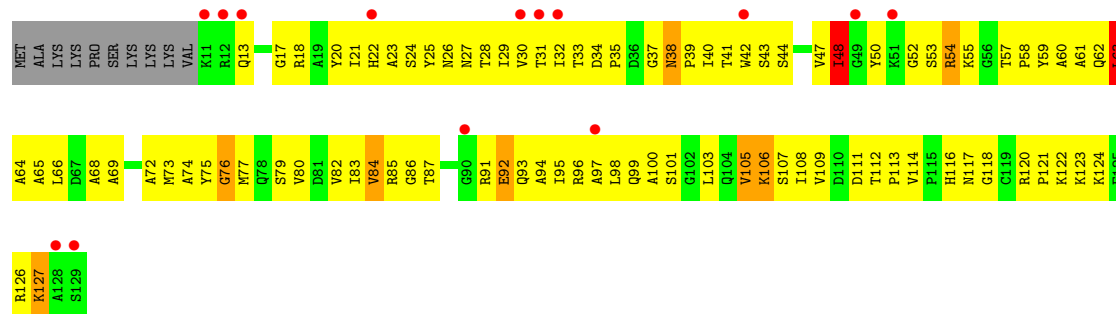
- Molecule 11: 30S ribosomal protein S11

Chain AK:



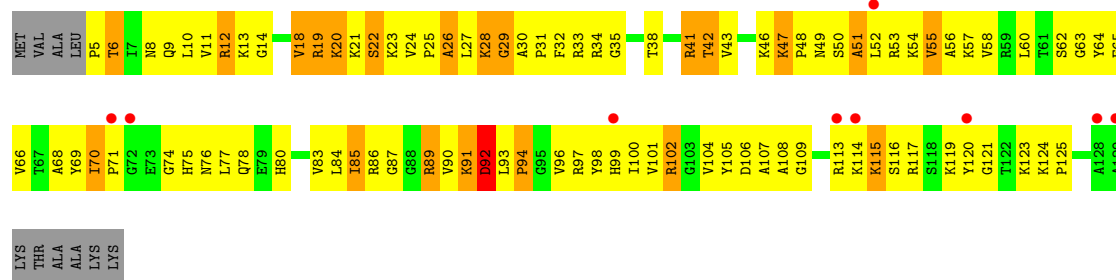
- Molecule 11: 30S ribosomal protein S11

Chain CK:



- Molecule 12: 30S ribosomal protein S12

Chain AL:



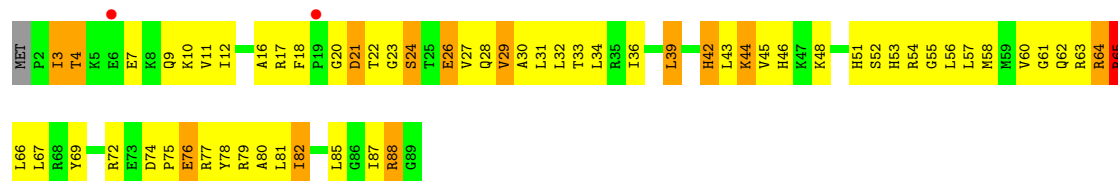
- Chain CL:





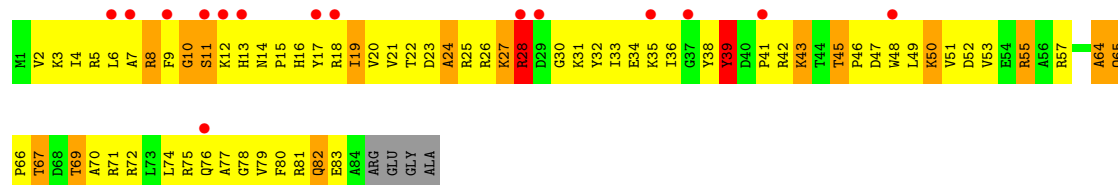
• Molecule 15: 30S ribosomal protein S15

Chain CO:



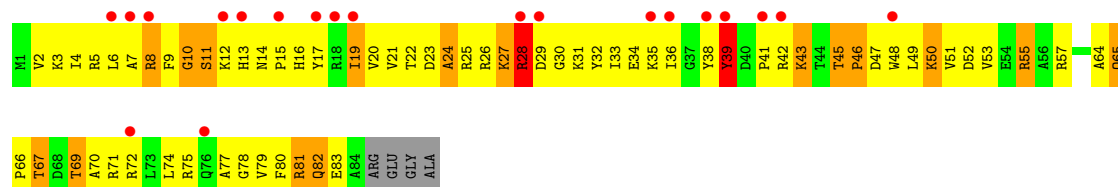
• Molecule 16: 30S ribosomal protein S16

Chain AP:



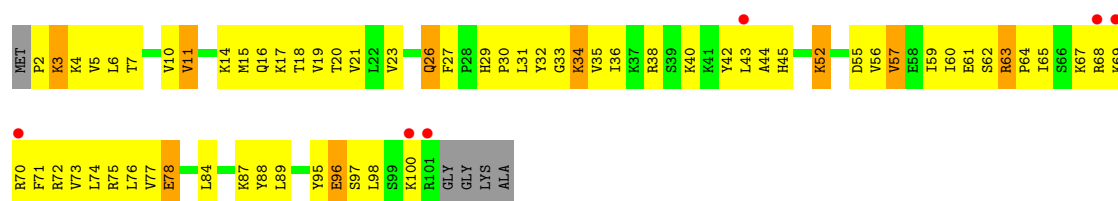
• Molecule 16: 30S ribosomal protein S16

Chain CP:



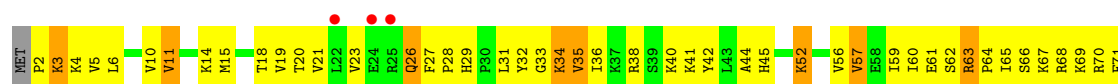
• Molecule 17: 30S ribosomal protein S17

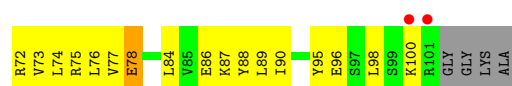
Chain AQ:



• Molecule 17: 30S ribosomal protein S17

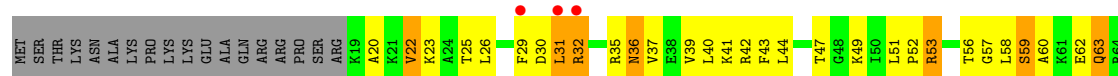
Chain CQ:





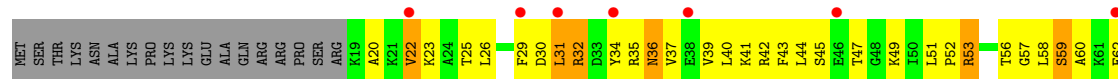
• Molecule 18: 30S ribosomal protein S18

Chain AR:



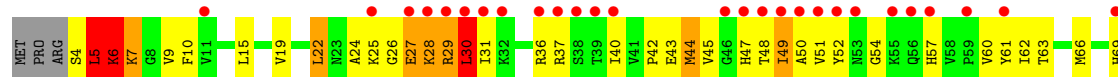
• Molecule 18: 30S ribosomal protein S18

Chain CR:



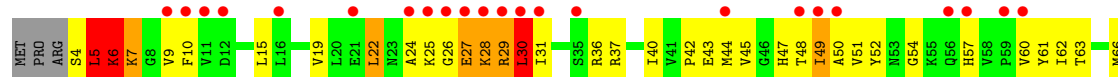
• Molecule 19: 30S ribosomal protein S19

Chain AS:



• Molecule 19: 30S ribosomal protein S19

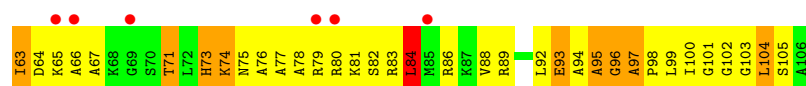
Chain CS:



• Molecule 20: 30S ribosomal protein S20

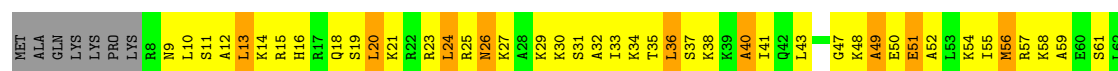
Chain AT:





- Molecule 20: 30S ribosomal protein S20

Chain CT:



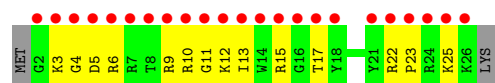
- Molecule 21: 30S ribosomal protein Thx

Chain AU:



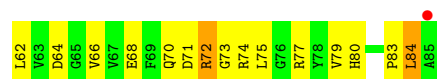
- Molecule 21: 30S ribosomal protein Thx

Chain CU:



- Molecule 22: 50S ribosomal protein L27

Chain B0:



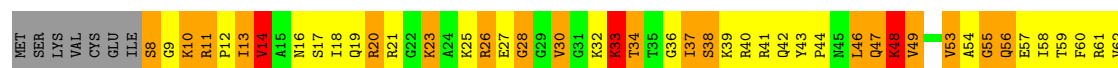
- Molecule 22: 50S ribosomal protein L27

Chain D0:



- Molecule 23: 50S ribosomal protein L28

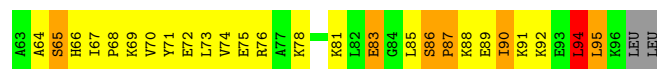
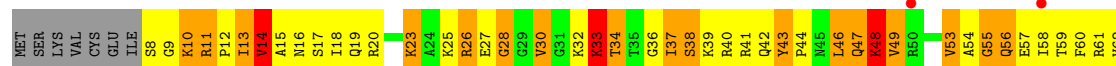
Chain B1:





- Molecule 23: 50S ribosomal protein L28

Chain D1:



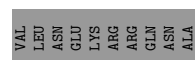
- Molecule 24: 50S ribosomal protein L29

Chain B2:



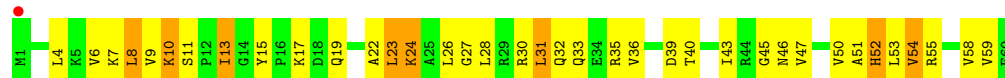
- Molecule 24: 50S ribosomal protein L29

Chain D2:



- Molecule 25: 50S ribosomal protein L30

Chain B3:



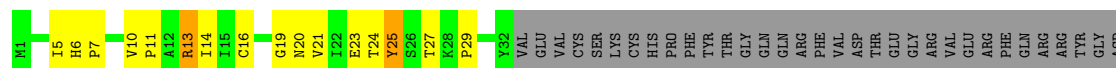
- Molecule 25: 50S ribosomal protein L30

Chain D3:



- Molecule 26: 50S ribosomal protein L31

Chain B4:



SER
TYR
ARG
LYS
GLY
ARG

- Molecule 26: 50S ribosomal protein L31

Chain D4:

M1 K2 E3 G4 I5 H6 P7 K8 L9 V10 P11 A12 R13 I14 I15 C16 G19 N20 V21 T22 E23 T24 Y25 S26 T27 T28 K29 P29 E30 I31 V32 VAL GLU VAL CYS SER LYS CYS HIS PRO PHE THR GLY GLN ARG PHE VAL ASP THR GLU GLY ARG VAL GLN ARG PHE ARG

ARG
TYR
GLY
ASP
SER
ARG
LYS
GLY
ARG

- Molecule 27: 50S ribosomal protein L32

Chain B5:

MET A2 K3 H4 P5 V6 P7 K8 K9 T10 K11 T11 S12 K13 R16 D17 A18 R19 R20 S21 H22 H23 A24 L25 T26 T29 L30 V31 P32 C33 P34 E35 C36 K37 A38 M39 K40 P41 P42 H43 T44 V45 C46 P47 E48 C49 G50 Y51 Y52 A53 G54 R55 K56 V57 L58 E59 V60

- Molecule 27: 50S ribosomal protein L32

Chain D5:

MET A2 K3 H4 P5 V6 P7 K8 K9 T10 K11 T11 S12 K13 R16 D17 A18 R19 R20 S21 H22 H23 A24 L25 T26 T29 L30 V31 P32 C33 P34 E35 C36 K37 A38 M39 K40 P41 P42 H43 T44 V45 C46 P47 E48 C49 G50 Y51 Y52 A53 G54 R55 K56 V57 L58 E59 V60

- Molecule 28: 50S ribosomal protein L33

Chain B6:

MET ALA SER GLU VAL ARG ILE LYS L9 L10 L11 E12 C13 T14 E15 K17 R18 R19 N20 Y21 A22 T23 E24 K25 N26 T27 R28 N29 T30 P31 N32 K33 L34 E35 L36 R37 K38 Y39 C40 P41 W42 C43 R44 K45 H46 T47 V48 H49 R50 E51 V52 K53 ILE

- Molecule 28: 50S ribosomal protein L33

Chain D6:

MET ALA SER GLU VAL ARG ILE LYS L9 L10 L11 E12 C13 T14 E15 K17 R18 R19 N20 Y21 A22 T23 E24 K25 N26 T27 R28 N29 T30 P31 N32 K33 L34 E35 L36 R37 K38 Y39 C40 P41 W42 C43 R44 K45 H46 T47 V48 H49 R50 E51 V52 K53 ILE

- Molecule 29: 50S ribosomal protein L34

Chain B7:

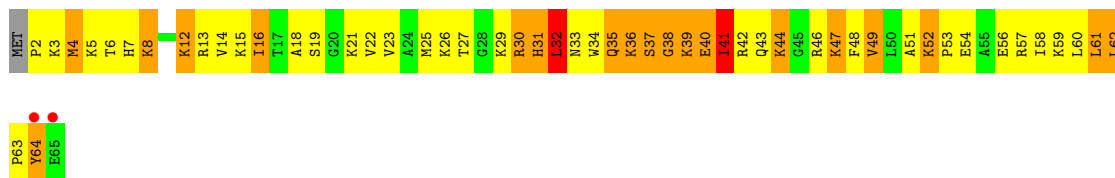
K1 K2 W5 Q6 P7 N8 R9 R10 K11 R12 A13 K14 T15 H16 G17 F18 R19 R22 R23 T24 P25 G26 G27 R28 V30 L31 K32 K33 R34 K37 G38 R39 W40 L42 T43 P44 R47 K48 R49

- Molecule 29: 50S ribosomal protein L34

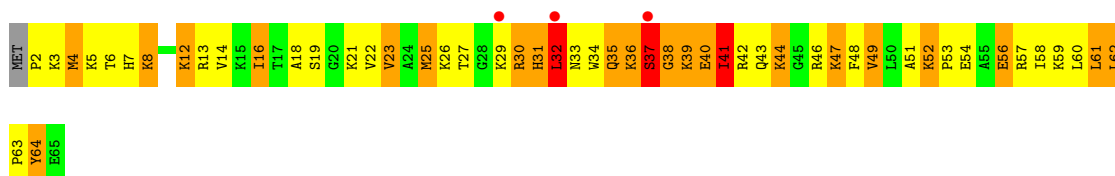
Chain D7:

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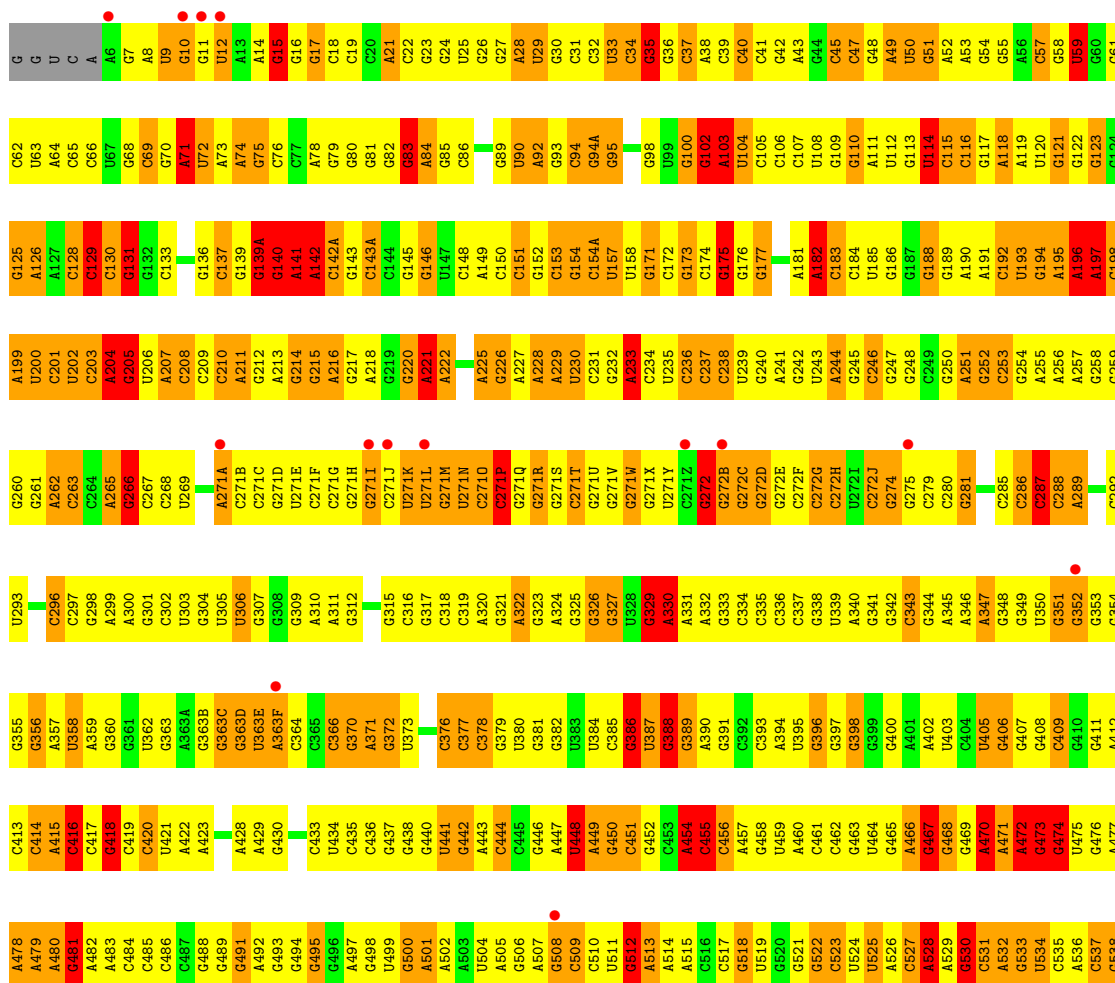
- Chain B8:



- Chain D8:



- Chain BA:



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G1456	A1396	U1334	A1213	C1152	C1038	G978	A918	U851	C791	C731	G668	G605	C541
U1457	U1397	U1335	A1214	C1153	G1039	G979	A919	G852	C792	C732	G669	U606	C542
C1458	C1398	U1336	G1215	G1154	C1040	A980	G920	G853	A794	C734	A670	U607	C543
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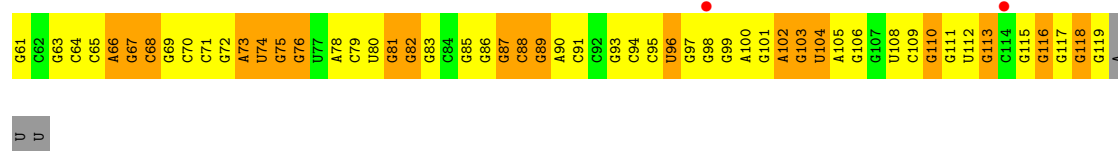
WORLDWIDE
PDB
PROTEIN DATA BANK



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G1355	C1234	G1174	U1112	A1000	U941	G873	U813	A752	G689	G625	U566	A502	G440
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G1373	C1251	G1192	U1130	G1016	A957	A896	A829	G768	A705	G541	G583	U519	C456
C1374	G1252	A1193	G1131	G1017	U958	C897	G830	G769	A706	G642	C584	G520	A457
G1375	A1253	U1194	U1132	U1018	A959	C898	G831	G770	G707	A643	G585	G521	U459
C1376	C1254	G1195	U1133	U1019	A960	A899	G832	G771	C645	A644	A586	G522	A460
U1377	U1255	C1196	C1135	A1020	C961	A900	U833	G772	U709	G646	U588	C523	C461
G1378	G1256	G1197	G1136	A1021	G962	A901	C834	U773	G710	A646	C589	U524	G462
A1379	C1257	U1198	U1137	G1022	U963	C902	A835	A774	G711	G647	G590	U525	G463
G1380	U1258	U1199	G1138	U1023	C964	C903	G836	G775	G712	G648	A591	A526	U464
C1381	G1259	G1199	U1139	G1024	C965	C904	C837	G776	G591	G649	C591	C527	G465
G1382	C1260	C1200	G1139	G1025	G966	U905	C838	A777	G592	C650	G592	A528	A466
C1383	C1261	C1201	C1140	U1026	C967	G906	U839	G778	G651	A718	G593	A529	G467
A1384	U1262	C1202	U1141	A1027	G968	U907	C840	U779	U594	C652	U594	G530	G468
G1385	G1263	G1203	U1142	A1028	U969	C908	A841	G780	C595	U657	C595	C531	G469
C1386	U1264	A1204	A1142A	A1029	C970	A909	G842	A781	G596	U657	U597	A532	A470
U1387	G1265	U1205	A1143	G1030	C971	A910	G843	A782	G597	C658	G533	A471	G470
G1388	G1266	C1206	G1144	U1031	G972	A911	C844	A783	G723	C659	G599	A472	A472
C1327	U1267	C1207	C1145	A1032	A973	C912	G845	A784	U724	G660	G599		

