



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 09:34 PM BST

PDB ID : 4V5K
Title : Structure of cytotoxic domain of colicin E3 bound to the 70S ribosome
Authors : Ng, C.L.; Lang, K.; Meenan, N.A.G.; Sharma, A.; Kelley, A.C.; Kleanthous, C.; Ramakrishnan, V.
Deposited on : 2010-05-29
Resolution : 3.20 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>

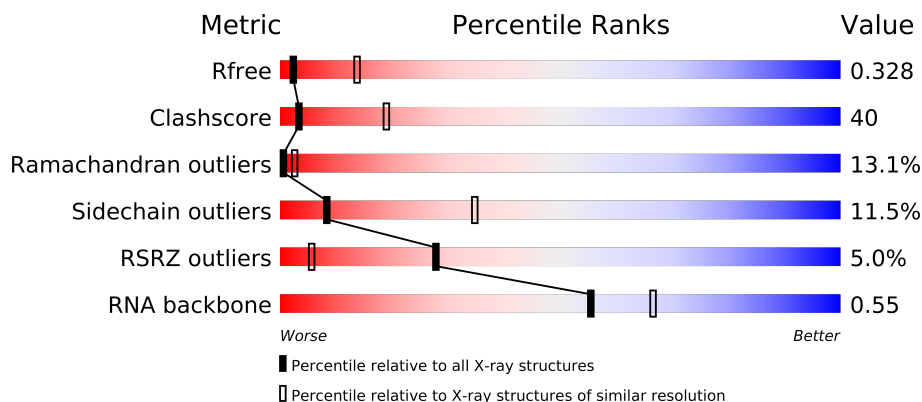
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	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	

Continued on next page...

Continued from previous page...

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	AV	77	
22	AW	77	
22	CV	77	
22	CW	77	
23	AX	25	
24	AY	97	
24	CY	97	
25	B0	85	
25	D0	85	
26	B1	98	
26	D1	98	
27	B2	72	




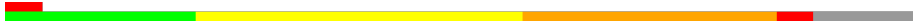
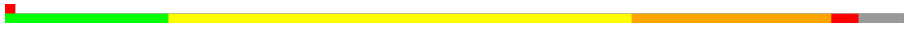
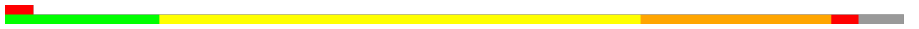


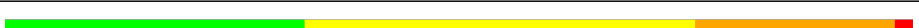
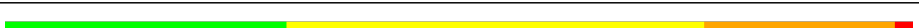
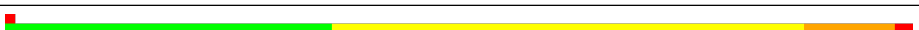
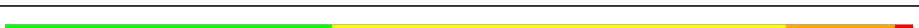
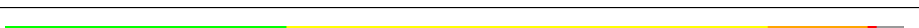

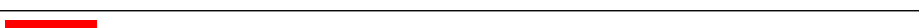
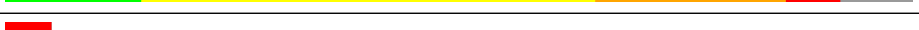

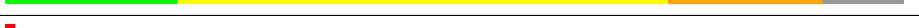


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2848	
35	DA	2848	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	
39	DE	206	
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BI	148	
43	DI	148	
44	BJ	130	
45	BN	140	
45	DN	140	
46	BO	122	
46	DO	122	
47	BP	150	
47	DP	150	
48	BQ	141	
48	DQ	141	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
49	BR	118	
49	DR	118	
50	BS	112	
50	DS	112	
51	BT	146	
51	DT	146	
52	BU	118	
52	DU	118	
53	BV	101	
53	DV	101	
54	BW	113	
54	DW	113	
55	BX	96	
55	DX	96	
56	BY	110	
56	DY	110	
57	BZ	206	
57	DZ	206	
58	CX	25	
59	DJ	131	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 296762 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	1508	Total	C	N	O	P	0	0	0
			32412	14427	6003	10475	1507			
1	CA	1508	Total	C	N	O	P	0	0	0
			32413	14427	6004	10475	1507			

- 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	1
			1692	1060	336	289	7			
4	CD	208	Total	C	N	O	S	0	0	1
			1692	1060	336	289	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				

- 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			

Continued on next page...