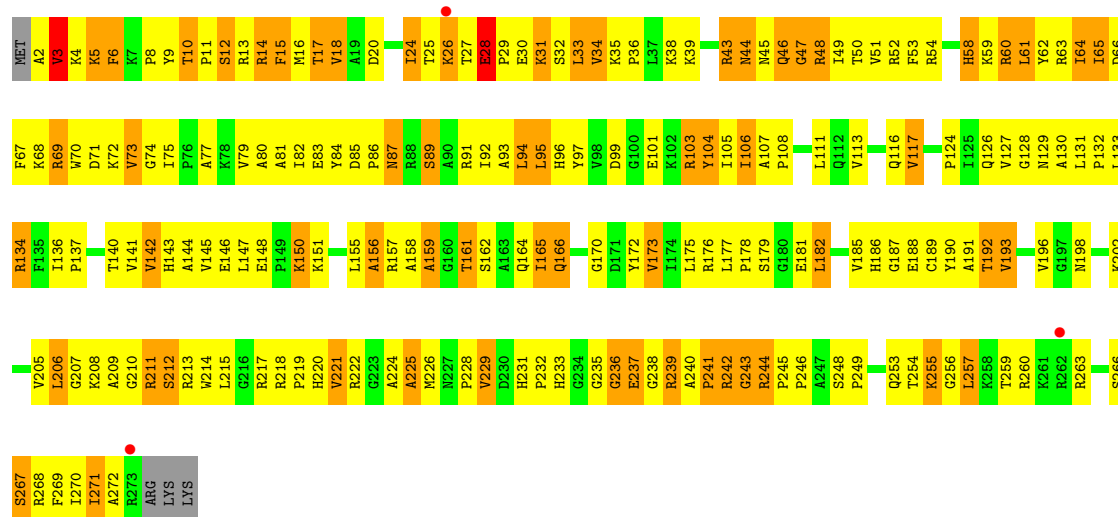
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C2314	G2250	U	U2091	A2031	A1969	C1837	U1777	A1701	A1579	A1509A	A1449	U1390
G2315	G2251	G	U2092	G2032	A1970	G1838	U1778	G1702	G1642	A1509B	G1450	U1391
G2316	G2252	G	G2093	A2033	A1971	G1839	U1779	G1703	G1643	G1500	G1450A	A1392
G2317	G2253		G2094	A2034	A1972		A1780	G1704	G1644	C1511	C1451	A1393
G2318			C2095	G2035	A1973		C1781	G1705	G1645	U1512	A1452	U1394
G2319			U2096	C2036	C1974		C1782	U1706	C1846	C1513	U1453	A1395
A2320	U2257		C2097	G2037	C1975		A1783	G1707	A1845	U1514	U1456	U1396
G2321	G2258		U2098	G2038	U1976		A1784	G1708	A1846	G1515	G1456	U1397
G2322	G2259		G2099	G2039	A1977		A1785	U1709	G1648	A1587	G1457	C1398
G2323	C2261		G2100	C2040	A1978		A1786	G1710	G1649	C1588	A1457	C1399
G2324	U2262		G2101	A2041			A1787	G1711	G1650	C1589	G1458	G1400
G2325	C2263		U2102	A2042	A1981		C1788	C1712	G1651	U1590	G1459	G1401
G2326	G2264		C2103	C2043	C1982		A1789	U1713	A1852	G1591	A1460	G1402
G2327	U2265		G2104	C2044	C1983		U1790	G1714	C1853	C1592	G1461	C1403
A2328	U2266		C2105	C2045	C1984		C1790	G1717	A1854	G1593	C1462	C1404
G2329	A2267		G2106	G2046	G1987		A1791	G1718	A1855	G1594	G1463	U1405
G2330	A2268			U2047	G1988		C1792	G1719	G1856	G1595	G1464	U1406
G2331	A2269			G2048	C1989		G1793	U1720	A1857	A1596	G1465	G1407
U2332	G2270			G2049	G1990		U1794	G1721	G1858	A1597	G1466	C1408
A2333	G2271			C2050	A1992		C1795	A1722	U1859	C1598	G1467	C1409
G2334	U2272			G2051	U1991		U1796	G1723	G1888	G1599	G1468	C1408
A2335	A2273			G2052	G1992		C1797	U1739	G1889	C1600	A1469	G1410
A2336	A2274			G2053	U1993		U1798	G1740	G1890	C1601	G1470	C1411
G2337	C2275			U2054	G1994		G1799	A1741	C1663	U1602	A1471	A1412
G2338	G2276			C2055	U1995		G1800	G1742	A1664	G1532	A1472	G1413
G2339	G2277			G2056	C1996		G1801	C1743	A1665	G1533	A1473	G1414
G2340	A2278			A2057	G1997		A1802	C1744	G1666	C1534	G1474	U1415
G2341	G2279			G2058	C1998		A1803	C1745	G1667	A1544	G1475	A1416
G2342	U2280			A2059	G1999		A1804	G1746	A1668	A1545	G1476	C1417
G2343	G2281			G2060	A2000		U1805	A1746	A1669	G1546	A1477	G1418
G2344	G2282			C2061	A2001		A1806	G1747	A1670	C1547	G1478	A1419
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A2346	G2284			C2063	G2003		U1808	G1748	C1672	C1549	G1480	G1421
G2347	C2285			G2064	A1940		A1809	U1749	G1673	C1550	G1481	G1422
U2348	A2286			C2065	C1941		A1810	G1750	G1674	C1551	G1482	G1423
G2349	A2287			G2066	C1942		G1811	C1751	A1675	A1552	G1483	G1424
G2350	A2288			G2067	U1943		A1812	G1752	A1676	A1553	G1484	G1425
G2351	G2289			C2068	U1944		G1813	G1753	A1677	A1554	G1485	G1426
	G2290			U2069	G1945		G1814	C1754	C1678	G1555	A1486	G1427
G2354	U2291			C2070	U1946		A1815	A1755	A1618	C1556	G1487	A1428
G2355	C2292			G2071	C1947		G1816	G1756	U1679	C1557	G1488	C1429
C2356	C2293			G2072	G1948		U1757	G1757	U1680	A1558	U1489	G1430
				G2073	G1949		U1817	G1758	G1681	G1559	A1490	U1431
G2358	C2297			C2074	G1950		A1818	A1759	G1682	G1560	G1491	G1432
A2359	G2298			C2075	U1951		U1820	A1760	G1683	G1561	G1492	U1433
G2360	G2299			U2076	A1952		A1821	C1761	C1684	C1562	C1493	U1434
G2361	G2300			A2077	C1953		G1822	A1762	C1685	G1563	A1494	A1435
C2362	C2301			C2078	G1954		G1823	G1763	C1686	C1564	A1495	G1436
G2363	G2302			U2079	U1955		G1824	G1764	G1687	C1565	A1496	G1437
G2364	G2303			C2080	U1956		A1825	C1765	U1688	A1566	U1497	U1438
G2365	A2304			G2081	C1957		G1826	U1766	A1689	G1567	C1498	A1439
A2366	C2305			C2082	C1958		U1827	C1767	C1690	G1568	C1499	A1440
G2367	C2306			U2083	G1959		G1828	U1768	A1631A	A1569	G1500	G1441
G2368	G2307			G2084	U1960		A1829	G1769	A1632	A1570	C1501	G1442
G2369	U2308			C2085	A1901		C1830	G1770	U1692	A1571	C1502	G1443
A2370	G2309			U2086	G1902		G1831	C1771	G1693	A1572	U1503	G1444
G2371	A2310			G2087	G1903		C1832	G1772	G1694	G1573	G1504	G1445
G2372	C2311			U2088	G1904		U1833	C1773	G1695	C1574	C1505	A1446
G2373	U2312			C2089	C1905		G1906	U1775	A1697	C1575	C1506	C1445A
				U2099	C1966		C1967		A1698	U1576	A1507	G1447





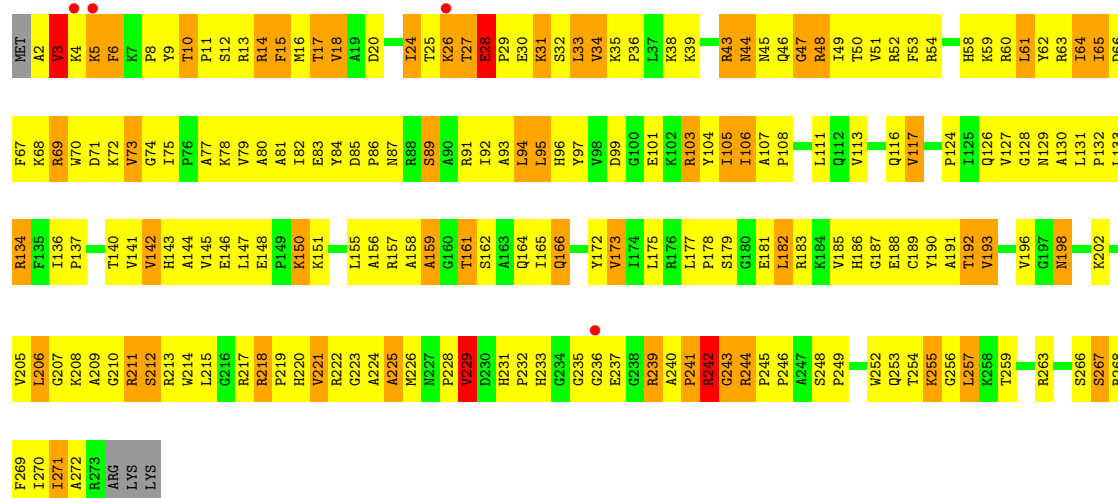
• Molecule 33: 50S ribosomal protein L2

Chain BD:



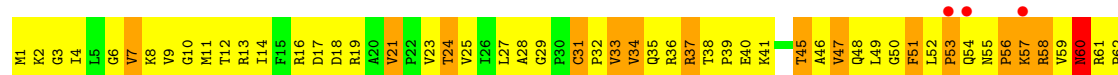
• Molecule 33: 50S ribosomal protein L2

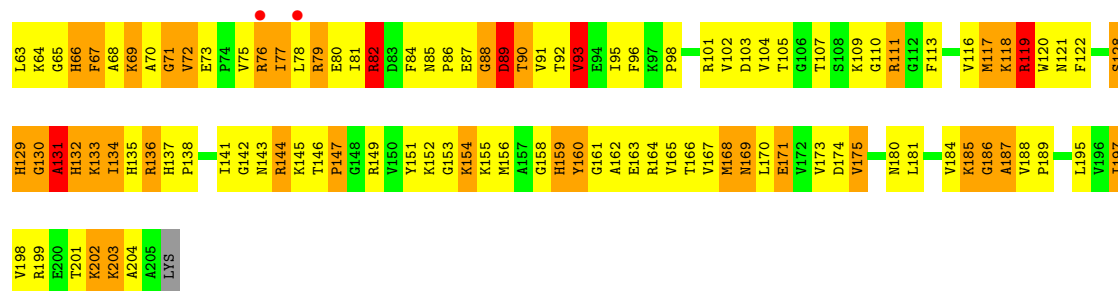
Chain DD:



• Molecule 34: 50S ribosomal protein L3

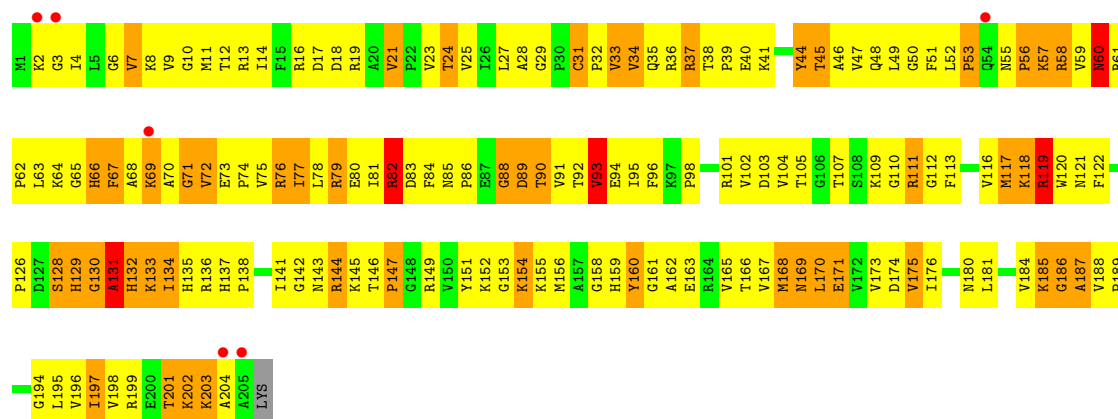
Chain BE:





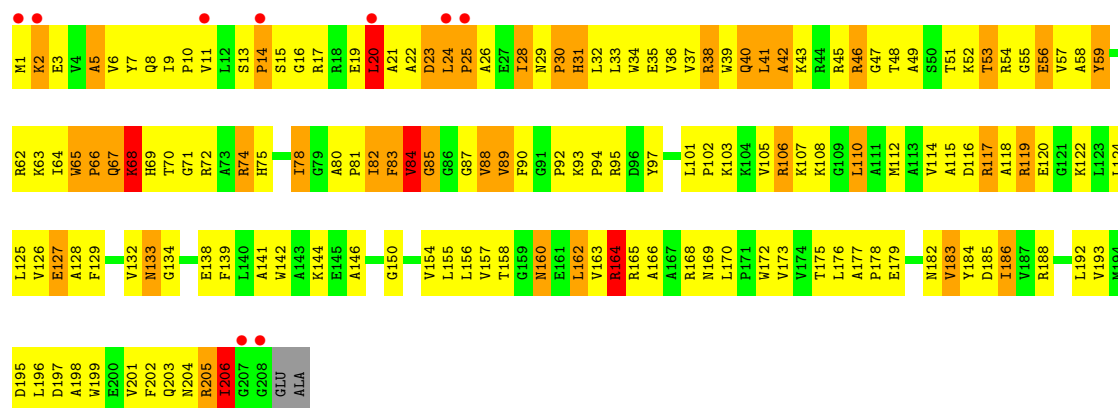
• Molecule 34: 50S ribosomal protein L3

Chain DE:



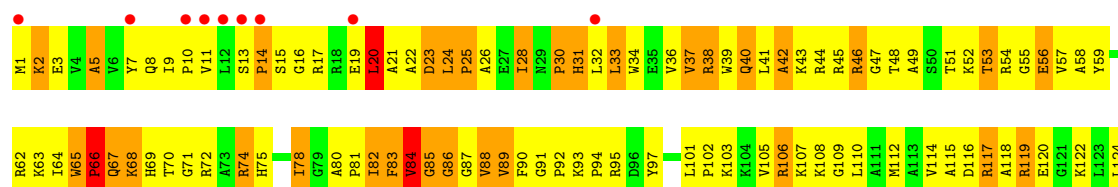
• Molecule 35: 50S ribosomal protein L4

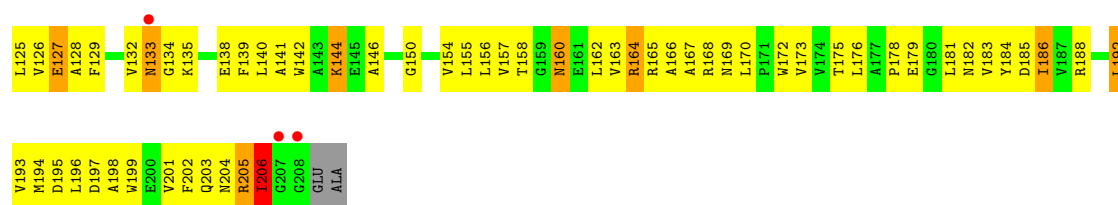
Chain BF:



• Molecule 35: 50S ribosomal protein L4

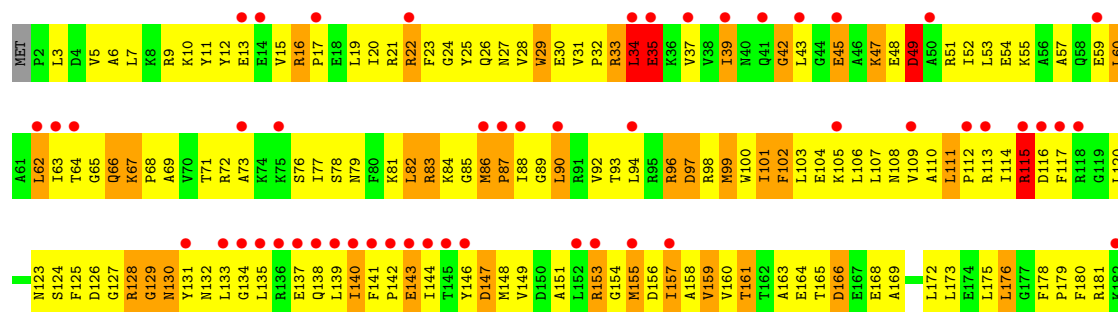
Chain DF:





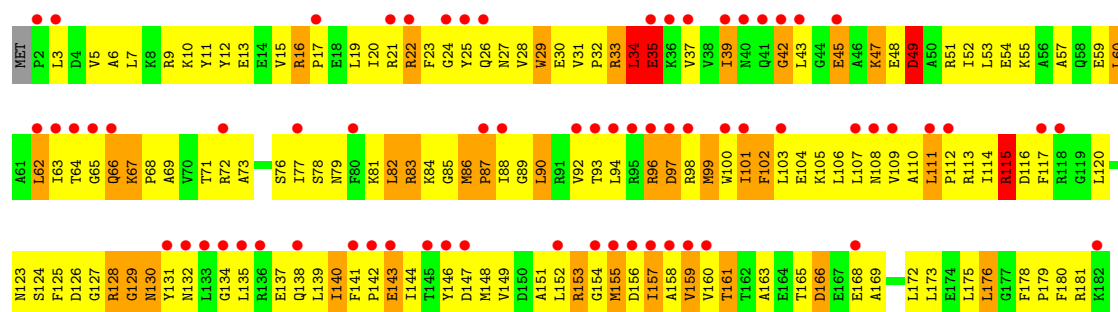
• Molecule 36: 50S ribosomal protein L5

Chain BG:



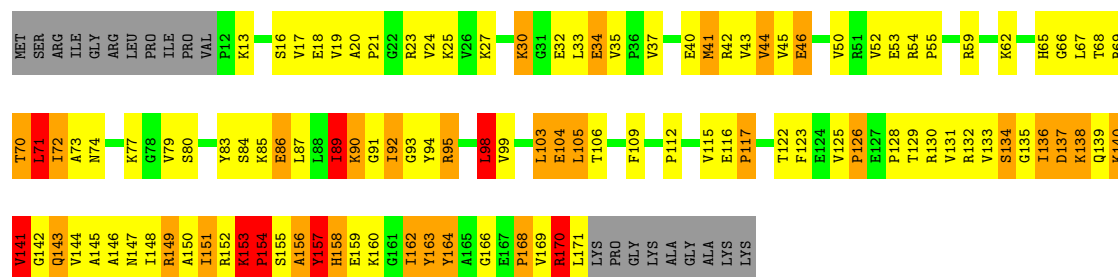
• Molecule 36: 50S ribosomal protein L5

Chain DG:



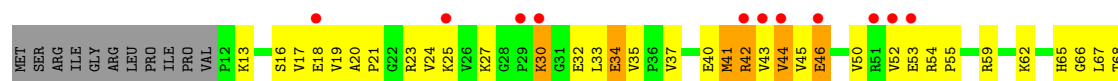
• Molecule 37: 50S ribosomal protein L6

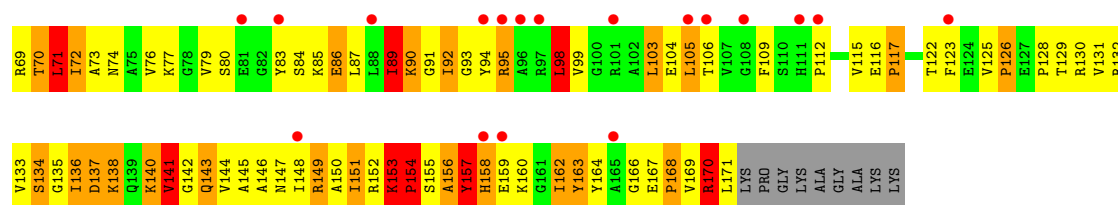
Chain BH:



• Molecule 37: 50S ribosomal protein L6

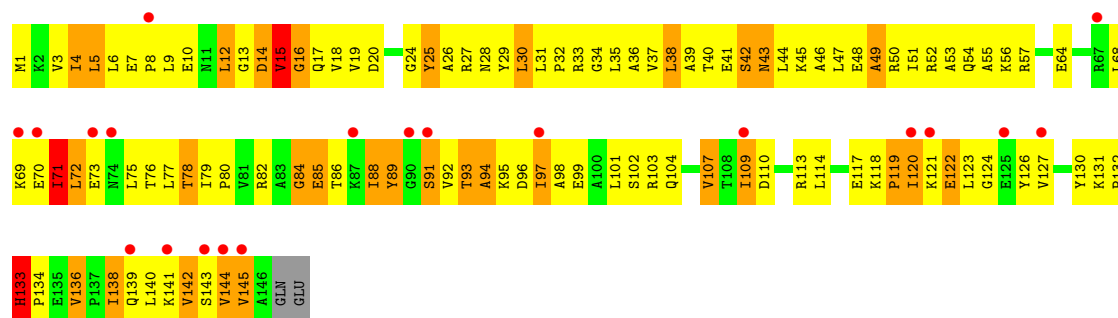
Chain DH:





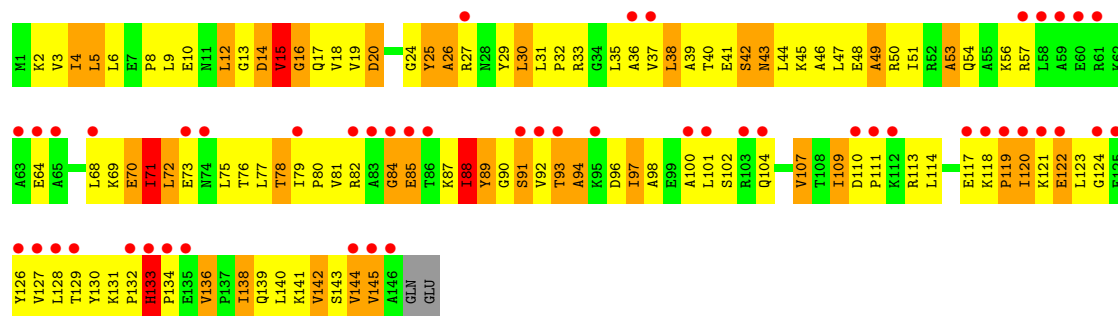
• Molecule 38: 50S ribosomal protein L9

Chain BI:



• Molecule 38: 50S ribosomal protein L9

Chain DI:



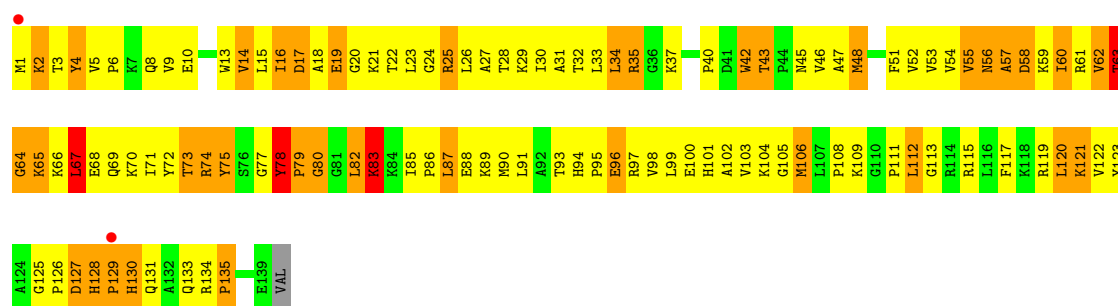
• Molecule 39: 50S ribosomal protein L13

Chain BN:



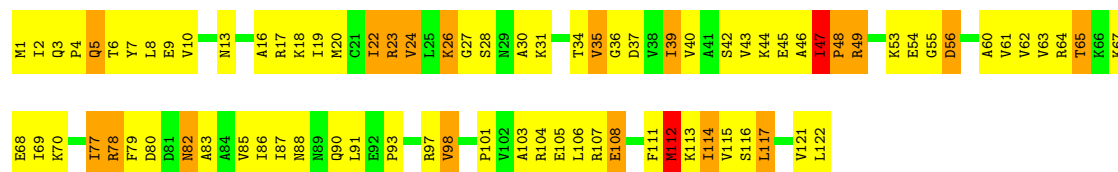
• Molecule 39: 50S ribosomal protein L13

Chain DN:



- Molecule 40: 50S ribosomal protein L14

Chain BO:



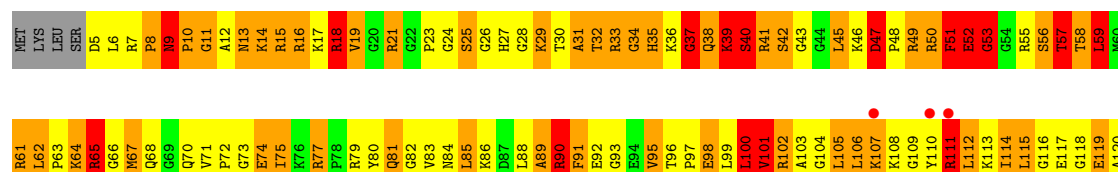
- Molecule 40: 50S ribosomal protein L14

Chain DO:



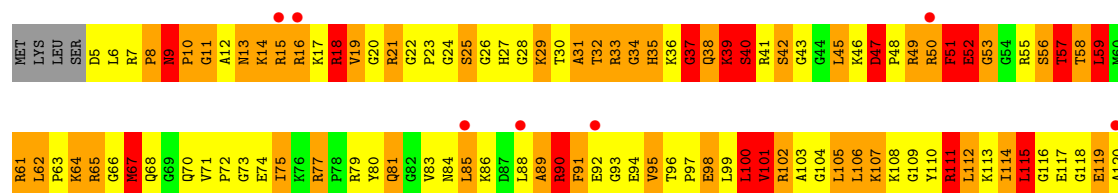
- Molecule 41: 50S ribosomal protein L15

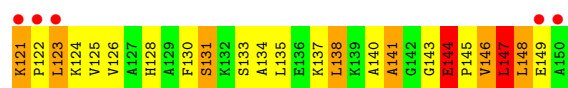
Chain BP:



- Molecule 41: 50S ribosomal protein L15

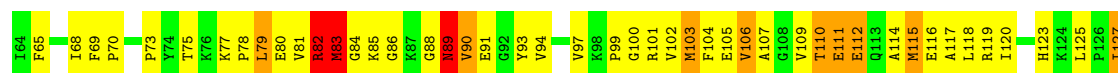
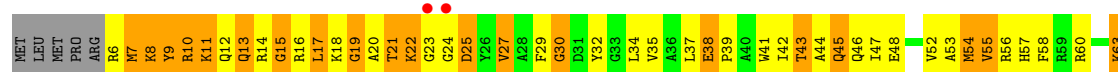
Chain DP:





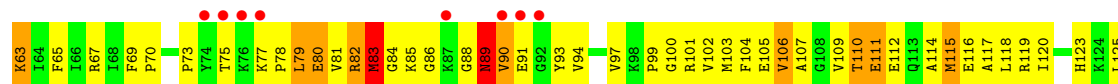
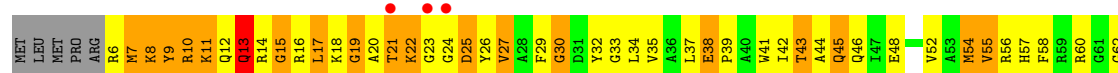
- Molecule 42: 50S ribosomal protein L16

Chain BQ:



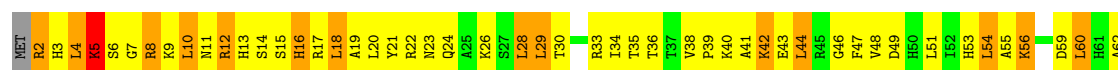
- Molecule 42: 50S ribosomal protein L16

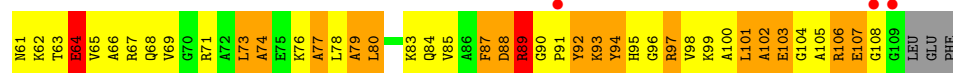
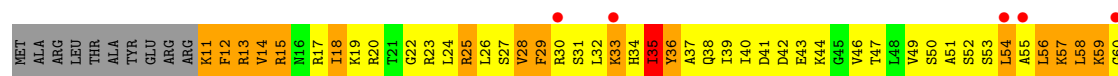
Chain DQ:



- Molecule 43: 50S ribosomal protein L17

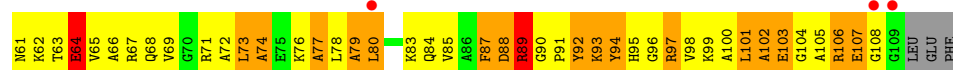
Chain BR:





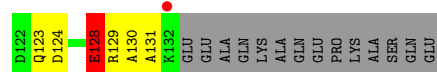
• Molecule 44: 50S ribosomal protein L18

Chain DS:



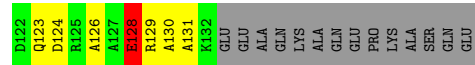
• Molecule 45: 50S ribosomal protein L19

Chain BT:



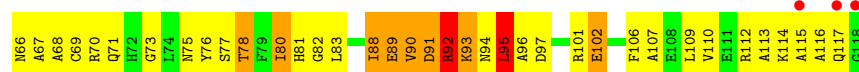
• Molecule 45: 50S ribosomal protein L19

Chain DT:



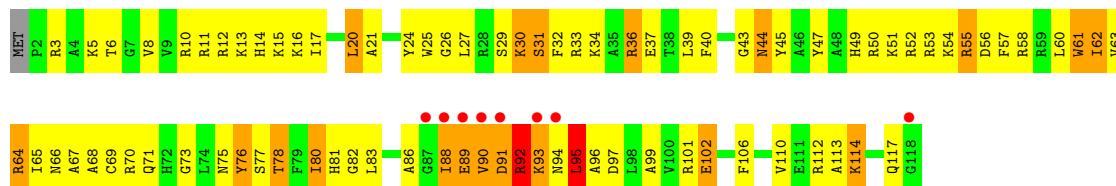
• Molecule 46: 50S ribosomal protein L20

Chain BU:



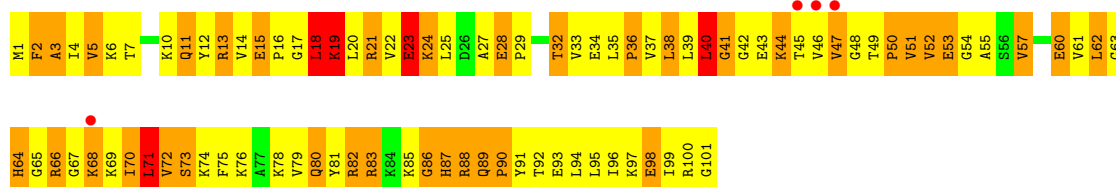
- Molecule 46: 50S ribosomal protein L20

Chain DU:



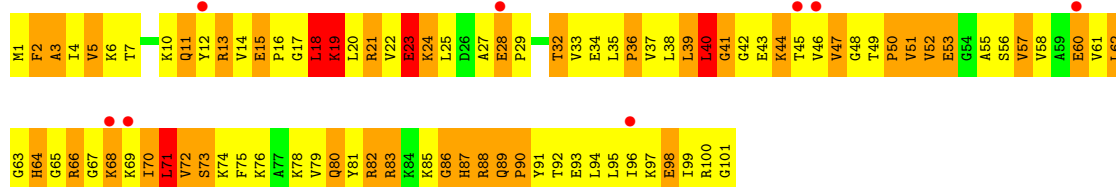
- Molecule 47: 50S ribosomal protein L21

Chain BV:



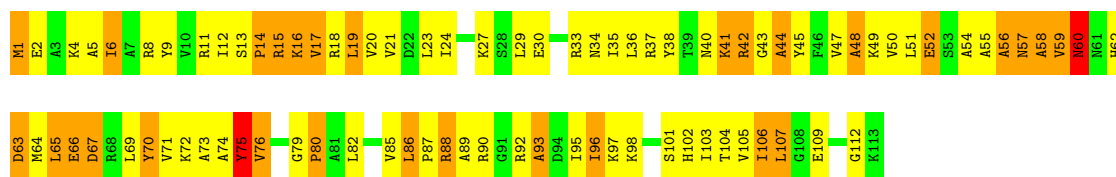
- Molecule 47: 50S ribosomal protein L21

Chain DV:



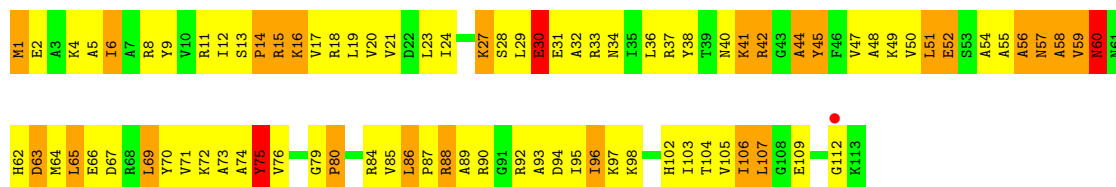
- Molecule 48: 50S ribosomal protein L22

Chain BW:



- Molecule 48: 50S ribosomal protein L22

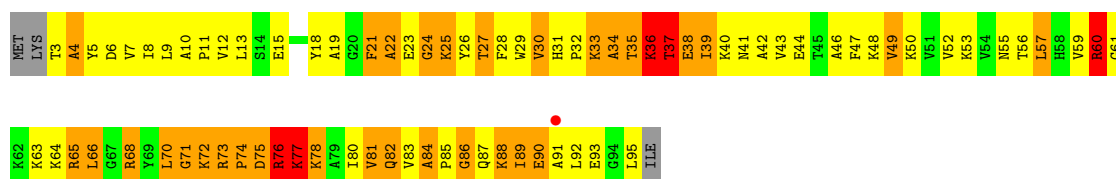
Chain DW:



- Molecule 49: 50S ribosomal protein L23

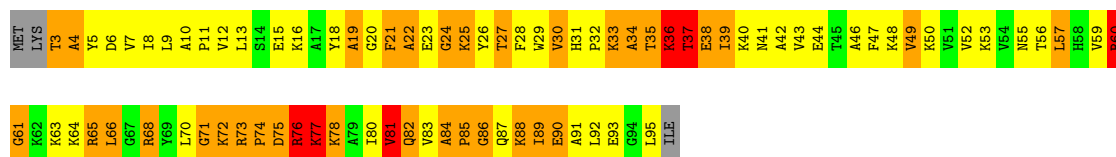
Chain BX:





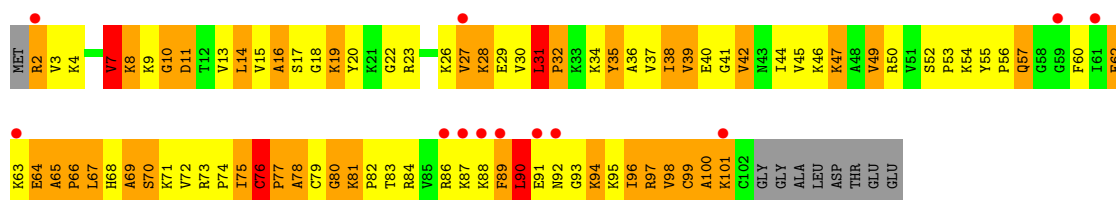
• Molecule 49: 50S ribosomal protein L23

Chain DX:



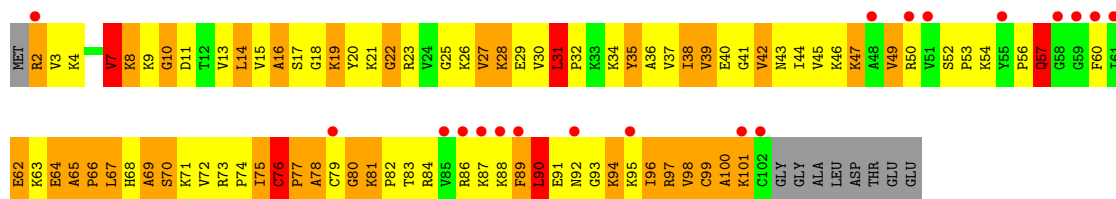
• Molecule 50: 50S ribosomal protein L24

Chain BY:



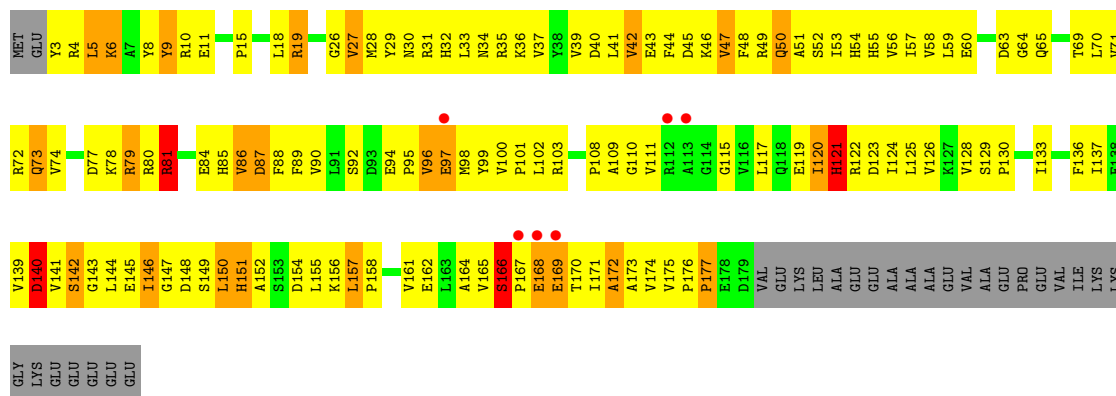
• Molecule 50: 50S ribosomal protein L24

Chain DY:



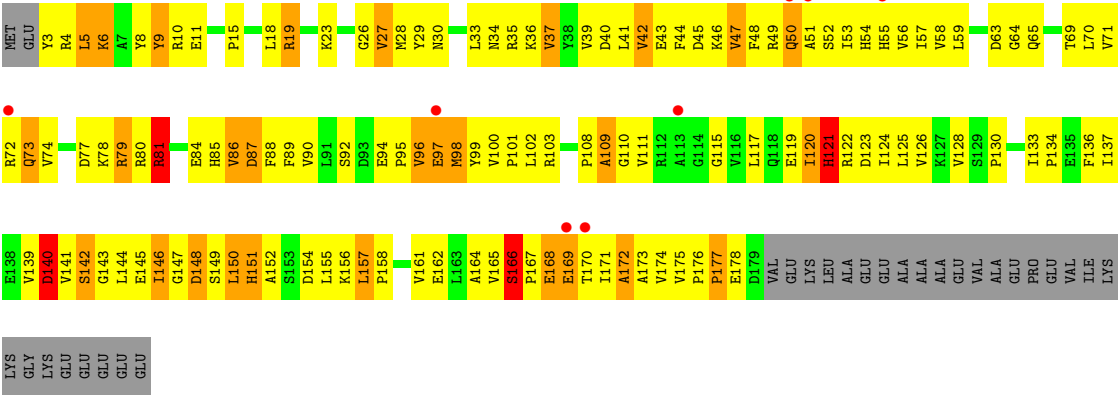
• Molecule 51: 50S ribosomal protein L25

Chain BZ:



• Molecule 51: 50S ribosomal protein L25

Chain DZ: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	207.32Å 437.99Å 614.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 3.10 48.97 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.97-3.10) 91.4 (48.97-3.10)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.12Å)	Xtriage
Refinement program	Phenix	Depositor
R, R_{free}	0.246 , 0.284 0.247 , 0.283	Depositor DCC
R_{free} test set	45921 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	88.4	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 914156 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	278037	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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, MG, TEL, 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	2/36190 (0.0%)	0.91	51/56486 (0.1%)
1	CA	0.52	2/36190 (0.0%)	0.92	61/56486 (0.1%)
2	AB	0.28	0/1936	0.49	0/2611
2	CB	0.28	0/1936	0.48	0/2611
3	AC	0.27	0/1637	0.45	0/2207
3	CC	0.27	0/1637	0.44	0/2207
4	AD	0.32	0/1733	0.54	0/2318
4	CD	0.34	0/1733	0.55	0/2318
5	AE	0.36	0/1163	0.55	0/1566
5	CE	0.34	0/1163	0.55	0/1566
6	AF	0.35	0/856	0.57	0/1154
6	CF	0.35	0/856	0.56	0/1154
7	AG	0.26	0/1276	0.43	0/1709
7	CG	0.26	0/1276	0.43	0/1709
8	AH	0.36	0/1136	0.56	0/1527
8	CH	0.35	0/1136	0.56	0/1527
9	AI	0.28	0/1028	0.44	0/1375
9	CI	0.28	0/1028	0.44	0/1375
10	AJ	0.27	0/808	0.48	0/1087
10	CJ	0.27	0/808	0.48	0/1087
11	AK	0.34	0/900	0.55	0/1213
11	CK	0.33	0/900	0.55	0/1213
12	AL	0.40	0/987	0.65	0/1322
12	CL	0.40	0/987	0.66	0/1322
13	AM	0.28	0/928	0.48	0/1238
13	CM	0.28	0/928	0.48	0/1238
14	AN	0.28	0/501	0.46	0/664
14	CN	0.29	0/501	0.46	0/664
15	AO	0.35	0/745	0.55	0/992
15	CO	0.34	0/745	0.54	0/992
16	AP	0.34	0/717	0.55	0/965
16	CP	0.34	0/717	0.56	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.35	0/837	0.56	0/1119
17	CQ	0.35	0/837	0.55	0/1119
18	AR	0.35	0/579	0.57	0/768
18	CR	0.34	0/579	0.57	0/768
19	AS	0.28	0/643	0.45	0/867
19	CS	0.29	0/643	0.45	0/867
20	AT	0.34	0/765	0.53	0/1007
20	CT	0.34	0/765	0.54	0/1007
21	AU	0.26	0/213	0.42	0/279
21	CU	0.28	0/213	0.43	0/279
22	B0	0.60	0/658	0.75	0/878
22	D0	0.54	0/658	0.73	0/878
23	B1	0.69	0/700	0.97	0/931
23	D1	0.61	0/700	0.92	1/931 (0.1%)
24	B2	0.61	0/423	0.92	1/560 (0.2%)
24	D2	0.55	0/423	0.88	1/560 (0.2%)
25	B3	0.62	0/473	0.71	0/636
25	D3	0.45	0/473	0.66	0/636
26	B4	0.26	0/156	0.53	0/215
26	D4	0.28	0/156	0.52	0/215
27	B5	0.83	2/473 (0.4%)	1.04	3/639 (0.5%)
27	D5	0.67	0/473	1.01	3/639 (0.5%)
28	B6	0.73	0/387	0.91	2/517 (0.4%)
28	D6	0.60	0/387	0.85	1/517 (0.2%)
29	B7	0.67	0/427	0.83	0/563
29	D7	0.61	0/427	0.81	0/563
30	B8	0.72	0/516	0.98	1/681 (0.1%)
30	D8	0.61	0/516	0.94	1/681 (0.1%)
31	BA	1.17	111/65745 (0.2%)	1.49	1343/102639 (1.3%)
31	DA	0.89	28/65745 (0.0%)	1.45	1209/102639 (1.2%)
32	BB	0.87	0/2853	1.26	35/4451 (0.8%)
32	DB	0.63	0/2853	1.18	25/4451 (0.6%)
33	BD	0.63	0/2155	0.85	3/2907 (0.1%)
33	DD	0.58	0/2155	0.82	2/2907 (0.1%)
34	BE	0.69	0/1597	0.87	2/2155 (0.1%)
34	DE	0.58	0/1597	0.83	0/2155
35	BF	0.65	2/1659 (0.1%)	0.77	0/2246
35	DF	0.53	1/1659 (0.1%)	0.74	0/2246
36	BG	0.37	0/1498	0.61	1/2013 (0.0%)
36	DG	0.35	0/1498	0.59	1/2013 (0.0%)
37	BH	0.57	0/1246	0.71	0/1684
37	DH	0.41	0/1246	0.66	0/1684
38	BI	0.40	0/1147	0.65	0/1553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DI	0.43	0/1147	0.66	1/1553 (0.1%)
39	BN	0.71	0/1132	0.83	0/1527
39	DN	0.56	0/1132	0.76	0/1527
40	BO	0.62	0/943	0.74	0/1269
40	DO	0.53	0/943	0.73	0/1269
41	BP	0.65	0/1131	0.98	5/1504 (0.3%)
41	DP	0.56	0/1131	0.94	4/1504 (0.3%)
42	BQ	0.66	0/1100	0.80	1/1470 (0.1%)
42	DQ	0.55	0/1100	0.74	0/1470
43	BR	0.69	0/974	0.82	1/1302 (0.1%)
43	DR	0.57	0/974	0.80	2/1302 (0.2%)
44	BS	0.52	0/779	0.75	0/1038
44	DS	0.43	0/779	0.72	0/1038
45	BT	0.58	0/1114	0.82	0/1488
45	DT	0.52	0/1114	0.79	0/1488
46	BU	0.70	0/975	0.80	2/1297 (0.2%)
46	DU	0.56	0/975	0.74	1/1297 (0.1%)
47	BV	0.69	0/789	0.89	0/1054
47	DV	0.54	0/789	0.84	1/1054 (0.1%)
48	BW	0.76	0/907	0.91	1/1216 (0.1%)
48	DW	0.61	0/907	0.88	0/1216
49	BX	0.72	0/740	0.92	0/995
49	DX	0.63	0/740	0.90	0/995
50	BY	0.65	0/789	0.86	0/1053
50	DY	0.53	0/789	0.81	0/1053
51	BZ	0.46	0/1436	0.62	1/1951 (0.1%)
51	DZ	0.40	0/1436	0.61	1/1951 (0.1%)
All	All	0.79	148/301000 (0.0%)	1.17	2768/449812 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	CA	1	0
22	B0	0	1
22	D0	0	1
23	B1	0	1
23	D1	0	1
24	B2	0	1
24	D2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
27	B5	0	1
27	D5	0	1
31	BA	18	0
31	DA	18	0
33	BD	0	4
33	DD	0	2
34	BE	0	2
34	DE	0	2
37	BH	0	1
37	DH	0	1
41	BP	0	5
41	DP	0	3
42	BQ	0	1
42	DQ	0	1
43	BR	0	1
43	DR	0	1
45	BT	0	1
45	DT	0	1
47	BV	0	1
47	DV	0	2
49	BX	0	2
49	DX	0	3
All	All	37	42

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BA	1142(A)	A	N9-C4	-11.15	1.31	1.37
31	BA	783	A	N9-C4	-10.64	1.31	1.37
31	BA	669	G	C4'-C3'	-10.15	1.42	1.53
31	BA	774	A	N9-C4	-9.61	1.32	1.37
31	DA	1142(A)	A	N9-C4	-9.23	1.32	1.37

The worst 5 of 2768 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	55	A	C8-N9-C4	-18.55	98.38	105.80
1	AA	55	A	N7-C8-N9	17.45	122.53	113.80
31	BA	1332	G	N3-C4-C5	16.73	136.96	128.60
31	BA	1332	G	N3-C4-N9	-16.73	115.96	126.00
31	BA	814	C	C6-N1-C2	15.82	126.63	120.30

5 of 37 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	BA	472	A	C3'
31	BA	669	G	C4',C3',C1'
31	BA	945	A	C1'
31	BA	1300	U	C4',C3'
31	BA	1379	A	C1'

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	B0	11	ARG	Peptide
23	B1	30	VAL	Peptide
24	B2	54	LYS	Peptide
27	B5	51	TYR	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	2214	12
1	CA	32329	0	16318	2202	2
2	AB	1901	0	1951	203	0
2	CB	1901	0	1951	204	0
3	AC	1613	0	1677	143	0
3	CC	1613	0	1677	145	0
4	AD	1703	0	1763	229	0
4	CD	1703	0	1764	232	0
5	AE	1147	0	1207	126	0
5	CE	1147	0	1207	145	0
6	AF	843	0	857	116	0
6	CF	843	0	857	125	0
7	AG	1257	0	1296	77	0
7	CG	1257	0	1296	81	0
8	AH	1116	0	1177	144	0
8	CH	1116	0	1177	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AI	1011	0	1042	112	0
9	CI	1011	0	1042	107	0
10	AJ	795	0	840	102	0
10	CJ	795	0	840	105	0
11	AK	885	0	904	109	0
11	CK	885	0	904	116	0
12	AL	971	0	1057	136	0
12	CL	971	0	1057	131	0
13	AM	921	0	976	97	0
13	CM	921	0	976	91	0
14	AN	492	0	532	46	0
14	CN	492	0	529	49	0
15	AO	734	0	771	81	0
15	CO	734	0	771	79	0
16	AP	701	0	720	103	0
16	CP	701	0	720	110	0
17	AQ	824	0	891	81	0
17	CQ	824	0	891	78	0
18	AR	574	0	644	86	0
18	CR	574	0	644	86	0
19	AS	630	0	652	53	0
19	CS	630	0	652	50	0
20	AT	763	0	861	93	0
20	CT	763	0	861	94	0
21	AU	209	0	221	14	0
21	CU	209	0	221	12	0
22	B0	650	0	654	90	0
22	D0	650	0	654	95	0
23	B1	693	0	764	149	0
23	D1	693	0	764	156	0
24	B2	421	0	461	141	0
24	D2	421	0	461	136	0
25	B3	468	0	523	47	0
25	D3	468	0	523	70	0
26	B4	157	0	69	7	0
26	D4	157	0	69	8	0
27	B5	459	0	480	100	0
27	D5	459	0	480	100	0
28	B6	381	0	390	102	0
28	D6	381	0	390	95	0
29	B7	419	0	467	54	0
29	D7	419	0	467	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B8	508	0	576	156	0
30	D8	508	0	576	151	0
31	BA	58698	0	29589	4119	0
31	DA	58698	0	29591	4387	0
32	BB	2551	0	1295	239	0
32	DB	2551	0	1295	231	0
33	BD	2105	0	2182	402	0
33	DD	2105	0	2182	406	0
34	BE	1564	0	1629	278	0
34	DE	1564	0	1629	278	0
35	BF	1624	0	1677	214	0
35	DF	1624	0	1677	209	0
36	BG	1474	0	1534	220	0
36	DG	1474	0	1534	223	0
37	BH	1223	0	1282	170	0
37	DH	1223	0	1282	162	0
38	BI	1132	0	1218	167	2
38	DI	1132	0	1218	158	12
39	BN	1105	0	1180	231	0
39	DN	1105	0	1180	231	0
40	BO	933	0	996	138	0
40	DO	933	0	996	133	0
41	BP	1114	0	1187	372	0
41	DP	1114	0	1187	345	0
42	BQ	1080	0	1127	195	0
42	DQ	1080	0	1127	195	0
43	BR	960	0	1021	136	0
43	DR	960	0	1021	146	0
44	BS	771	0	832	166	0
44	DS	771	0	832	172	0
45	BT	1100	0	1164	210	0
45	DT	1100	0	1164	213	0
46	BU	958	0	1015	171	0
46	DU	958	0	1015	177	0
47	BV	779	0	851	265	0
47	DV	779	0	851	258	0
48	BW	896	0	953	110	0
48	DW	896	0	953	128	0
49	BX	726	0	778	203	0
49	DX	726	0	777	199	0
50	BY	776	0	870	193	0
50	DY	776	0	870	191	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	BZ	1404	0	1432	190	0
51	DZ	1404	0	1432	196	0
52	AA	52	0	0	0	0
52	B0	1	0	0	0	0
52	B1	1	0	0	0	0
52	B5	2	0	0	0	0
52	B7	1	0	0	0	0
52	BA	360	0	0	0	0
52	BB	7	0	0	0	0
52	BD	2	0	0	0	0
52	BF	1	0	0	0	0
52	BP	3	0	0	0	0
52	BQ	2	0	0	0	0
52	BR	1	0	0	0	0
52	BU	1	0	0	0	0
52	BX	1	0	0	0	0
52	CA	50	0	0	0	0
52	D5	1	0	0	0	0
52	D7	1	0	0	0	0
52	D8	1	0	0	0	0
52	DA	318	0	0	0	0
52	DB	3	0	0	0	0
52	DD	2	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	2	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	0	0
53	CN	1	0	0	0	0
54	BA	1	0	0	0	0
54	DA	1	0	0	0	0
55	BA	58	0	65	32	0
55	DA	58	0	65	34	0
All	All	278037	0	189235	24925	14

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 54.

The worst 5 of 24925 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:CA:921:U:H1'	1:CA:922:G:C4	1.55	1.40
55:DA:3320:TEL:C14	55:DA:3320:TEL:H11	1.64	1.28
55:BA:3362:TEL:C14	55:BA:3362:TEL:H11	1.64	1.24
33:BD:35:LYS:HD2	33:BD:104:TYR:CD1	1.73	1.22
26:B4:13:ARG:HA	36:BG:101:ILE:HG13	1.22	1.19

The worst 5 of 14 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:358:U:OP2	38:DI:90:GLY:N[2_655]	1.80	0.40
1:AA:55:A:O4'	38:DI:82:ARG:NE[2_655]	1.98	0.22
1:AA:55:A:C8	38:DI:82:ARG:NE[2_655]	1.98	0.22
1:AA:358:U:O4'	38:DI:89:TYR:CD1[2_655]	1.99	0.21
1:AA:359:U:O5'	38:DI:87:LYS:O[2_655]	1.99	0.21

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%)	168 (72%)	49 (21%)	16 (7%)	2	13
2	CB	233/256 (91%)	169 (72%)	48 (21%)	16 (7%)	2	13
3	AC	205/239 (86%)	152 (74%)	40 (20%)	13 (6%)	2	16
3	CC	205/239 (86%)	153 (75%)	40 (20%)	12 (6%)	2	17
4	AD	206/209 (99%)	131 (64%)	49 (24%)	26 (13%)	0	3
4	CD	206/209 (99%)	130 (63%)	48 (23%)	28 (14%)	0	2
5	AE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	1	6
5	CE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	1	6
6	AF	99/101 (98%)	69 (70%)	18 (18%)	12 (12%)	1	4
6	CF	99/101 (98%)	66 (67%)	20 (20%)	13 (13%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	153/156 (98%)	126 (82%)	22 (14%)	5 (3%)	6	33
7	CG	153/156 (98%)	127 (83%)	21 (14%)	5 (3%)	6	33
8	AH	136/138 (99%)	100 (74%)	26 (19%)	10 (7%)	2	11
8	CH	136/138 (99%)	99 (73%)	28 (21%)	9 (7%)	2	15
9	AI	123/128 (96%)	85 (69%)	27 (22%)	11 (9%)	1	8
9	CI	123/128 (96%)	86 (70%)	26 (21%)	11 (9%)	1	8
10	AJ	97/105 (92%)	75 (77%)	19 (20%)	3 (3%)	7	36
10	CJ	97/105 (92%)	76 (78%)	18 (19%)	3 (3%)	7	36
11	AK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	2	14
11	CK	117/129 (91%)	86 (74%)	23 (20%)	8 (7%)	2	14
12	AL	123/135 (91%)	76 (62%)	26 (21%)	21 (17%)	0	0
12	CL	123/135 (91%)	77 (63%)	24 (20%)	22 (18%)	0	0
13	AM	107/126 (85%)	75 (70%)	26 (24%)	6 (6%)	3	19
13	CM	107/126 (85%)	74 (69%)	27 (25%)	6 (6%)	3	19
14	AN	58/61 (95%)	48 (83%)	5 (9%)	5 (9%)	1	9
14	CN	58/61 (95%)	48 (83%)	5 (9%)	5 (9%)	1	9
15	AO	86/89 (97%)	56 (65%)	21 (24%)	9 (10%)	1	5
15	CO	86/89 (97%)	56 (65%)	21 (24%)	9 (10%)	1	5
16	AP	82/88 (93%)	48 (58%)	21 (26%)	13 (16%)	0	1
16	CP	82/88 (93%)	48 (58%)	21 (26%)	13 (16%)	0	1
17	AQ	98/105 (93%)	76 (78%)	17 (17%)	5 (5%)	3	22
17	CQ	98/105 (93%)	76 (78%)	17 (17%)	5 (5%)	3	22
18	AR	68/88 (77%)	43 (63%)	20 (29%)	5 (7%)	2	11
18	CR	68/88 (77%)	42 (62%)	19 (28%)	7 (10%)	1	6
19	AS	77/93 (83%)	56 (73%)	15 (20%)	6 (8%)	1	11
19	CS	77/93 (83%)	56 (73%)	15 (20%)	6 (8%)	1	11
20	AT	97/106 (92%)	58 (60%)	24 (25%)	15 (16%)	0	1
20	CT	97/106 (92%)	53 (55%)	29 (30%)	15 (16%)	0	1
21	AU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	4	26
21	CU	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	4	26
22	B0	83/85 (98%)	67 (81%)	9 (11%)	7 (8%)	1	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	D0	83/85 (98%)	62 (75%)	14 (17%)	7 (8%)	1	9
23	B1	87/98 (89%)	43 (49%)	27 (31%)	17 (20%)	0	0
23	D1	87/98 (89%)	44 (51%)	26 (30%)	17 (20%)	0	0
24	B2	49/72 (68%)	25 (51%)	14 (29%)	10 (20%)	0	0
24	D2	49/72 (68%)	26 (53%)	13 (26%)	10 (20%)	0	0
25	B3	58/60 (97%)	48 (83%)	9 (16%)	1 (2%)	14	54
25	D3	58/60 (97%)	44 (76%)	13 (22%)	1 (2%)	14	54
26	B4	30/71 (42%)	7 (23%)	11 (37%)	12 (40%)	0	0
26	D4	30/71 (42%)	6 (20%)	11 (37%)	13 (43%)	0	0
27	B5	57/60 (95%)	37 (65%)	8 (14%)	12 (21%)	0	0
27	D5	57/60 (95%)	36 (63%)	8 (14%)	13 (23%)	0	0
28	B6	41/54 (76%)	19 (46%)	10 (24%)	12 (29%)	0	0
28	D6	41/54 (76%)	18 (44%)	11 (27%)	12 (29%)	0	0
29	B7	47/49 (96%)	44 (94%)	2 (4%)	1 (2%)	11	48
29	D7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	11	48
30	B8	62/65 (95%)	37 (60%)	15 (24%)	10 (16%)	0	1
30	D8	62/65 (95%)	38 (61%)	13 (21%)	11 (18%)	0	0
33	BD	270/276 (98%)	203 (75%)	50 (18%)	17 (6%)	2	16
33	DD	270/276 (98%)	202 (75%)	52 (19%)	16 (6%)	2	17
34	BE	203/206 (98%)	133 (66%)	43 (21%)	27 (13%)	0	2
34	DE	203/206 (98%)	136 (67%)	39 (19%)	28 (14%)	0	2
35	BF	206/210 (98%)	138 (67%)	44 (21%)	24 (12%)	1	4
35	DF	206/210 (98%)	137 (66%)	45 (22%)	24 (12%)	1	4
36	BG	177/182 (97%)	110 (62%)	46 (26%)	21 (12%)	1	4
36	DG	177/182 (97%)	109 (62%)	47 (27%)	21 (12%)	1	4
37	BH	158/180 (88%)	98 (62%)	38 (24%)	22 (14%)	0	2
37	DH	158/180 (88%)	97 (61%)	37 (23%)	24 (15%)	0	1
38	BI	144/148 (97%)	86 (60%)	36 (25%)	22 (15%)	0	1
38	DI	144/148 (97%)	83 (58%)	38 (26%)	23 (16%)	0	1
39	BN	137/140 (98%)	93 (68%)	29 (21%)	15 (11%)	1	5
39	DN	137/140 (98%)	97 (71%)	25 (18%)	15 (11%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BO	120/122 (98%)	96 (80%)	19 (16%)	5 (4%)	4	27
40	DO	120/122 (98%)	98 (82%)	17 (14%)	5 (4%)	4	27
41	BP	144/150 (96%)	72 (50%)	31 (22%)	41 (28%)	0	0
41	DP	144/150 (96%)	72 (50%)	29 (20%)	43 (30%)	0	0
42	BQ	134/141 (95%)	92 (69%)	29 (22%)	13 (10%)	1	6
42	DQ	134/141 (95%)	91 (68%)	29 (22%)	14 (10%)	1	5
43	BR	115/118 (98%)	70 (61%)	34 (30%)	11 (10%)	1	7
43	DR	115/118 (98%)	71 (62%)	34 (30%)	10 (9%)	1	9
44	BS	97/112 (87%)	43 (44%)	26 (27%)	28 (29%)	0	0
44	DS	97/112 (87%)	41 (42%)	29 (30%)	27 (28%)	0	0
45	BT	130/146 (89%)	80 (62%)	25 (19%)	25 (19%)	0	0
45	DT	130/146 (89%)	80 (62%)	26 (20%)	24 (18%)	0	0
46	BU	115/118 (98%)	78 (68%)	29 (25%)	8 (7%)	2	13
46	DU	115/118 (98%)	82 (71%)	24 (21%)	9 (8%)	1	11
47	BV	97/101 (96%)	49 (50%)	24 (25%)	24 (25%)	0	0
47	DV	97/101 (96%)	47 (48%)	25 (26%)	25 (26%)	0	0
48	BW	111/113 (98%)	81 (73%)	11 (10%)	19 (17%)	0	0
48	DW	111/113 (98%)	78 (70%)	15 (14%)	18 (16%)	0	0
49	BX	91/96 (95%)	45 (50%)	22 (24%)	24 (26%)	0	0
49	DX	91/96 (95%)	45 (50%)	21 (23%)	25 (28%)	0	0
50	BY	99/110 (90%)	41 (41%)	25 (25%)	33 (33%)	0	0
50	DY	99/110 (90%)	41 (41%)	27 (27%)	31 (31%)	0	0
51	BZ	175/206 (85%)	117 (67%)	41 (23%)	17 (10%)	1	6
51	DZ	175/206 (85%)	116 (66%)	41 (23%)	18 (10%)	1	6
All	All	11148/12060 (92%)	7385 (66%)	2386 (21%)	1377 (12%)	1	3