Continued from previous page...

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	118	Total	C	N	O	S	0	0	1
			934	577	193	162	2			
13	CM	118	Total	C	N	O	S	0	0	1
			934	577	193	162	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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	85	Total	C	N	O	S	0	0	1
			671	427	124	118	2			
19	CS	85	Total	C	N	O	S	0	0	1
			671	427	124	118	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 RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	AW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	CV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	CW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	16	Total	C	N	O	P	0	0	0
			341	155	66	105	15			

- Molecule 24 is a protein called COLICIN-E3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AY	97	Total	C	N	O	0	0	0
			769	483	144	142			
24	CY	16	Total	C	N	O	0	0	1
			126	82	23	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	58	ALA	HIS	ENGINEERED MUTATION	UNP P06646
CY	58	ALA	HIS	ENGINEERED MUTATION	UNP P00646

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

Continued on next page...

Continued from previous page...

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			734	460	148	125	1			
26	D1	94	Total	C	N	O	S	0	0	1
			734	460	148	125	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	ARG	LYS	CONFLICT	UNP P60494
D1	81	ARG	LYS	CONFLICT	UNP P60494

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	56	Total	C	N	O	S	0	0	1
			434	274	75	81	4			
29	D4	56	Total	C	N	O	S	0	0	1
			434	274	75	81	4			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

- Molecule 35 is a RNA chain called RNA (2848-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	DA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

- Molecule 36 is a RNA chain called RNA (119-MER).

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			
42	DH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BI	145	Total	C	N	O	S	0	0	1
			1125	718	200	206	1			
43	DI	145	Total	C	N	O	S	0	0	1
			1125	718	200	206	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O	0	0	0
			651	390	130	131			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

Continued on next page...

Continued from previous page...

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	187	Total	C	N	O	S	0	0	1
			1482	944	264	272	2			
57	DZ	187	Total	C	N	O	S	0	0	1
			1482	944	264	272	2			

- Molecule 58 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	CX	8	Total	C	N	O	P	0	0	0
			173	79	37	50	7			

- Molecule 59 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
59	DJ	131	Total	C	N	O	0	0	1
			651	390	131	130			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AP	1	Total	Mg	0	0
			1	1		
60	BA	709	Total	Mg	0	0
			709	709		
60	CA	184	Total	Mg	0	0
			184	184		
60	DN	3	Total	Mg	0	0
			3	3		
60	CH	1	Total	Mg	0	0
			1	1		
60	DF	3	Total	Mg	0	0
			3	3		
60	CV	12	Total	Mg	0	0
			12	12		
60	D2	1	Total	Mg	0	0
			1	1		
60	BE	4	Total	Mg	0	0
			4	4		
60	DU	4	Total	Mg	0	0
			4	4		
60	B1	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AN	2	Total 2	Mg 2	0	0
60	BP	4	Total 4	Mg 4	0	0
60	AX	4	Total 4	Mg 4	0	0
60	D6	2	Total 2	Mg 2	0	0
60	CY	1	Total 1	Mg 1	0	0
60	DD	6	Total 6	Mg 6	0	0
60	B5	3	Total 3	Mg 3	0	0
60	BB	6	Total 6	Mg 6	0	0
60	BT	1	Total 1	Mg 1	0	0
60	DO	1	Total 1	Mg 1	0	0
60	D3	1	Total 1	Mg 1	0	0
60	BF	1	Total 1	Mg 1	0	0
60	AV	7	Total 7	Mg 7	0	0
60	DR	2	Total 2	Mg 2	0	0
60	D8	1	Total 1	Mg 1	0	0
60	AA	373	Total 373	Mg 373	0	0
60	BQ	1	Total 1	Mg 1	0	0
60	CQ	1	Total 1	Mg 1	0	0
60	D7	4	Total 4	Mg 4	0	0
60	B6	1	Total 1	Mg 1	0	0
60	BU	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CC	3	Total 3	Mg 3	0	0
60	AD	3	Total 3	Mg 3	0	0
60	BN	1	Total 1	Mg 1	0	0
60	D0	4	Total 4	Mg 4	0	0
60	AI	3	Total 3	Mg 3	0	0
60	BY	1	Total 1	Mg 1	0	0
60	DE	4	Total 4	Mg 4	0	0
60	D9	1	Total 1	Mg 1	0	0
60	CJ	2	Total 2	Mg 2	0	0
60	BR	5	Total 5	Mg 5	0	0
60	CP	1	Total 1	Mg 1	0	0
60	DA	897	Total 897	Mg 897	0	0
60	DW	1	Total 1	Mg 1	0	0
60	D5	3	Total 3	Mg 3	0	0
60	B7	1	Total 1	Mg 1	0	0
60	AL	6	Total 6	Mg 6	0	0
60	CM	3	Total 3	Mg 3	0	0
60	BO	1	Total 1	Mg 1	0	0
60	AQ	3	Total 3	Mg 3	0	0
60	D1	2	Total 2	Mg 2	0	0
60	AH	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

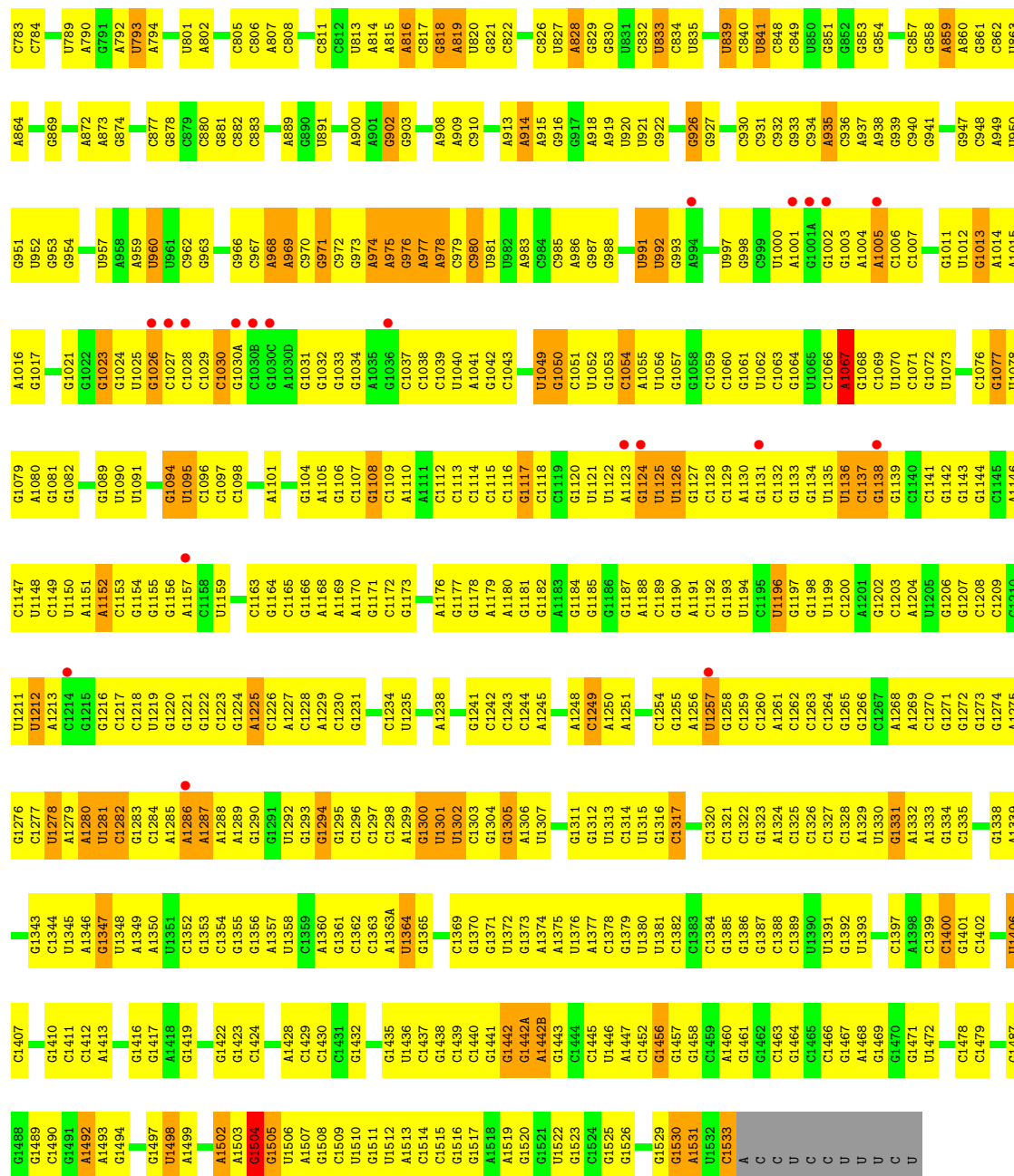
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DP	6	Total 6	Mg 6	0	0
60	AC	2	Total 2	Mg 2	0	0
60	DY	1	Total 1	Mg 1	0	0
60	DB	11	Total 11	Mg 11	0	0
60	CS	2	Total 2	Mg 2	0	0
60	CD	1	Total 1	Mg 1	0	0
60	BD	5	Total 5	Mg 5	0	0
60	AT	1	Total 1	Mg 1	0	0
60	DT	1	Total 1	Mg 1	0	0
60	B0	2	Total 2	Mg 2	0	0
60	AO	2	Total 2	Mg 2	0	0
60	AY	3	Total 3	Mg 3	0	0
60	BH	4	Total 4	Mg 4	0	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AD	2	Total 2	Zn 2	0	0
61	CD	1	Total 1	Zn 1	0	0
61	AN	1	Total 1	Zn 1	0	0