5 of 1377 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	34	ALA
2	AB	165	VAL
2	AB	194	PRO
3	AC	54	ARG

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%)	182 (90%)	20 (10%)	11	39
2	CB	202/220 (92%)	183 (91%)	19 (9%)	13	43
3	AC	160/188 (85%)	154 (96%)	6 (4%)	44	84
3	CC	160/188 (85%)	154 (96%)	6 (4%)	44	84
4	AD	180/181 (99%)	157 (87%)	23 (13%)	6	24
4	CD	180/181 (99%)	156 (87%)	24 (13%)	6	22
5	AE	115/123 (94%)	101 (88%)	14 (12%)	7	26
5	CE	115/123 (94%)	101 (88%)	14 (12%)	7	26
6	AF	90/90 (100%)	80 (89%)	10 (11%)	9	33
6	CF	90/90 (100%)	80 (89%)	10 (11%)	9	33
7	AG	126/127 (99%)	120 (95%)	6 (5%)	35	77
7	CG	126/127 (99%)	120 (95%)	6 (5%)	35	77
8	AH	119/119 (100%)	104 (87%)	15 (13%)	7	24
8	CH	119/119 (100%)	105 (88%)	14 (12%)	8	29
9	AI	98/99 (99%)	87 (89%)	11 (11%)	9	33
9	CI	98/99 (99%)	88 (90%)	10 (10%)	11	37
10	AJ	88/92 (96%)	75 (85%)	13 (15%)	4	17
10	CJ	88/92 (96%)	76 (86%)	12 (14%)	5	21
11	AK	90/99 (91%)	83 (92%)	7 (8%)	18	57
11	CK	90/99 (91%)	83 (92%)	7 (8%)	18	57
12	AL	104/111 (94%)	94 (90%)	10 (10%)	12	42
12	CL	104/111 (94%)	94 (90%)	10 (10%)	12	42
13	AM	93/101 (92%)	85 (91%)	8 (9%)	15	51
13	CM	93/101 (92%)	85 (91%)	8 (9%)	15	51
14	AN	49/50 (98%)	46 (94%)	3 (6%)	26	67
14	CN	49/50 (98%)	46 (94%)	3 (6%)	26	67
15	AO	79/80 (99%)	71 (90%)	8 (10%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CO	79/80 (99%)	71 (90%)	8 (10%)	11	38
16	AP	72/74 (97%)	61 (85%)	11 (15%)	4	15
16	CP	72/74 (97%)	61 (85%)	11 (15%)	4	15
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	15	51
17	CQ	94/97 (97%)	86 (92%)	8 (8%)	15	51
18	AR	61/77 (79%)	55 (90%)	6 (10%)	12	40
18	CR	61/77 (79%)	55 (90%)	6 (10%)	12	40
19	AS	69/80 (86%)	60 (87%)	9 (13%)	6	23
19	CS	69/80 (86%)	60 (87%)	9 (13%)	6	23
20	AT	76/82 (93%)	65 (86%)	11 (14%)	5	18
20	CT	76/82 (93%)	64 (84%)	12 (16%)	4	14
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%)	48 (79%)	13 (21%)	1	7
22	D0	61/67 (91%)	48 (79%)	13 (21%)	1	7
23	B1	73/83 (88%)	51 (70%)	22 (30%)	0	1
23	D1	73/83 (88%)	53 (73%)	20 (27%)	0	1
24	B2	46/67 (69%)	28 (61%)	18 (39%)	0	0
24	D2	46/67 (69%)	28 (61%)	18 (39%)	0	0
25	B3	51/52 (98%)	41 (80%)	10 (20%)	2	8
25	D3	51/52 (98%)	42 (82%)	9 (18%)	3	10
27	B5	51/52 (98%)	39 (76%)	12 (24%)	1	5
27	D5	51/52 (98%)	41 (80%)	10 (20%)	2	8
28	B6	43/52 (83%)	27 (63%)	16 (37%)	0	0
28	D6	43/52 (83%)	28 (65%)	15 (35%)	0	0
29	B7	41/42 (98%)	32 (78%)	9 (22%)	1	6
29	D7	41/42 (98%)	31 (76%)	10 (24%)	1	4
30	B8	53/55 (96%)	36 (68%)	17 (32%)	0	0
30	D8	53/55 (96%)	35 (66%)	18 (34%)	0	0
33	BD	213/218 (98%)	160 (75%)	53 (25%)	1	3
33	DD	213/218 (98%)	157 (74%)	56 (26%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
34	BE	165/166 (99%)	127 (77%)	38 (23%)	1	5	
34	DE	165/166 (99%)	126 (76%)	39 (24%)	1	5	
35	BF	165/166 (99%)	130 (79%)	35 (21%)	1	7	
35	DF	165/166 (99%)	132 (80%)	33 (20%)	2	8	
36	BG	155/156 (99%)	126 (81%)	29 (19%)	2	9	
36	DG	155/156 (99%)	126 (81%)	29 (19%)	2	9	
37	BH	132/148 (89%)	105 (80%)	27 (20%)	2	8	
37	DH	132/148 (89%)	107 (81%)	25 (19%)	2	9	
38	BI	122/124 (98%)	99 (81%)	23 (19%)	2	9	
38	DI	122/124 (98%)	100 (82%)	22 (18%)	2	10	
39	BN	117/119 (98%)	80 (68%)	37 (32%)	0	1	
39	DN	117/119 (98%)	81 (69%)	36 (31%)	0	1	
40	BO	100/100 (100%)	82 (82%)	18 (18%)	2	10	
40	DO	100/100 (100%)	80 (80%)	20 (20%)	2	8	
41	BP	112/116 (97%)	67 (60%)	45 (40%)	0	0	
41	DP	112/116 (97%)	67 (60%)	45 (40%)	0	0	
42	BQ	106/111 (96%)	81 (76%)	25 (24%)	1	5	
42	DQ	106/111 (96%)	82 (77%)	24 (23%)	1	5	
43	BR	100/101 (99%)	76 (76%)	24 (24%)	1	4	
43	DR	100/101 (99%)	76 (76%)	24 (24%)	1	4	
44	BS	77/88 (88%)	59 (77%)	18 (23%)	1	5	
44	DS	77/88 (88%)	59 (77%)	18 (23%)	1	5	
45	BT	116/127 (91%)	76 (66%)	40 (34%)	0	0	
45	DT	116/127 (91%)	77 (66%)	39 (34%)	0	0	
46	BU	92/94 (98%)	74 (80%)	18 (20%)	2	8	
46	DU	92/94 (98%)	71 (77%)	21 (23%)	1	5	
47	BV	82/82 (100%)	56 (68%)	26 (32%)	0	1	
47	DV	82/82 (100%)	57 (70%)	25 (30%)	0	1	
48	BW	91/92 (99%)	67 (74%)	24 (26%)	1	2	
48	DW	91/92 (99%)	69 (76%)	22 (24%)	1	4	
49	BX	74/78 (95%)	55 (74%)	19 (26%)	1	2	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	DX	74/78 (95%)	54 (73%)	20 (27%)	1	2
50	BY	84/91 (92%)	67 (80%)	17 (20%)	2	8
50	DY	84/91 (92%)	66 (79%)	18 (21%)	1	7
51	BZ	155/179 (87%)	132 (85%)	23 (15%)	4	17
51	DZ	155/179 (87%)	131 (84%)	24 (16%)	4	14
All	All	9322/9876 (94%)	7617 (82%)	1705 (18%)	2	10

5 of 1705 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BV	98	GLU
9	CI	114	TYR
46	DU	8	VAL
48	BW	101	SER
2	CB	145	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 256 such sidechains are listed below:

Mol	Chain	Res	Type
45	BT	90	GLN
5	CE	78	HIS
43	DR	31	HIS
48	BW	34	ASN
2	CB	146	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	307 (20%)	30 (1%)
1	CA	1503/1522 (98%)	307 (20%)	30 (1%)
31	BA	2723/2787 (97%)	822 (30%)	77 (2%)
31	DA	2723/2787 (97%)	827 (30%)	75 (2%)
32	BB	118/122 (96%)	42 (35%)	0
32	DB	118/122 (96%)	42 (35%)	0
All	All	8688/8862 (98%)	2347 (27%)	212 (2%)

5 of 2347 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	47	C

5 of 212 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	BA	2422	A
1	CA	484	G
31	DA	2288	A
31	BA	2542	A
1	CA	30	U

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 827 ligands modelled in this entry, 825 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	TEL	BA	3362	-	62,62,62	1.80	7 (11%)	92,92,92	3.08	29 (31%)
55	TEL	DA	3320	-	62,62,62	1.80	7 (11%)	92,92,92	3.08	29 (31%)

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	TEL	BA	3362	-	1/1/19/19	0/73/108/108	0/5/5/5
55	TEL	DA	3320	-	1/1/19/19	0/73/108/108	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	3320	TEL	C43-C40	-7.12	1.37	1.48
55	BA	3362	TEL	C43-C40	-7.07	1.37	1.48
55	BA	3362	TEL	O5-C2	-4.64	1.40	1.47
55	DA	3320	TEL	O5-C2	-4.63	1.40	1.47
55	DA	3320	TEL	C37-N31	-4.53	1.29	1.36

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BA	3362	TEL	C8-C4-C2	-16.81	92.52	115.55
55	DA	3320	TEL	C8-C4-C2	-16.81	92.52	115.55
55	DA	3320	TEL	O9-C15-C21	9.87	121.11	110.84
55	BA	3362	TEL	O9-C15-C21	9.87	121.11	110.84
55	BA	3362	TEL	C2-O5-C10	-9.78	102.94	108.92

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
55	DA	3320	TEL	C21
55	BA	3362	TEL	C21

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	DG	112:PRO	C	113:ARG	N	5.74
1	BG	112:PRO	C	113:ARG	N	5.73
1	CM	69:GLU	C	70:LEU	N	4.94
1	AM	69:GLU	C	70:LEU	N	4.93
1	D6	46:HIS	C	47:THR	N	4.90

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%)	0.68	200 (13%) 4 1	64, 134, 200, 203	0
1	CA	1504/1522 (98%)	0.73	202 (13%) 4 1	67, 134, 200, 203	0
2	AB	235/256 (91%)	0.51	20 (8%) 11 2	122, 175, 196, 201	0
2	CB	235/256 (91%)	0.76	37 (15%) 3 1	123, 175, 196, 202	0
3	AC	207/239 (86%)	0.56	18 (8%) 10 2	122, 174, 194, 197	0
3	CC	207/239 (86%)	0.68	23 (11%) 6 1	122, 175, 195, 199	0
4	AD	208/209 (99%)	0.51	17 (8%) 12 2	89, 149, 187, 193	0
4	CD	208/209 (99%)	0.22	6 (2%) 49 7	86, 148, 186, 193	0
5	AE	151/162 (93%)	0.37	9 (5%) 21 3	88, 127, 174, 197	0
5	CE	151/162 (93%)	0.73	20 (13%) 4 1	90, 128, 174, 197	0
6	AF	101/101 (100%)	0.16	0 100 100	95, 151, 183, 196	0
6	CF	101/101 (100%)	0.31	2 (1%) 62 12	96, 154, 184, 198	0
7	AG	155/156 (99%)	0.73	28 (18%) 2 0	146, 184, 197, 200	0
7	CG	155/156 (99%)	1.31	35 (22%) 1 0	146, 185, 197, 199	0
8	AH	138/138 (100%)	0.04	1 (0%) 84 32	92, 129, 167, 189	0
8	CH	138/138 (100%)	0.08	0 100 100	92, 129, 166, 189	0
9	AI	127/128 (99%)	1.26	31 (24%) 1 0	143, 190, 200, 202	0
9	CI	127/128 (99%)	1.80	48 (37%) 1 0	144, 190, 199, 202	0
10	AJ	99/105 (94%)	1.35	22 (22%) 1 0	130, 184, 199, 200	0
10	CJ	99/105 (94%)	2.11	50 (50%) 0 0	134, 185, 199, 202	0
11	AK	119/129 (92%)	0.81	17 (14%) 3 1	87, 142, 187, 200	0
11	CK	119/129 (92%)	0.88	14 (11%) 5 1	86, 144, 189, 200	0
12	AL	125/135 (92%)	0.43	9 (7%) 15 2	76, 114, 168, 200	0
12	CL	125/135 (92%)	0.70	15 (12%) 5 1	80, 114, 169, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	AM	115/126 (91%)	1.43	37 (32%)	1 0	147, 192, 199, 201	0
13	CM	115/126 (91%)	1.55	36 (31%)	1 0	148, 192, 199, 202	0
14	AN	60/61 (98%)	1.14	11 (18%)	2 0	141, 183, 196, 199	0
14	CN	60/61 (98%)	0.78	7 (11%)	5 1	142, 182, 196, 198	0
15	AO	88/89 (98%)	0.25	1 (1%)	77 22	85, 123, 173, 189	0
15	CO	88/89 (98%)	0.39	2 (2%)	57 9	87, 124, 176, 186	0
16	AP	84/88 (95%)	0.82	15 (17%)	2 0	97, 128, 177, 192	0
16	CP	84/88 (95%)	0.92	20 (23%)	1 0	97, 126, 175, 191	0
17	AQ	100/105 (95%)	0.33	6 (6%)	21 3	82, 113, 158, 175	0
17	CQ	100/105 (95%)	0.20	5 (5%)	28 4	82, 114, 158, 176	0
18	AR	70/88 (79%)	0.60	4 (5%)	23 3	102, 140, 183, 193	0
18	CR	70/88 (79%)	1.12	13 (18%)	2 0	103, 140, 182, 196	0
19	AS	79/93 (84%)	2.23	36 (45%)	1 0	160, 194, 199, 199	0
19	CS	79/93 (84%)	1.75	31 (39%)	1 0	158, 193, 199, 200	0
20	AT	99/106 (93%)	0.46	8 (8%)	12 2	97, 133, 181, 196	0
20	CT	99/106 (93%)	0.62	15 (15%)	3 1	97, 132, 180, 197	0
21	AU	25/27 (92%)	2.94	17 (68%)	0 0	153, 185, 194, 195	0
21	CU	25/27 (92%)	4.29	23 (92%)	0 0	156, 186, 195, 196	0
22	B0	85/85 (100%)	0.31	6 (7%)	16 3	56, 78, 183, 200	0
22	D0	85/85 (100%)	0.18	7 (8%)	12 2	62, 82, 179, 199	0
23	B1	89/98 (90%)	0.18	0	100 100	54, 86, 160, 184	0
23	D1	89/98 (90%)	0.36	2 (2%)	59 11	57, 88, 162, 191	0
24	B2	51/72 (70%)	0.43	1 (1%)	62 12	63, 105, 166, 192	0
24	D2	51/72 (70%)	0.32	4 (7%)	13 2	68, 110, 167, 192	0
25	B3	60/60 (100%)	-0.07	1 (1%)	67 15	49, 77, 143, 193	0
25	D3	60/60 (100%)	0.29	1 (1%)	67 15	54, 79, 145, 186	0
26	B4	32/71 (45%)	-0.03	0	100 100	140, 177, 199, 200	0
26	D4	32/71 (45%)	0.51	4 (12%)	5 1	139, 180, 199, 201	0
27	B5	58/60 (96%)	0.19	3 (5%)	26 4	40, 65, 182, 197	0
27	D5	58/60 (96%)	0.23	3 (5%)	26 4	42, 69, 186, 197	0
28	B6	45/54 (83%)	0.45	1 (2%)	59 11	52, 100, 167, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/54 (83%)	0.75	9 (20%) 2 0	57, 102, 169, 189	0
29	B7	49/49 (100%)	0.36	0 100 100	42, 51, 132, 180	0
29	D7	49/49 (100%)	0.78	1 (2%) 62 12	45, 54, 132, 180	0
30	B8	64/65 (98%)	0.36	2 (3%) 47 7	53, 76, 137, 169	0
30	D8	64/65 (98%)	0.30	3 (4%) 30 4	55, 79, 140, 168	0
31	BA	2725/2787 (97%)	0.14	69 (2%) 54 9	38, 66, 177, 204	0
31	DA	2725/2787 (97%)	0.05	97 (3%) 41 6	44, 71, 181, 203	0
32	BB	119/122 (97%)	0.44	8 (6%) 17 3	56, 123, 191, 200	0
32	DB	119/122 (97%)	0.41	9 (7%) 14 2	64, 127, 194, 203	0
33	BD	272/276 (98%)	0.01	3 (1%) 77 22	42, 70, 130, 172	0
33	DD	272/276 (98%)	0.11	4 (1%) 70 16	47, 73, 128, 175	0
34	BE	205/206 (99%)	0.22	5 (2%) 56 9	40, 75, 166, 194	0
34	DE	205/206 (99%)	0.25	6 (2%) 49 7	46, 78, 169, 195	0
35	BF	208/210 (99%)	0.38	9 (4%) 34 5	39, 86, 178, 198	0
35	DF	208/210 (99%)	0.29	12 (5%) 22 3	44, 89, 182, 199	0
36	BG	181/182 (99%)	1.63	51 (28%) 1 0	116, 186, 200, 203	0
36	DG	181/182 (99%)	1.95	67 (37%) 1 0	119, 188, 200, 203	0
37	BH	160/180 (88%)	0.28	0 100 100	81, 136, 181, 190	0
37	DH	160/180 (88%)	1.03	29 (18%) 2 0	87, 142, 186, 195	0
38	BI	146/148 (98%)	0.61	20 (13%) 4 1	74, 178, 197, 200	0
38	DI	146/148 (98%)	1.96	50 (34%) 1 0	76, 180, 198, 201	0
39	BN	139/140 (99%)	0.09	3 (2%) 59 11	51, 87, 154, 186	0
39	DN	139/140 (99%)	0.07	2 (1%) 72 17	56, 90, 155, 190	0
40	BO	122/122 (100%)	0.02	0 100 100	51, 79, 133, 168	0
40	DO	122/122 (100%)	-0.05	0 100 100	54, 84, 136, 173	0
41	BP	146/150 (97%)	0.44	6 (4%) 35 5	43, 106, 165, 199	0
41	DP	146/150 (97%)	0.54	12 (8%) 12 2	42, 109, 168, 198	0
42	BQ	136/141 (96%)	0.25	5 (3%) 39 6	55, 88, 159, 190	0
42	DQ	136/141 (96%)	0.39	14 (10%) 7 2	59, 90, 160, 191	0
43	BR	117/118 (99%)	-0.00	0 100 100	43, 65, 134, 180	0
43	DR	117/118 (99%)	0.09	2 (1%) 67 15	47, 68, 136, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BS	99/112 (88%)	0.63	8 (8%) 12 2	79, 134, 189, 198	0
44	DS	99/112 (88%)	1.10	15 (15%) 3 1	83, 136, 192, 198	0
45	BT	132/146 (90%)	0.25	7 (5%) 25 4	60, 105, 179, 192	0
45	DT	132/146 (90%)	0.32	8 (6%) 21 3	65, 107, 179, 195	0
46	BU	117/118 (99%)	0.15	3 (2%) 53 8	43, 71, 142, 190	0
46	DU	117/118 (99%)	0.42	8 (6%) 17 3	48, 76, 145, 194	0
47	BV	101/101 (100%)	0.37	4 (3%) 36 5	44, 117, 183, 198	0
47	DV	101/101 (100%)	0.60	8 (7%) 13 2	49, 120, 186, 197	0
48	BW	113/113 (100%)	-0.21	0 100 100	41, 58, 127, 188	0
48	DW	113/113 (100%)	-0.22	1 (0%) 81 25	43, 62, 130, 191	0
49	BX	93/96 (96%)	0.21	1 (1%) 77 22	50, 82, 151, 186	0
49	DX	93/96 (96%)	0.01	0 100 100	57, 84, 153, 186	0
50	BY	101/110 (91%)	0.72	12 (11%) 5 1	61, 120, 197, 199	0
50	DY	101/110 (91%)	0.93	19 (18%) 2 0	68, 121, 195, 199	0
51	BZ	177/206 (85%)	0.18	6 (3%) 43 6	76, 129, 182, 196	0
51	DZ	177/206 (85%)	0.26	8 (4%) 32 5	80, 133, 185, 196	0
All	All	20062/20922 (95%)	0.46	1750 (8%) 10 2	38, 110, 197, 204	0

The worst 5 of 1750 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BF	208	GLY	21.4
31	DA	2802	G	18.9
31	BA	2796	U	16.8
1	CA	84	U	15.8
35	BF	207	GLY	15.7

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	3098	1/1	0.21	-	76,76,76,76	0
52	MG	CA	1614	1/1	0.12	-	80,80,80,80	0
52	MG	DA	3065	1/1	0.50	-	70,70,70,70	0
52	MG	BA	3352	1/1	0.46	-	53,53,53,53	0
52	MG	BA	3093	1/1	0.76	-	57,57,57,57	0
52	MG	BA	3015	1/1	0.17	-	46,46,46,46	0
52	MG	DA	3318	1/1	0.07	-	83,83,83,83	0
52	MG	BA	3309	1/1	0.33	-	70,70,70,70	0
52	MG	DA	3104	1/1	0.41	-	85,85,85,85	0
52	MG	BA	3313	1/1	0.50	-	61,61,61,61	0
52	MG	DA	3049	1/1	0.22	-	54,54,54,54	0
52	MG	CA	1635	1/1	1.21	-	80,80,80,80	0
52	MG	DA	3084	1/1	0.35	-	27,27,27,27	0
52	MG	BA	3332	1/1	0.23	-	65,65,65,65	0
52	MG	BA	3010	1/1	0.50	-	53,53,53,53	0
52	MG	BA	3174	1/1	0.31	-	51,51,51,51	0
52	MG	AA	1648	1/1	0.68	-	57,57,57,57	0
52	MG	BA	3186	1/1	0.40	-	44,44,44,44	0
52	MG	DA	3177	1/1	0.48	-	48,48,48,48	0
52	MG	DA	3018	1/1	0.64	-	34,34,34,34	0
52	MG	BA	3193	1/1	0.41	-	51,51,51,51	0
52	MG	DA	3207	1/1	0.18	-	53,53,53,53	0
52	MG	BA	3005	1/1	0.35	-	56,56,56,56	0
52	MG	BA	3055	1/1	0.32	-	31,31,31,31	0
52	MG	DA	3302	1/1	0.26	-	64,64,64,64	0
52	MG	DR	202	1/1	0.53	-	50,50,50,50	0
52	MG	BA	3217	1/1	0.54	-	34,34,34,34	0
52	MG	DA	3130	1/1	0.18	-	83,83,83,83	0
52	MG	BA	3232	1/1	0.45	-	43,43,43,43	0
52	MG	BA	3226	1/1	0.42	-	42,42,42,42	0
52	MG	BA	3268	1/1	0.13	-	60,60,60,60	0
52	MG	CA	1628	1/1	0.61	-	92,92,92,92	0
52	MG	BA	3154	1/1	0.22	-	73,73,73,73	0
52	MG	AA	1623	1/1	0.40	-	50,50,50,50	0
52	MG	DA	3037	1/1	0.46	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3116	1/1	0.36	-	67,67,67,67	0
52	MG	DA	3268	1/1	0.58	-	72,72,72,72	0
52	MG	DA	3303	1/1	0.27	-	57,57,57,57	0
52	MG	DU	201	1/1	0.34	-	75,75,75,75	0
52	MG	DA	3226	1/1	0.63	-	73,73,73,73	0
52	MG	CA	1646	1/1	0.46	-	68,68,68,68	0
52	MG	DA	3172	1/1	0.64	-	59,59,59,59	0
52	MG	DA	3070	1/1	0.35	-	52,52,52,52	0
52	MG	CA	1621	1/1	0.47	-	78,78,78,78	0
52	MG	BA	3052	1/1	0.32	-	17,17,17,17	0
52	MG	DA	3147	1/1	0.53	-	35,35,35,35	0
52	MG	DA	3249	1/1	0.44	-	69,69,69,69	0
52	MG	DA	3017	1/1	0.23	-	55,55,55,55	0
52	MG	DA	3089	1/1	0.20	-	54,54,54,54	0
52	MG	BA	3244	1/1	0.39	-	44,44,44,44	0
52	MG	CA	1612	1/1	0.19	-	70,70,70,70	0
52	MG	BA	3182	1/1	0.45	-	54,54,54,54	0
52	MG	BA	3167	1/1	0.26	-	27,27,27,27	0
52	MG	BA	3327	1/1	0.72	-	70,70,70,70	0
52	MG	BA	3160	1/1	0.98	-	78,78,78,78	0
52	MG	BA	3339	1/1	0.29	-	74,74,74,74	0
52	MG	BA	3184	1/1	0.18	-	62,62,62,62	0
52	MG	AA	1615	1/1	0.64	-	72,72,72,72	0
52	MG	DA	3244	1/1	0.47	-	69,69,69,69	0
52	MG	DA	3178	1/1	0.39	-	52,52,52,52	0
52	MG	DA	3317	1/1	0.12	-	60,60,60,60	0
52	MG	CA	1604	1/1	0.31	-	98,98,98,98	0
52	MG	DA	3028	1/1	0.31	-	68,68,68,68	0
52	MG	DA	3221	1/1	0.35	-	62,62,62,62	0
52	MG	DA	3094	1/1	0.36	-	75,75,75,75	0
54	K	DA	3319	1/1	0.14	-	82,82,82,82	0
52	MG	DA	3195	1/1	0.22	-	62,62,62,62	0
52	MG	BA	3275	1/1	0.13	-	47,47,47,47	0
52	MG	BA	3140	1/1	0.24	-	78,78,78,78	0
52	MG	BA	3172	1/1	0.18	-	50,50,50,50	0
52	MG	D7	101	1/1	0.51	-	58,58,58,58	0
52	MG	BA	3287	1/1	0.34	-	59,59,59,59	0
52	MG	BA	3103	1/1	0.22	-	31,31,31,31	0
52	MG	DA	3285	1/1	0.58	-	70,70,70,70	0
52	MG	CA	1602	1/1	0.79	-	73,73,73,73	0
52	MG	DA	3127	1/1	0.28	-	40,40,40,40	0
52	MG	DA	3225	1/1	0.60	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	AA	1638	1/1	0.36	-	91,91,91,91	0
52	MG	BA	3281	1/1	0.15	-	45,45,45,45	0
52	MG	BA	3265	1/1	0.50	-	51,51,51,51	0
54	K	BA	3361	1/1	0.09	-	69,69,69,69	0
52	MG	DA	3006	1/1	0.47	-	40,40,40,40	0
52	MG	DA	3041	1/1	0.31	-	55,55,55,55	0
52	MG	BA	3004	1/1	0.24	-	31,31,31,31	0
52	MG	DA	3259	1/1	0.42	-	60,60,60,60	0
52	MG	BA	3025	1/1	0.41	-	64,64,64,64	0
52	MG	BA	3044	1/1	0.42	-	19,19,19,19	0
52	MG	AA	1643	1/1	0.45	-	85,85,85,85	0
52	MG	BA	3155	1/1	0.37	-	42,42,42,42	0
52	MG	DA	3047	1/1	0.16	-	28,28,28,28	0
52	MG	DA	3269	1/1	0.80	-	64,64,64,64	0
52	MG	DA	3202	1/1	0.47	-	73,73,73,73	0
52	MG	BA	3206	1/1	0.30	-	36,36,36,36	0
52	MG	DA	3288	1/1	0.24	-	32,32,32,32	0
52	MG	BA	3261	1/1	0.24	-	34,34,34,34	0
52	MG	DA	3251	1/1	0.44	-	91,91,91,91	0
52	MG	BA	3234	1/1	0.52	-	40,40,40,40	0
52	MG	AA	1620	1/1	0.69	-	95,95,95,95	0
52	MG	DA	3253	1/1	0.15	-	51,51,51,51	0
52	MG	AA	1637	1/1	0.28	-	54,54,54,54	0
52	MG	BA	3341	1/1	0.25	-	67,67,67,67	0
52	MG	DA	3211	1/1	0.76	-	62,62,62,62	0
52	MG	DA	3267	1/1	0.33	-	57,57,57,57	0
52	MG	DA	3263	1/1	0.64	-	55,55,55,55	0
52	MG	BA	3300	1/1	0.16	-	56,56,56,56	0
52	MG	DA	3295	1/1	0.34	-	65,65,65,65	0
52	MG	BA	3026	1/1	0.29	-	58,58,58,58	0
52	MG	BA	3188	1/1	0.16	-	80,80,80,80	0
52	MG	CA	1630	1/1	0.58	-	74,74,74,74	0
52	MG	BA	3021	1/1	0.33	-	30,30,30,30	0
52	MG	B5	101	1/1	0.33	-	54,54,54,54	0
52	MG	DA	3242	1/1	0.15	-	84,84,84,84	0
52	MG	DA	3255	1/1	0.45	-	91,91,91,91	0
52	MG	DA	3158	1/1	0.67	-	71,71,71,71	0
52	MG	DA	3109	1/1	0.31	-	60,60,60,60	0
52	MG	BX	101	1/1	0.33	-	58,58,58,58	0
52	MG	BA	3049	1/1	0.44	-	26,26,26,26	0
52	MG	DA	3091	1/1	0.59	-	44,44,44,44	0
52	MG	BA	3269	1/1	0.42	-	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	3129	1/1	0.10	-	55,55,55,55	0
52	MG	DA	3313	1/1	0.52	-	64,64,64,64	0
52	MG	BA	3057	1/1	0.23	-	40,40,40,40	0
52	MG	BA	3113	1/1	0.43	-	28,28,28,28	0
52	MG	DA	3101	1/1	0.54	-	57,57,57,57	0
52	MG	BA	3007	1/1	0.63	-	57,57,57,57	0
52	MG	DA	3274	1/1	0.21	-	68,68,68,68	0
52	MG	DR	201	1/1	0.60	-	45,45,45,45	0
52	MG	BA	3131	1/1	0.16	-	17,17,17,17	0
52	MG	BA	3296	1/1	0.23	-	54,54,54,54	0
52	MG	DA	3183	1/1	1.15	-	80,80,80,80	0
52	MG	BB	206	1/1	0.77	-	66,66,66,66	0
52	MG	BA	3156	1/1	0.50	-	31,31,31,31	0
52	MG	BA	3038	1/1	0.52	-	25,25,25,25	0
52	MG	AA	1632	1/1	0.66	-	70,70,70,70	0
52	MG	BA	3252	1/1	0.22	-	72,72,72,72	0
52	MG	DA	3118	1/1	0.49	-	72,72,72,72	0
52	MG	AA	1625	1/1	0.26	-	73,73,73,73	0
52	MG	BA	3073	1/1	0.34	-	24,24,24,24	0
52	MG	CA	1625	1/1	0.34	-	70,70,70,70	0
52	MG	BA	3161	1/1	0.40	-	65,65,65,65	0
52	MG	DA	3266	1/1	0.96	-	55,55,55,55	0
52	MG	DA	3161	1/1	0.27	-	72,72,72,72	0
52	MG	DA	3167	1/1	0.28	-	45,45,45,45	0
52	MG	DA	3029	1/1	0.22	-	36,36,36,36	0
52	MG	DA	3265	1/1	0.36	-	61,61,61,61	0
52	MG	DA	3250	1/1	0.22	-	62,62,62,62	0
52	MG	DA	3069	1/1	0.28	-	54,54,54,54	0
52	MG	DA	3233	1/1	0.24	-	57,57,57,57	0
52	MG	BA	3040	1/1	0.62	-	49,49,49,49	0
52	MG	CA	1615	1/1	0.42	-	69,69,69,69	0
52	MG	AA	1650	1/1	1.42	-	86,86,86,86	0
52	MG	BA	3331	1/1	0.37	-	52,52,52,52	0
52	MG	DA	3082	1/1	0.36	-	50,50,50,50	0
52	MG	DA	3137	1/1	0.53	-	49,49,49,49	0
52	MG	BA	3047	1/1	0.62	-	41,41,41,41	0
52	MG	DA	3194	1/1	0.56	-	56,56,56,56	0
52	MG	DA	3136	1/1	0.16	-	81,81,81,81	0
52	MG	AA	1652	1/1	0.17	-	83,83,83,83	0
52	MG	BA	3124	1/1	0.30	-	12,12,12,12	0
52	MG	BA	3152	1/1	0.13	-	58,58,58,58	0
52	MG	CA	1648	1/1	0.82	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3308	1/1	0.22	-	55,55,55,55	0
52	MG	DA	3090	1/1	0.48	-	53,53,53,53	0
52	MG	DA	3224	1/1	0.55	-	47,47,47,47	0
52	MG	BA	3280	1/1	0.29	-	80,80,80,80	0
52	MG	DA	3227	1/1	0.96	-	79,79,79,79	0
52	MG	BA	3338	1/1	0.35	-	61,61,61,61	0
52	MG	CA	1644	1/1	0.31	-	86,86,86,86	0
52	MG	BA	3162	1/1	0.42	-	69,69,69,69	0
52	MG	AA	1614	1/1	0.27	-	81,81,81,81	0
52	MG	DA	3128	1/1	0.52	-	62,62,62,62	0
52	MG	DA	3193	1/1	0.47	-	54,54,54,54	0
52	MG	BA	3020	1/1	0.29	-	24,24,24,24	0
52	MG	BA	3258	1/1	0.18	-	57,57,57,57	0
52	MG	BA	3037	1/1	0.40	-	14,14,14,14	0
52	MG	BA	3170	1/1	0.83	-	44,44,44,44	0
52	MG	DA	3003	1/1	0.68	-	61,61,61,61	0
52	MG	DA	3046	1/1	0.35	-	49,49,49,49	0
52	MG	DA	3198	1/1	0.39	-	53,53,53,53	0
52	MG	BA	3034	1/1	0.34	-	69,69,69,69	0
52	MG	BA	3351	1/1	0.60	-	53,53,53,53	0
52	MG	BA	3197	1/1	0.41	-	46,46,46,46	0
52	MG	DA	3105	1/1	0.41	-	74,74,74,74	0
52	MG	BA	3242	1/1	0.57	-	71,71,71,71	0
52	MG	CA	1650	1/1	0.17	-	66,66,66,66	0
52	MG	DA	3125	1/1	0.11	-	54,54,54,54	0
52	MG	BA	3209	1/1	0.16	-	51,51,51,51	0
52	MG	DA	3054	1/1	0.61	-	47,47,47,47	0
52	MG	DA	3062	1/1	0.55	-	76,76,76,76	0
52	MG	BA	3058	1/1	0.22	-	47,47,47,47	0
52	MG	AA	1622	1/1	0.28	-	64,64,64,64	0
52	MG	BA	3183	1/1	0.39	-	55,55,55,55	0
52	MG	CA	1647	1/1	0.44	-	78,78,78,78	0
52	MG	BA	3150	1/1	0.45	-	50,50,50,50	0
52	MG	BA	3279	1/1	0.83	-	62,62,62,62	0
52	MG	BA	3255	1/1	0.29	-	46,46,46,46	0
52	MG	DA	3106	1/1	0.59	-	50,50,50,50	0
52	MG	BA	3029	1/1	0.26	-	30,30,30,30	0
52	MG	DA	3146	1/1	0.42	-	59,59,59,59	0
52	MG	DA	3180	1/1	0.53	-	56,56,56,56	0
52	MG	DA	3292	1/1	0.72	-	60,60,60,60	0
52	MG	DA	3145	1/1	0.17	-	57,57,57,57	0
52	MG	DA	3197	1/1	0.53	-	59,59,59,59	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	0.41	-	34,34,34,34	0
52	MG	DA	3152	1/1	0.44	-	66,66,66,66	0
52	MG	DA	3058	1/1	0.54	-	42,42,42,42	0
52	MG	BA	3147	1/1	0.67	-	55,55,55,55	0
52	MG	BA	3298	1/1	0.80	-	65,65,65,65	0
52	MG	BA	3159	1/1	0.69	-	58,58,58,58	0
52	MG	DA	3005	1/1	0.12	-	69,69,69,69	0
52	MG	BA	3343	1/1	0.51	-	51,51,51,51	0
52	MG	DA	3311	1/1	0.79	-	86,86,86,86	0
52	MG	BA	3273	1/1	0.33	-	44,44,44,44	0
52	MG	BA	3344	1/1	0.15	-	43,43,43,43	0
52	MG	BA	3134	1/1	0.17	-	52,52,52,52	0
52	MG	BA	3210	1/1	0.59	-	46,46,46,46	0
52	MG	DA	3140	1/1	0.59	-	46,46,46,46	0
52	MG	B7	101	1/1	0.26	-	42,42,42,42	0
52	MG	DA	3247	1/1	0.38	-	61,61,61,61	0
52	MG	BB	203	1/1	0.11	-	82,82,82,82	0
52	MG	CA	1632	1/1	0.32	-	76,76,76,76	0
52	MG	BA	3233	1/1	0.49	-	54,54,54,54	0
52	MG	BA	3316	1/1	0.11	-	43,43,43,43	0
52	MG	BA	3087	1/1	0.08	-	18,18,18,18	0
52	MG	DA	3149	1/1	0.49	-	51,51,51,51	0
52	MG	CA	1622	1/1	0.45	-	75,75,75,75	0
52	MG	BA	3302	1/1	0.26	-	67,67,67,67	0
52	MG	DA	3050	1/1	0.43	-	39,39,39,39	0
52	MG	AA	1611	1/1	0.50	-	50,50,50,50	0
52	MG	BA	3056	1/1	0.10	-	31,31,31,31	0
52	MG	AA	1639	1/1	1.17	-	77,77,77,77	0
52	MG	BA	3125	1/1	0.14	-	53,53,53,53	0
52	MG	DA	3280	1/1	0.20	-	67,67,67,67	0
52	MG	BA	3310	1/1	0.60	-	74,74,74,74	0
52	MG	DA	3022	1/1	0.39	-	38,38,38,38	0
52	MG	BA	3322	1/1	0.22	-	44,44,44,44	0
52	MG	BA	3117	1/1	0.27	-	58,58,58,58	0
52	MG	DA	3066	1/1	0.19	-	52,52,52,52	0
52	MG	DA	3108	1/1	0.35	-	56,56,56,56	0
52	MG	BA	3074	1/1	0.66	-	67,67,67,67	0
52	MG	DA	3060	1/1	0.45	-	50,50,50,50	0
52	MG	DA	3116	1/1	0.39	-	65,65,65,65	0
52	MG	CA	1623	1/1	0.17	-	79,79,79,79	0
52	MG	BA	3018	1/1	0.23	-	25,25,25,25	0
52	MG	BA	3350	1/1	0.66	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3272	1/1	0.67	-	78,78,78,78	0
52	MG	BA	3303	1/1	0.46	-	36,36,36,36	0
52	MG	DA	3185	1/1	0.25	-	65,65,65,65	0
52	MG	BA	3076	1/1	0.14	-	29,29,29,29	0
52	MG	BA	3195	1/1	0.17	-	40,40,40,40	0
52	MG	BA	3330	1/1	0.55	-	64,64,64,64	0
52	MG	DA	3068	1/1	0.26	-	80,80,80,80	0
52	MG	BA	3089	1/1	0.20	-	20,20,20,20	0
52	MG	DA	3059	1/1	0.15	-	55,55,55,55	0
52	MG	BQ	201	1/1	0.18	-	32,32,32,32	0
52	MG	BA	3165	1/1	0.16	-	57,57,57,57	0
52	MG	AA	1629	1/1	0.69	-	83,83,83,83	0
52	MG	BA	3204	1/1	0.52	-	49,49,49,49	0
52	MG	AA	1646	1/1	0.48	-	53,53,53,53	0
52	MG	DA	3115	1/1	0.36	-	58,58,58,58	0
52	MG	DA	3114	1/1	0.21	-	75,75,75,75	0
52	MG	DA	3304	1/1	0.10	-	67,67,67,67	0
52	MG	BA	3253	1/1	0.06	-	42,42,42,42	0
52	MG	DA	3206	1/1	0.95	-	74,74,74,74	0
52	MG	DA	3160	1/1	0.56	-	51,51,51,51	0
52	MG	BA	3218	1/1	0.80	-	38,38,38,38	0
52	MG	AA	1601	1/1	0.08	-	68,68,68,68	0
52	MG	BA	3272	1/1	0.45	-	38,38,38,38	0
52	MG	DA	3179	1/1	0.23	-	67,67,67,67	0
52	MG	BA	3099	1/1	0.23	-	45,45,45,45	0
52	MG	BA	3009	1/1	0.32	-	44,44,44,44	0
52	MG	BA	3213	1/1	0.24	-	34,34,34,34	0
52	MG	DA	3107	1/1	0.24	-	42,42,42,42	0