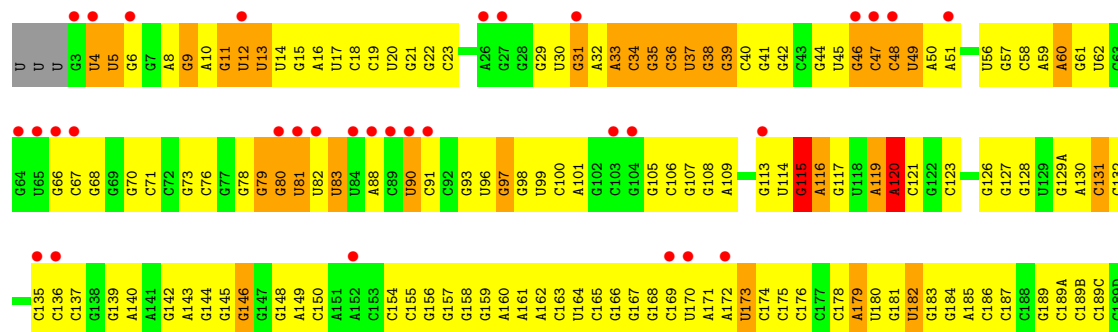
- Molecule 62 is water.

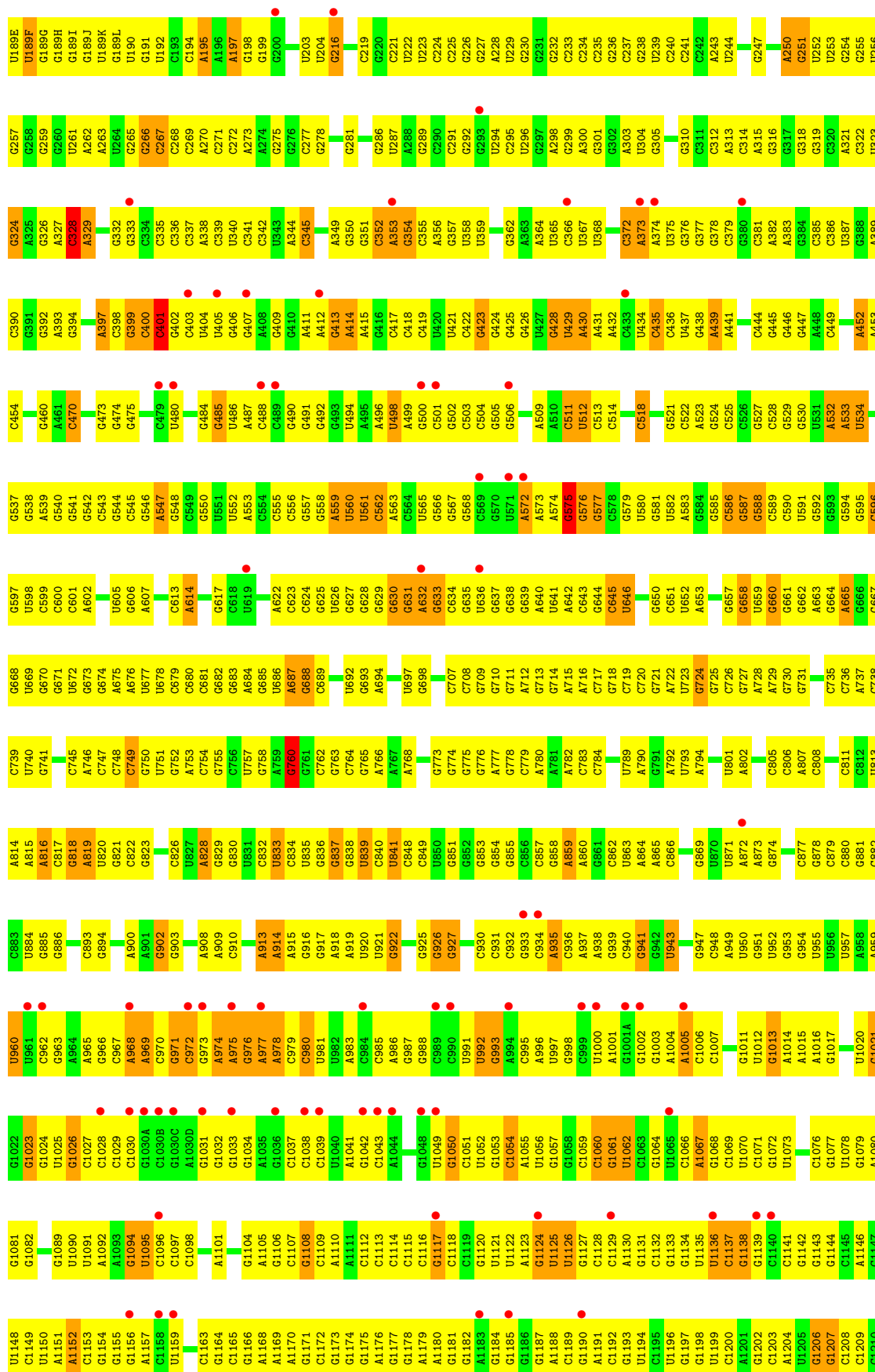
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AA	2	Total 2	O 2	0	0