52	MG	BA	3241	1/1	0.57	-	69,69,69,69	0
52	MG	DA	3032	1/1	0.41	-	51,51,51,51	0
52	MG	DA	3013	1/1	0.39	-	77,77,77,77	0
52	MG	BA	3215	1/1	0.36	-	37,37,37,37	0
52	MG	DA	3232	1/1	0.73	-	56,56,56,56	0
52	MG	DA	3045	1/1	0.43	-	51,51,51,51	0
52	MG	BA	3045	1/1	0.32	-	22,22,22,22	0
52	MG	CA	1634	1/1	0.29	-	88,88,88,88	0
52	MG	BA	3094	1/1	0.69	-	47,47,47,47	0
52	MG	DA	3129	1/1	0.17	-	48,48,48,48	0
52	MG	BA	3247	1/1	0.43	-	77,77,77,77	0
52	MG	DA	3262	1/1	0.48	-	55,55,55,55	0
52	MG	BA	3069	1/1	0.43	-	46,46,46,46	0
52	MG	BA	3092	1/1	0.33	-	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3081	1/1	0.43	-	58,58,58,58	0
52	MG	BA	3085	1/1	0.11	-	0,0,0,0	0
52	MG	BA	3245	1/1	0.27	-	48,48,48,48	0
52	MG	CA	1620	1/1	0.19	-	70,70,70,70	0
52	MG	DA	3261	1/1	0.32	-	38,38,38,38	0
52	MG	DA	3048	1/1	0.50	-	51,51,51,51	0
52	MG	DA	3023	1/1	0.20	-	39,39,39,39	0
52	MG	DA	3110	1/1	0.60	-	46,46,46,46	0
52	MG	BA	3039	1/1	0.97	-	57,57,57,57	0
52	MG	BA	3356	1/1	0.50	-	75,75,75,75	0
52	MG	DA	3234	1/1	0.14	-	73,73,73,73	0
52	MG	BA	3079	1/1	0.17	-	48,48,48,48	0
52	MG	DA	3239	1/1	0.15	-	65,65,65,65	0
52	MG	BA	3319	1/1	0.38	-	60,60,60,60	0
52	MG	DA	3168	1/1	0.47	-	64,64,64,64	0
52	MG	BA	3175	1/1	0.29	-	50,50,50,50	0
52	MG	BA	3181	1/1	0.51	-	54,54,54,54	0
52	MG	BA	3110	1/1	0.37	-	23,23,23,23	0
52	MG	DA	3092	1/1	0.23	-	61,61,61,61	0
52	MG	DA	3043	1/1	0.38	-	43,43,43,43	0
52	MG	BA	3107	1/1	0.13	-	20,20,20,20	0
52	MG	BA	3064	1/1	0.25	-	45,45,45,45	0
52	MG	BA	3151	1/1	0.57	-	68,68,68,68	0
52	MG	DA	3038	1/1	0.81	-	68,68,68,68	0
52	MG	DB	203	1/1	0.44	-	47,47,47,47	0
52	MG	DA	3245	1/1	0.44	-	44,44,44,44	0
52	MG	BA	3054	1/1	0.18	-	50,50,50,50	0
52	MG	DA	3063	1/1	0.75	-	72,72,72,72	0
53	ZN	CN	101	1/1	0.13	-	164,164,164,164	0
52	MG	BA	3359	1/1	0.22	-	81,81,81,81	0
52	MG	DA	3314	1/1	0.64	-	54,54,54,54	0
52	MG	DA	3222	1/1	0.22	-	72,72,72,72	0
52	MG	CA	1639	1/1	0.98	-	87,87,87,87	0
52	MG	BA	3115	1/1	0.14	-	71,71,71,71	0
52	MG	BA	3138	1/1	0.75	-	42,42,42,42	0
52	MG	AA	1604	1/1	0.53	-	100,100,100,100	0
52	MG	AA	1636	1/1	0.34	-	88,88,88,88	0
52	MG	AA	1651	1/1	0.23	-	81,81,81,81	0
52	MG	BA	3179	1/1	0.63	-	55,55,55,55	0
52	MG	BA	3237	1/1	0.50	-	60,60,60,60	0
52	MG	BB	204	1/1	0.42	-	47,47,47,47	0
52	MG	BA	3328	1/1	0.26	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3031	1/1	0.34	-	66,66,66,66	0
52	MG	DA	3200	1/1	0.55	-	47,47,47,47	0
52	MG	BA	3003	1/1	0.49	-	34,34,34,34	0
52	MG	BA	3311	1/1	1.00	-	69,69,69,69	0
52	MG	DA	3184	1/1	0.23	-	96,96,96,96	0
52	MG	DA	3159	1/1	0.48	-	39,39,39,39	0
52	MG	DA	3277	1/1	0.23	-	66,66,66,66	0
52	MG	DA	3051	1/1	0.41	-	53,53,53,53	0
52	MG	BA	3012	1/1	0.53	-	61,61,61,61	0
52	MG	BA	3317	1/1	0.39	-	49,49,49,49	0
52	MG	AA	1612	1/1	0.26	-	84,84,84,84	0
52	MG	DA	3124	1/1	0.10	-	63,63,63,63	0
52	MG	AA	1628	1/1	0.52	-	65,65,65,65	0
52	MG	DA	3275	1/1	0.65	-	72,72,72,72	0
52	MG	DA	3020	1/1	0.48	-	74,74,74,74	0
52	MG	DA	3290	1/1	0.17	-	74,74,74,74	0
52	MG	BA	3223	1/1	0.59	-	45,45,45,45	0
52	MG	BA	3277	1/1	0.26	-	49,49,49,49	0
52	MG	DA	3097	1/1	0.40	-	51,51,51,51	0
52	MG	DA	3135	1/1	0.42	-	74,74,74,74	0
52	MG	BA	3335	1/1	0.57	-	55,55,55,55	0
52	MG	AA	1644	1/1	1.19	-	94,94,94,94	0
52	MG	DA	3257	1/1	0.22	-	72,72,72,72	0
52	MG	BA	3090	1/1	0.39	-	22,22,22,22	0
52	MG	DA	3204	1/1	0.15	-	48,48,48,48	0
52	MG	BA	3333	1/1	0.19	-	48,48,48,48	0
52	MG	BA	3212	1/1	0.09	-	29,29,29,29	0
52	MG	DA	3187	1/1	0.64	-	53,53,53,53	0
52	MG	DA	3298	1/1	0.23	-	46,46,46,46	0
52	MG	BA	3294	1/1	0.25	-	40,40,40,40	0
52	MG	BA	3248	1/1	0.09	-	57,57,57,57	0
52	MG	BA	3321	1/1	0.32	-	69,69,69,69	0
52	MG	DA	3316	1/1	0.34	-	75,75,75,75	0
52	MG	DA	3205	1/1	0.42	-	64,64,64,64	0
52	MG	BA	3254	1/1	0.08	-	58,58,58,58	0
52	MG	BA	3169	1/1	0.70	-	49,49,49,49	0
52	MG	BA	3137	1/1	0.22	-	16,16,16,16	0
52	MG	BA	3122	1/1	0.38	-	61,61,61,61	0
52	MG	DA	3223	1/1	0.26	-	62,62,62,62	0
52	MG	DE	301	1/1	0.15	-	34,34,34,34	0
52	MG	BA	3173	1/1	0.55	-	46,46,46,46	0
52	MG	BA	3123	1/1	0.39	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3216	1/1	0.17	-	46,46,46,46	0
52	MG	DA	3203	1/1	0.64	-	55,55,55,55	0
52	MG	BB	202	1/1	0.39	-	44,44,44,44	0
52	MG	CA	1617	1/1	0.62	-	74,74,74,74	0
52	MG	DA	3024	1/1	0.38	-	54,54,54,54	0
52	MG	BA	3236	1/1	0.48	-	38,38,38,38	0
52	MG	BA	3146	1/1	0.42	-	56,56,56,56	0
52	MG	DA	3294	1/1	0.21	-	50,50,50,50	0
52	MG	DA	3191	1/1	0.39	-	48,48,48,48	0
52	MG	BA	3353	1/1	0.25	-	73,73,73,73	0
52	MG	DA	3236	1/1	0.69	-	76,76,76,76	0
52	MG	BA	3112	1/1	0.20	-	43,43,43,43	0
52	MG	BA	3231	1/1	0.20	-	31,31,31,31	0
52	MG	CA	1638	1/1	0.23	-	62,62,62,62	0
52	MG	AA	1642	1/1	0.17	-	58,58,58,58	0
52	MG	CA	1605	1/1	0.29	-	102,102,102,102	0
52	MG	BA	3288	1/1	0.08	-	55,55,55,55	0
52	MG	BA	3274	1/1	0.22	-	36,36,36,36	0
52	MG	CA	1606	1/1	1.03	-	73,73,73,73	0
52	MG	BA	3304	1/1	0.31	-	41,41,41,41	0
52	MG	AA	1645	1/1	0.46	-	104,104,104,104	0
52	MG	AA	1602	1/1	0.59	-	50,50,50,50	0
52	MG	CA	1645	1/1	0.81	-	64,64,64,64	0
52	MG	CA	1640	1/1	0.30	-	74,74,74,74	0
52	MG	BA	3238	1/1	0.28	-	70,70,70,70	0
52	MG	BA	3163	1/1	0.34	-	45,45,45,45	0
52	MG	BR	201	1/1	0.50	-	27,27,27,27	0
52	MG	BA	3358	1/1	0.06	-	34,34,34,34	0
52	MG	DA	3033	1/1	0.42	-	63,63,63,63	0
52	MG	DA	3034	1/1	0.58	-	51,51,51,51	0
52	MG	DA	3026	1/1	0.53	-	32,32,32,32	0
52	MG	BA	3301	1/1	0.41	-	52,52,52,52	0
52	MG	DA	3132	1/1	0.13	-	72,72,72,72	0
52	MG	CA	1631	1/1	0.24	-	95,95,95,95	0
52	MG	DA	3213	1/1	0.41	-	44,44,44,44	0
52	MG	BA	3306	1/1	0.61	-	70,70,70,70	0
52	MG	DA	3036	1/1	0.94	-	54,54,54,54	0
52	MG	DA	3238	1/1	0.17	-	80,80,80,80	0
52	MG	DA	3083	1/1	0.33	-	43,43,43,43	0
52	MG	BA	3024	1/1	0.18	-	37,37,37,37	0
52	MG	BA	3346	1/1	0.17	-	61,61,61,61	0
52	MG	BA	3357	1/1	0.16	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3342	1/1	0.14	-	39,39,39,39	0
52	MG	BA	3187	1/1	0.76	-	60,60,60,60	0
52	MG	DA	3229	1/1	0.48	-	78,78,78,78	0
52	MG	DA	3019	1/1	0.46	-	42,42,42,42	0
52	MG	BA	3105	1/1	0.32	-	32,32,32,32	0
52	MG	DA	3015	1/1	0.46	-	40,40,40,40	0
52	MG	DA	3080	1/1	0.60	-	59,59,59,59	0
52	MG	BA	3102	1/1	0.37	-	41,41,41,41	0
52	MG	DA	3121	1/1	0.87	-	64,64,64,64	0
53	ZN	AN	101	1/1	0.16	-	181,181,181,181	0
52	MG	BA	3282	1/1	0.30	-	49,49,49,49	0
52	MG	DA	3196	1/1	0.18	-	41,41,41,41	0
52	MG	DA	3256	1/1	0.28	-	77,77,77,77	0
52	MG	DA	3113	1/1	0.32	-	75,75,75,75	0
52	MG	BA	3006	1/1	0.49	-	27,27,27,27	0
52	MG	DA	3201	1/1	0.67	-	46,46,46,46	0
52	MG	DA	3230	1/1	0.25	-	69,69,69,69	0
52	MG	BA	3178	1/1	0.24	-	25,25,25,25	0
52	MG	DA	3053	1/1	0.69	-	90,90,90,90	0
52	MG	DA	3286	1/1	0.34	-	63,63,63,63	0
52	MG	CA	1616	1/1	0.23	-	74,74,74,74	0
52	MG	BA	3080	1/1	0.67	-	23,23,23,23	0
52	MG	DA	3212	1/1	0.36	-	71,71,71,71	0
52	MG	BA	3114	1/1	0.51	-	49,49,49,49	0
52	MG	DA	3270	1/1	0.48	-	92,92,92,92	0
52	MG	BA	3266	1/1	0.59	-	63,63,63,63	0
52	MG	BA	3091	1/1	0.22	-	44,44,44,44	0
53	ZN	AD	301	1/1	0.27	-	110,110,110,110	0
53	ZN	CD	301	1/1	0.20	-	105,105,105,105	0
52	MG	DA	3188	1/1	0.72	-	81,81,81,81	0
52	MG	BA	3224	1/1	0.17	-	43,43,43,43	0
52	MG	CA	1626	1/1	0.60	-	70,70,70,70	0
52	MG	BA	3014	1/1	0.45	-	46,46,46,46	0
52	MG	BA	3062	1/1	0.16	-	38,38,38,38	0
52	MG	BA	3203	1/1	0.37	-	53,53,53,53	0
52	MG	DA	3163	1/1	0.10	-	77,77,77,77	0
52	MG	DA	3279	1/1	0.25	-	55,55,55,55	0
52	MG	BA	3136	1/1	0.33	-	51,51,51,51	0
52	MG	BA	3347	1/1	0.32	-	58,58,58,58	0
52	MG	DA	3309	1/1	0.06	-	76,76,76,76	0
52	MG	AA	1606	1/1	0.32	-	63,63,63,63	0
52	MG	DA	3067	1/1	0.59	-	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	BA	3041	1/1	0.27	-	22,22,22,22	0
52	MG	DA	3258	1/1	0.39	-	70,70,70,70	0
52	MG	DA	3009	1/1	0.28	-	52,52,52,52	0
55	TEL	DA	3320	58/58	0.29	-	110,110,110,110	0
52	MG	BA	3033	1/1	0.20	-	27,27,27,27	0
52	MG	DQ	201	1/1	0.18	-	63,63,63,63	0
52	MG	CA	1624	1/1	0.20	-	69,69,69,69	0
52	MG	DA	3134	1/1	0.87	-	61,61,61,61	0
52	MG	BA	3295	1/1	0.87	-	79,79,79,79	0
52	MG	BA	3360	1/1	0.05	-	68,68,68,68	0
52	MG	DA	3246	1/1	0.14	-	70,70,70,70	0
52	MG	BA	3072	1/1	0.68	-	59,59,59,59	0
52	MG	BA	3292	1/1	0.29	-	67,67,67,67	0
52	MG	DA	3086	1/1	0.22	-	61,61,61,61	0
52	MG	DA	3014	1/1	0.49	-	76,76,76,76	0
52	MG	BB	205	1/1	0.08	-	90,90,90,90	0
52	MG	BA	3128	1/1	0.18	-	63,63,63,63	0
52	MG	BA	3325	1/1	0.44	-	49,49,49,49	0
52	MG	DA	3074	1/1	0.46	-	56,56,56,56	0
52	MG	DA	3181	1/1	0.26	-	62,62,62,62	0
52	MG	BA	3314	1/1	0.47	-	63,63,63,63	0
52	MG	BA	3065	1/1	0.23	-	37,37,37,37	0
52	MG	DA	3209	1/1	0.57	-	58,58,58,58	0
52	MG	DA	3254	1/1	0.17	-	61,61,61,61	0
52	MG	BA	3143	1/1	0.39	-	34,34,34,34	0
52	MG	BA	3078	1/1	0.41	-	39,39,39,39	0
52	MG	BA	3017	1/1	0.51	-	46,46,46,46	0
52	MG	BA	3276	1/1	0.49	-	76,76,76,76	0
52	MG	BA	3284	1/1	0.33	-	34,34,34,34	0
52	MG	CA	1608	1/1	0.46	-	90,90,90,90	0
52	MG	DA	3190	1/1	0.23	-	49,49,49,49	0
52	MG	BA	3171	1/1	0.55	-	45,45,45,45	0
52	MG	DA	3310	1/1	0.47	-	54,54,54,54	0
52	MG	AA	1633	1/1	0.17	-	90,90,90,90	0
52	MG	BA	3185	1/1	0.51	-	61,61,61,61	0
52	MG	BA	3214	1/1	0.47	-	55,55,55,55	0
52	MG	CA	1649	1/1	0.17	-	80,80,80,80	0
52	MG	BP	201	1/1	0.26	-	17,17,17,17	0
52	MG	BA	3334	1/1	0.10	-	61,61,61,61	0
52	MG	BA	3061	1/1	0.39	-	36,36,36,36	0
52	MG	DA	3007	1/1	0.47	-	40,40,40,40	0
52	MG	BA	3177	1/1	0.34	-	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	3099	1/1	0.39	-	56,56,56,56	0
52	MG	BA	3157	1/1	0.17	-	24,24,24,24	0
52	MG	DA	3044	1/1	0.38	-	39,39,39,39	0
52	MG	BA	3249	1/1	0.19	-	56,56,56,56	0
52	MG	BA	3075	1/1	0.47	-	56,56,56,56	0
52	MG	BD	302	1/1	0.29	-	47,47,47,47	0
52	MG	DA	3173	1/1	0.49	-	48,48,48,48	0
52	MG	DA	3216	1/1	0.91	-	78,78,78,78	0
52	MG	AA	1613	1/1	0.31	-	76,76,76,76	0
52	MG	DA	3004	1/1	0.26	-	39,39,39,39	0
52	MG	BA	3267	1/1	0.31	-	40,40,40,40	0
52	MG	CA	1643	1/1	1.11	-	93,93,93,93	0
52	MG	BA	3219	1/1	0.43	-	75,75,75,75	0
52	MG	BA	3153	1/1	0.27	-	62,62,62,62	0
52	MG	BA	3019	1/1	0.46	-	26,26,26,26	0
52	MG	DA	3162	1/1	0.68	-	80,80,80,80	0
52	MG	DA	3252	1/1	0.23	-	55,55,55,55	0
52	MG	DA	3117	1/1	0.29	-	59,59,59,59	0
52	MG	BA	3307	1/1	0.99	-	70,70,70,70	0
52	MG	DA	3155	1/1	0.21	-	59,59,59,59	0
52	MG	DA	3027	1/1	0.28	-	43,43,43,43	0
52	MG	DA	3175	1/1	0.35	-	68,68,68,68	0
52	MG	DA	3151	1/1	0.18	-	66,66,66,66	0
52	MG	DA	3240	1/1	0.12	-	47,47,47,47	0
52	MG	AA	1630	1/1	0.70	-	75,75,75,75	0
52	MG	BA	3230	1/1	0.36	-	44,44,44,44	0
52	MG	DA	3210	1/1	0.20	-	49,49,49,49	0
52	MG	AA	1607	1/1	0.22	-	81,81,81,81	0
52	MG	DA	3088	1/1	0.52	-	53,53,53,53	0
52	MG	DA	3093	1/1	0.68	-	49,49,49,49	0
52	MG	BA	3168	1/1	0.31	-	59,59,59,59	0
52	MG	BA	3190	1/1	0.42	-	34,34,34,34	0
52	MG	DA	3030	1/1	0.24	-	66,66,66,66	0
52	MG	BA	3323	1/1	0.22	-	51,51,51,51	0
52	MG	CA	1636	1/1	0.48	-	74,74,74,74	0
52	MG	BA	3096	1/1	0.53	-	33,33,33,33	0
52	MG	BA	3051	1/1	0.28	-	22,22,22,22	0
52	MG	CA	1603	1/1	0.31	-	57,57,57,57	0
52	MG	DA	3241	1/1	0.32	-	48,48,48,48	0
52	MG	BA	3312	1/1	0.22	-	55,55,55,55	0
52	MG	DA	3235	1/1	0.17	-	48,48,48,48	0
52	MG	DA	3119	1/1	0.21	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3192	1/1	0.67	-	42,42,42,42	0
52	MG	DA	3217	1/1	0.95	-	55,55,55,55	0
52	MG	DA	3075	1/1	0.23	-	50,50,50,50	0
52	MG	BA	3011	1/1	0.47	-	22,22,22,22	0
52	MG	BA	3221	1/1	0.47	-	47,47,47,47	0
52	MG	BA	3059	1/1	0.38	-	46,46,46,46	0
52	MG	AA	1616	1/1	0.18	-	68,68,68,68	0
52	MG	DA	3142	1/1	0.47	-	69,69,69,69	0
52	MG	DA	3299	1/1	0.33	-	64,64,64,64	0
52	MG	BA	3164	1/1	0.22	-	40,40,40,40	0
52	MG	BA	3013	1/1	0.55	-	33,33,33,33	0