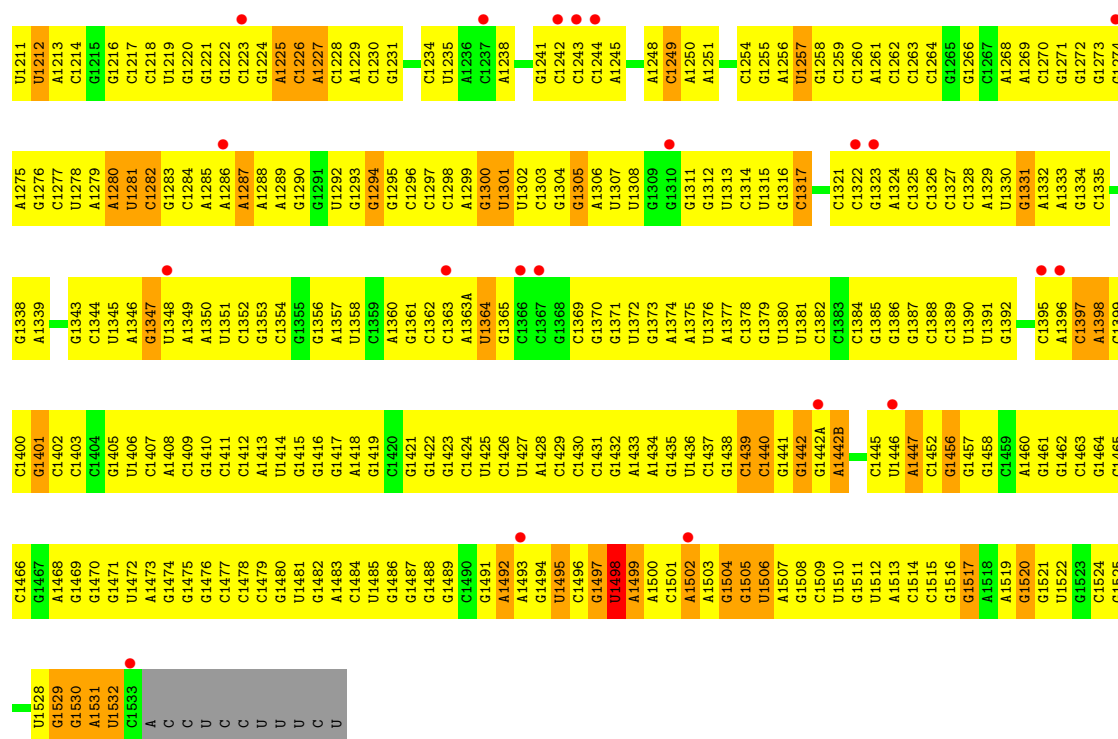


Molecule 1: 16S rRNA

Chain CA:

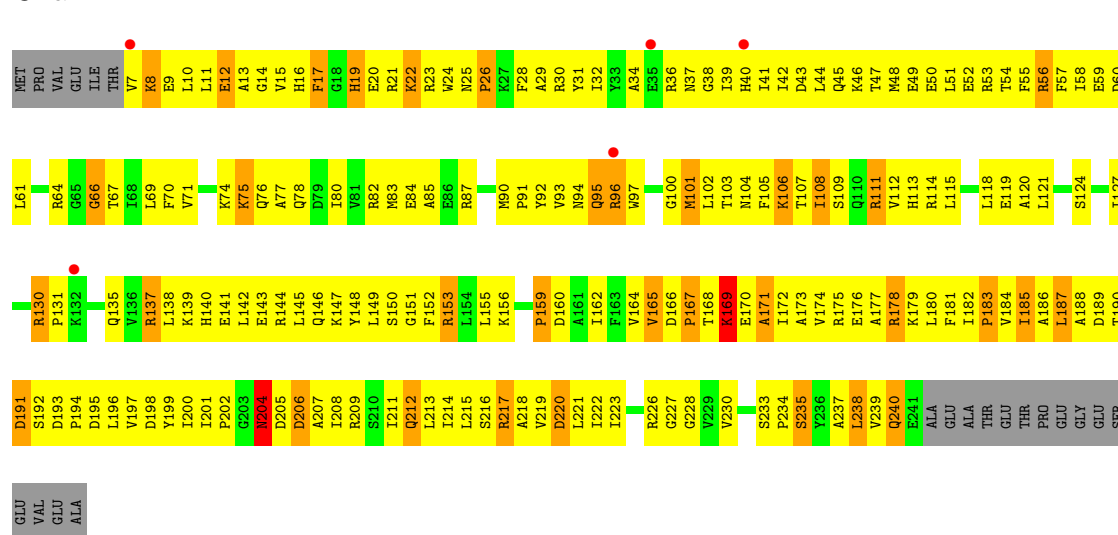






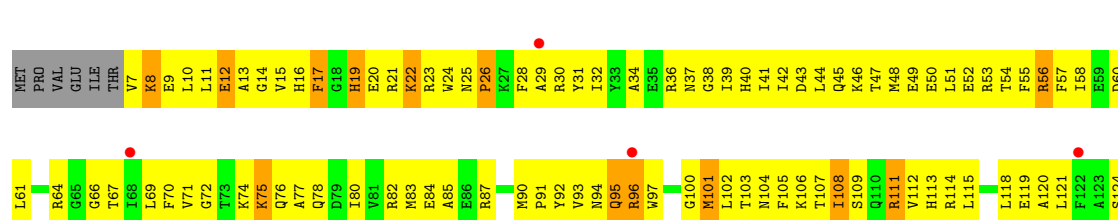
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