52	MG	BA	3264	1/1	0.23	-	58,58,58,58	0
52	MG	DA	3011	1/1	0.33	-	43,43,43,43	0
52	MG	DA	3055	1/1	0.45	-	38,38,38,38	0
52	MG	BA	3120	1/1	0.28	-	65,65,65,65	0
52	MG	BA	3133	1/1	0.25	-	38,38,38,38	0
52	MG	B5	102	1/1	0.40	-	80,80,80,80	0
52	MG	DA	3296	1/1	0.29	-	104,104,104,104	0
52	MG	BA	3228	1/1	0.83	-	56,56,56,56	0
52	MG	BQ	202	1/1	0.22	-	49,49,49,49	0
52	MG	BA	3293	1/1	0.04	-	51,51,51,51	0
52	MG	DA	3154	1/1	0.53	-	66,66,66,66	0
52	MG	BA	3135	1/1	0.49	-	30,30,30,30	0
52	MG	BA	3315	1/1	0.75	-	62,62,62,62	0
52	MG	DA	3169	1/1	0.60	-	49,49,49,49	0
52	MG	BA	3002	1/1	0.59	-	31,31,31,31	0
55	TEL	BA	3362	58/58	0.30	-	110,110,110,110	0
52	MG	DA	3170	1/1	0.71	-	76,76,76,76	0
52	MG	DA	3071	1/1	0.67	-	85,85,85,85	0
52	MG	DA	3248	1/1	0.65	-	72,72,72,72	0
52	MG	DA	3133	1/1	0.34	-	31,31,31,31	0
52	MG	DA	3122	1/1	0.16	-	61,61,61,61	0
52	MG	DA	3148	1/1	0.64	-	61,61,61,61	0
52	MG	CA	1611	1/1	0.31	-	72,72,72,72	0
52	MG	AA	1605	1/1	0.26	-	106,106,106,106	0
52	MG	DA	3293	1/1	0.38	-	60,60,60,60	0
52	MG	CA	1610	1/1	0.19	-	106,106,106,106	0
52	MG	DA	3138	1/1	0.49	-	35,35,35,35	0
52	MG	BA	3256	1/1	0.37	-	43,43,43,43	0
52	MG	BA	3260	1/1	0.17	-	46,46,46,46	0
52	MG	AA	1618	1/1	0.64	-	81,81,81,81	0
52	MG	DA	3111	1/1	0.43	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3060	1/1	0.34	-	59,59,59,59	0
52	MG	CA	1618	1/1	0.69	-	84,84,84,84	0
52	MG	BA	3176	1/1	0.84	-	68,68,68,68	0
52	MG	DA	3214	1/1	0.30	-	33,33,33,33	0
52	MG	BA	3063	1/1	0.40	-	57,57,57,57	0
52	MG	BA	3201	1/1	0.16	-	52,52,52,52	0
52	MG	BA	3290	1/1	0.52	-	87,87,87,87	0
52	MG	BA	3349	1/1	0.35	-	51,51,51,51	0
52	MG	DD	301	1/1	0.38	-	56,56,56,56	0
52	MG	BA	3189	1/1	0.45	-	40,40,40,40	0
52	MG	BA	3240	1/1	0.39	-	39,39,39,39	0
52	MG	BA	3191	1/1	0.48	-	59,59,59,59	0
52	MG	BA	3286	1/1	0.19	-	72,72,72,72	0
52	MG	DA	3012	1/1	0.51	-	29,29,29,29	0
52	MG	BA	3243	1/1	0.46	-	39,39,39,39	0
52	MG	DA	3102	1/1	0.77	-	54,54,54,54	0
52	MG	BA	3082	1/1	0.43	-	37,37,37,37	0
52	MG	BA	3035	1/1	0.34	-	23,23,23,23	0
52	MG	BA	3336	1/1	0.52	-	61,61,61,61	0
52	MG	AA	1610	1/1	0.28	-	115,115,115,115	0
52	MG	DA	3001	1/1	0.48	-	66,66,66,66	0
52	MG	BA	3048	1/1	0.34	-	20,20,20,20	0
52	MG	DA	3165	1/1	0.43	-	53,53,53,53	0
52	MG	BA	3340	1/1	0.08	-	83,83,83,83	0
52	MG	DA	3078	1/1	0.11	-	62,62,62,62	0
52	MG	DA	3100	1/1	0.19	-	59,59,59,59	0
52	MG	DA	3208	1/1	0.43	-	43,43,43,43	0
52	MG	BA	3202	1/1	0.24	-	49,49,49,49	0
52	MG	DA	3271	1/1	0.34	-	67,67,67,67	0
52	MG	BA	3262	1/1	0.40	-	68,68,68,68	0
52	MG	DA	3042	1/1	0.21	-	48,48,48,48	0
52	MG	BA	3180	1/1	0.15	-	68,68,68,68	0
52	MG	BA	3127	1/1	0.77	-	48,48,48,48	0
52	MG	BA	3355	1/1	0.20	-	78,78,78,78	0
52	MG	BA	3068	1/1	0.52	-	47,47,47,47	0
52	MG	DA	3315	1/1	0.16	-	69,69,69,69	0
52	MG	AA	1641	1/1	0.22	-	57,57,57,57	0
52	MG	BA	3139	1/1	0.40	-	60,60,60,60	0
52	MG	DA	3077	1/1	0.38	-	46,46,46,46	0
52	MG	BA	3148	1/1	0.49	-	28,28,28,28	0
52	MG	DX	101	1/1	0.45	-	76,76,76,76	0
52	MG	DA	3273	1/1	1.68	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	DA	3112	1/1	0.17	-	76,76,76,76	0
52	MG	BB	207	1/1	0.27	-	80,80,80,80	0
52	MG	CA	1642	1/1	0.26	-	80,80,80,80	0
52	MG	DA	3260	1/1	0.72	-	73,73,73,73	0
52	MG	BD	301	1/1	0.43	-	51,51,51,51	0
52	MG	BA	3100	1/1	0.45	-	40,40,40,40	0
52	MG	BA	3271	1/1	0.56	-	57,57,57,57	0
52	MG	DA	3052	1/1	0.47	-	44,44,44,44	0
52	MG	BA	3104	1/1	0.15	-	45,45,45,45	0
52	MG	DA	3061	1/1	0.15	-	40,40,40,40	0
52	MG	BA	3001	1/1	0.27	-	55,55,55,55	0
52	MG	DD	302	1/1	0.16	-	38,38,38,38	0
52	MG	BA	3235	1/1	0.49	-	43,43,43,43	0
52	MG	BA	3145	1/1	0.51	-	54,54,54,54	0
52	MG	DA	3308	1/1	0.46	-	75,75,75,75	0
52	MG	DA	3281	1/1	0.89	-	87,87,87,87	0
52	MG	DA	3276	1/1	1.17	-	87,87,87,87	0
52	MG	DA	3087	1/1	0.42	-	53,53,53,53	0
52	MG	DA	3297	1/1	0.23	-	93,93,93,93	0
52	MG	BA	3326	1/1	0.45	-	60,60,60,60	0
52	MG	BA	3095	1/1	0.31	-	43,43,43,43	0
52	MG	BA	3199	1/1	0.56	-	39,39,39,39	0
52	MG	DA	3002	1/1	0.52	-	41,41,41,41	0
52	MG	DA	3307	1/1	0.46	-	65,65,65,65	0
52	MG	BA	3097	1/1	0.41	-	53,53,53,53	0
52	MG	BA	3257	1/1	0.26	-	19,19,19,19	0
52	MG	AA	1624	1/1	0.39	-	55,55,55,55	0
52	MG	BA	3016	1/1	0.35	-	30,30,30,30	0
52	MG	DA	3176	1/1	0.80	-	41,41,41,41	0
52	MG	DA	3243	1/1	0.12	-	94,94,94,94	0
52	MG	BA	3225	1/1	0.44	-	23,23,23,23	0
52	MG	BA	3050	1/1	0.25	-	34,34,34,34	0
52	MG	BA	3043	1/1	0.20	-	39,39,39,39	0
52	MG	DA	3103	1/1	0.38	-	58,58,58,58	0
52	MG	DA	3144	1/1	0.50	-	65,65,65,65	0
52	MG	DA	3192	1/1	0.50	-	71,71,71,71	0
52	MG	DA	3306	1/1	0.26	-	63,63,63,63	0
52	MG	DA	3098	1/1	0.44	-	38,38,38,38	0
52	MG	BA	3289	1/1	0.15	-	66,66,66,66	0
52	MG	BA	3084	1/1	0.37	-	25,25,25,25	0
52	MG	AA	1608	1/1	0.44	-	71,71,71,71	0
52	MG	DA	3301	1/1	0.82	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	AA	1640	1/1	0.29	-	77,77,77,77	0
52	MG	DA	3123	1/1	0.24	-	67,67,67,67	0
52	MG	BA	3083	1/1	0.52	-	45,45,45,45	0
52	MG	BU	201	1/1	0.26	-	29,29,29,29	0
52	MG	BA	3046	1/1	0.34	-	38,38,38,38	0
52	MG	BA	3101	1/1	0.34	-	17,17,17,17	0
52	MG	BA	3070	1/1	0.25	-	25,25,25,25	0
52	MG	BA	3297	1/1	0.52	-	68,68,68,68	0
52	MG	DA	3139	1/1	0.65	-	48,48,48,48	0
52	MG	AA	1627	1/1	0.27	-	71,71,71,71	0
52	MG	DA	3064	1/1	0.23	-	46,46,46,46	0
52	MG	CA	1641	1/1	0.11	-	54,54,54,54	0
52	MG	CA	1601	1/1	0.21	-	85,85,85,85	0
52	MG	BA	3121	1/1	0.46	-	51,51,51,51	0
52	MG	DA	3289	1/1	0.32	-	71,71,71,71	0
52	MG	DA	3291	1/1	1.19	-	88,88,88,88	0
52	MG	DA	3072	1/1	0.26	-	42,42,42,42	0
52	MG	AA	1649	1/1	0.39	-	68,68,68,68	0
52	MG	BA	3144	1/1	0.74	-	43,43,43,43	0
52	MG	BP	202	1/1	0.79	-	66,66,66,66	0
52	MG	D5	101	1/1	0.54	-	51,51,51,51	0
52	MG	BB	201	1/1	0.35	-	47,47,47,47	0
52	MG	DA	3073	1/1	0.51	-	55,55,55,55	0
52	MG	DA	3282	1/1	0.22	-	59,59,59,59	0
52	MG	BA	3354	1/1	0.19	-	71,71,71,71	0
52	MG	CA	1633	1/1	1.03	-	77,77,77,77	0
52	MG	BA	3036	1/1	0.21	-	0,0,0,0	0
52	MG	AA	1631	1/1	0.08	-	63,63,63,63	0
52	MG	DA	3218	1/1	0.55	-	53,53,53,53	0
52	MG	DA	3284	1/1	0.22	-	70,70,70,70	0
52	MG	CA	1629	1/1	0.11	-	69,69,69,69	0
52	MG	DA	3010	1/1	0.56	-	45,45,45,45	0
52	MG	DA	3057	1/1	0.21	-	60,60,60,60	0
52	MG	DA	3096	1/1	0.35	-	42,42,42,42	0
52	MG	AA	1617	1/1	0.34	-	55,55,55,55	0
52	MG	BA	3345	1/1	0.23	-	70,70,70,70	0
52	MG	DA	3079	1/1	0.89	-	39,39,39,39	0
52	MG	B1	101	1/1	0.17	-	41,41,41,41	0
52	MG	BA	3030	1/1	0.15	-	26,26,26,26	0
52	MG	BA	3132	1/1	0.37	-	59,59,59,59	0
52	MG	DA	3264	1/1	0.38	-	87,87,87,87	0
52	MG	DA	3021	1/1	0.19	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	AA	1609	1/1	0.31	-	65,65,65,65	0
52	MG	BA	3086	1/1	0.20	-	28,28,28,28	0
52	MG	CA	1609	1/1	0.16	-	48,48,48,48	0
52	MG	B0	101	1/1	0.09	-	48,48,48,48	0
52	MG	DA	3016	1/1	0.53	-	54,54,54,54	0
52	MG	BA	3032	1/1	0.33	-	39,39,39,39	0
52	MG	DA	3278	1/1	0.80	-	83,83,83,83	0
52	MG	DA	3153	1/1	0.21	-	80,80,80,80	0
52	MG	DA	3056	1/1	0.35	-	51,51,51,51	0
52	MG	DA	3182	1/1	0.69	-	54,54,54,54	0
52	MG	AA	1626	1/1	0.42	-	84,84,84,84	0
52	MG	DA	3039	1/1	1.03	-	69,69,69,69	0
52	MG	DA	3228	1/1	0.18	-	57,57,57,57	0
52	MG	DA	3025	1/1	0.80	-	61,61,61,61	0
52	MG	BA	3305	1/1	0.52	-	72,72,72,72	0
52	MG	BA	3283	1/1	0.60	-	70,70,70,70	0
52	MG	AA	1603	1/1	0.29	-	45,45,45,45	0
52	MG	BA	3329	1/1	0.56	-	65,65,65,65	0
52	MG	DA	3215	1/1	0.14	-	61,61,61,61	0
52	MG	CA	1627	1/1	0.70	-	76,76,76,76	0
52	MG	BA	3196	1/1	1.04	-	66,66,66,66	0
52	MG	BA	3222	1/1	0.28	-	58,58,58,58	0
52	MG	BA	3239	1/1	0.24	-	61,61,61,61	0
52	MG	BA	3149	1/1	0.13	-	24,24,24,24	0
52	MG	BA	3023	1/1	0.28	-	31,31,31,31	0
52	MG	DA	3220	1/1	0.23	-	68,68,68,68	0
52	MG	BA	3263	1/1	0.39	-	54,54,54,54	0
52	MG	BA	3027	1/1	0.46	-	19,19,19,19	0
52	MG	BA	3278	1/1	0.23	-	62,62,62,62	0
52	MG	BA	3324	1/1	0.28	-	64,64,64,64	0
52	MG	DA	3095	1/1	0.18	-	56,56,56,56	0
52	MG	DA	3150	1/1	0.94	-	80,80,80,80	0
52	MG	BA	3028	1/1	0.30	-	30,30,30,30	0
52	MG	BA	3348	1/1	0.43	-	73,73,73,73	0
52	MG	BA	3066	1/1	0.36	-	36,36,36,36	0
52	MG	DA	3157	1/1	0.24	-	72,72,72,72	0
52	MG	BA	3071	1/1	0.41	-	32,32,32,32	0
52	MG	AA	1647	1/1	0.32	-	72,72,72,72	0
52	MG	BA	3227	1/1	0.25	-	21,21,21,21	0
52	MG	DA	3300	1/1	0.73	-	58,58,58,58	0
52	MG	DA	3219	1/1	0.51	-	49,49,49,49	0
52	MG	DB	202	1/1	0.33	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
52	MG	BA	3109	1/1	0.19	-	36,36,36,36	0
52	MG	DA	3312	1/1	0.36	-	53,53,53,53	0
52	MG	BA	3246	1/1	0.41	-	68,68,68,68	0
52	MG	BA	3158	1/1	0.33	-	32,32,32,32	0
52	MG	BA	3119	1/1	0.27	-	47,47,47,47	0
52	MG	AA	1634	1/1	0.37	-	54,54,54,54	0
52	MG	DA	3199	1/1	0.21	-	74,74,74,74	0
52	MG	CA	1637	1/1	0.15	-	85,85,85,85	0
52	MG	DA	3141	1/1	0.21	-	65,65,65,65	0
52	MG	BA	3194	1/1	0.24	-	27,27,27,27	0
52	MG	BA	3337	1/1	0.89	-	61,61,61,61	0
52	MG	DA	3035	1/1	0.57	-	41,41,41,41	0
52	MG	DA	3143	1/1	0.43	-	43,43,43,43	0
52	MG	BA	3118	1/1	0.32	-	44,44,44,44	0
52	MG	DA	3008	1/1	0.38	-	50,50,50,50	0
52	MG	BA	3111	1/1	0.21	-	19,19,19,19	0
52	MG	BA	3141	1/1	0.28	-	19,19,19,19	0
52	MG	CA	1613	1/1	0.82	-	87,87,87,87	0
52	MG	DA	3166	1/1	0.13	-	55,55,55,55	0
52	MG	DA	3126	1/1	0.35	-	57,57,57,57	0
52	MG	DA	3171	1/1	0.14	-	73,73,73,73	0
52	MG	DA	3237	1/1	0.28	-	56,56,56,56	0
52	MG	DA	3305	1/1	0.06	-	80,80,80,80	0
52	MG	BA	3022	1/1	0.33	-	45,45,45,45	0
52	MG	DA	3120	1/1	0.34	-	84,84,84,84	0
52	MG	BA	3042	1/1	0.25	-	31,31,31,31	0
52	MG	DA	3283	1/1	0.49	-	57,57,57,57	0
52	MG	DA	3076	1/1	0.24	-	56,56,56,56	0
52	MG	DA	3189	1/1	0.21	-	45,45,45,45	0
52	MG	DA	3085	1/1	0.34	-	62,62,62,62	0
52	MG	BA	3088	1/1	0.67	-	60,60,60,60	0
52	MG	BA	3166	1/1	0.58	-	75,75,75,75	0
52	MG	DA	3040	1/1	0.35	-	36,36,36,36	0
52	MG	BA	3320	1/1	0.17	-	48,48,48,48	0
52	MG	BA	3208	1/1	0.48	-	36,36,36,36	0
52	MG	AA	1619	1/1	0.54	-	55,55,55,55	0
52	MG	DA	3164	1/1	0.25	-	50,50,50,50	0
52	MG	BA	3126	1/1	0.24	-	56,56,56,56	0
52	MG	BA	3250	1/1	0.21	-	40,40,40,40	0
52	MG	DP	201	1/1	0.13	-	42,42,42,42	0
52	MG	BA	3067	1/1	0.45	-	38,38,38,38	0
52	MG	BA	3198	1/1	0.34	-	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	BA	3285	1/1	0.84	-	56,56,56,56	0
52	MG	BA	3251	1/1	0.67	-	44,44,44,44	0
52	MG	BA	3081	1/1	0.43	-	39,39,39,39	0
52	MG	BA	3008	1/1	0.48	-	36,36,36,36	0
52	MG	DA	3287	1/1	0.27	-	64,64,64,64	0
52	MG	BA	3299	1/1	0.77	-	43,43,43,43	0
52	MG	DA	3131	1/1	0.67	-	66,66,66,66	0
52	MG	BA	3318	1/1	0.29	-	55,55,55,55	0
52	MG	BA	3108	1/1	0.32	-	43,43,43,43	0
52	MG	AA	1621	1/1	0.50	-	51,51,51,51	0
52	MG	BA	3053	1/1	0.54	-	33,33,33,33	0
52	MG	BA	3270	1/1	0.18	-	24,24,24,24	0
52	MG	BA	3211	1/1	0.54	-	38,38,38,38	0
52	MG	AA	1635	1/1	0.63	-	50,50,50,50	0
52	MG	DA	3031	1/1	0.66	-	61,61,61,61	0
52	MG	BA	3259	1/1	0.12	-	47,47,47,47	0
52	MG	BA	3220	1/1	0.44	-	36,36,36,36	0
52	MG	BP	203	1/1	0.23	-	29,29,29,29	0
52	MG	DB	201	1/1	0.41	-	59,59,59,59	0
52	MG	DA	3156	1/1	0.45	-	44,44,44,44	0
52	MG	CA	1619	1/1	0.40	-	61,61,61,61	0
52	MG	BA	3077	1/1	0.22	-	40,40,40,40	0
52	MG	BA	3142	1/1	0.65	-	47,47,47,47	0
52	MG	D8	101	1/1	0.61	-	66,66,66,66	0
52	MG	CA	1607	1/1	0.42	-	74,74,74,74	0
52	MG	BA	3200	1/1	0.80	-	55,55,55,55	0
52	MG	BA	3205	1/1	1.08	-	68,68,68,68	0
52	MG	BA	3130	1/1	0.74	-	65,65,65,65	0
52	MG	DF	301	1/1	0.22	-	83,83,83,83	0
52	MG	DA	3174	1/1	0.42	-	35,35,35,35	0
52	MG	BA	3229	1/1	0.06	-	30,30,30,30	0
52	MG	BA	3106	1/1	0.82	-	43,43,43,43	0
52	MG	BA	3291	1/1	0.37	-	45,45,45,45	0
52	MG	BF	301	1/1	0.25	-	59,59,59,59	0
52	MG	DA	3186	1/1	0.37	-	58,58,58,58	0
52	MG	DA	3231	1/1	0.18	-	42,42,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.