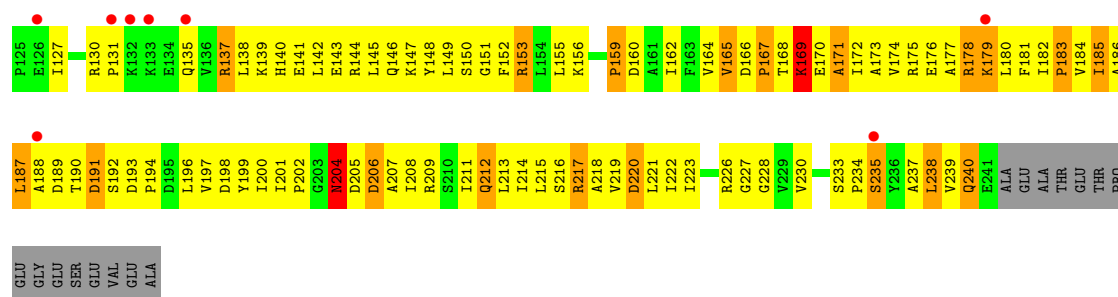
Chain AB:



• Molecule 2: 30S RIBOSOMAL PROTEIN S2

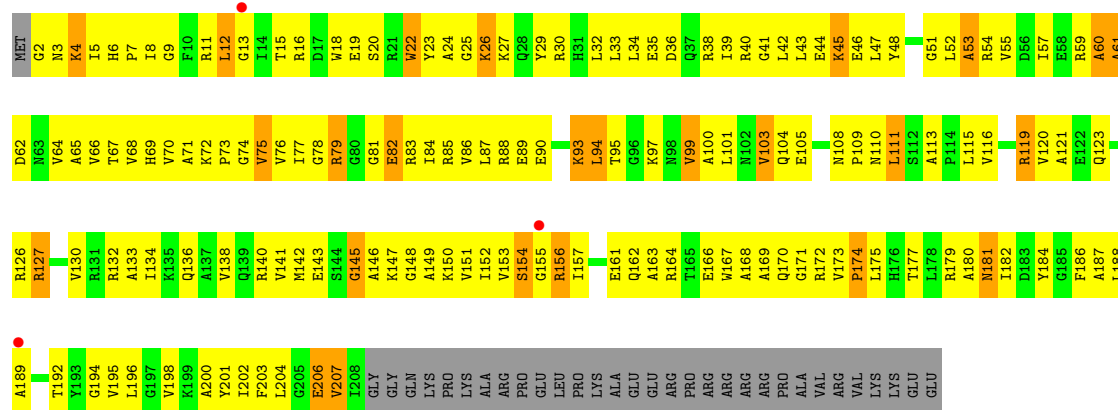
Chain CB:





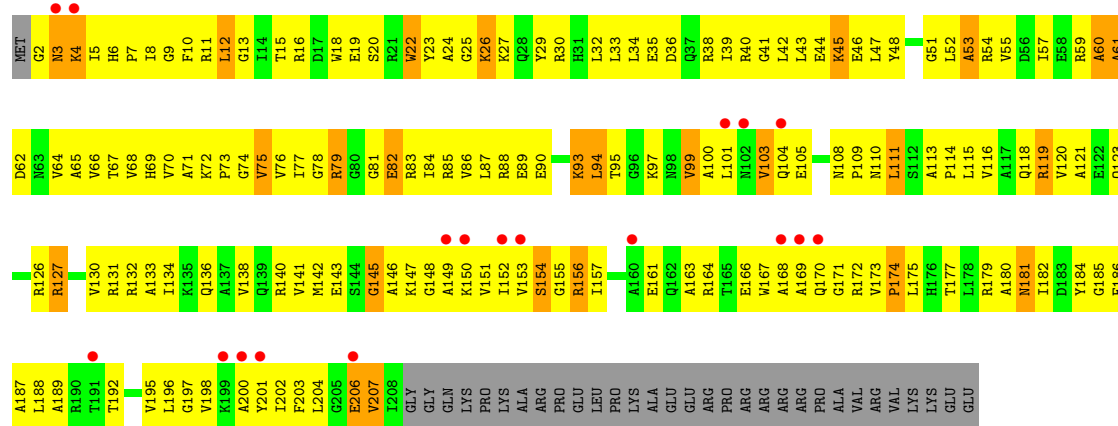
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:



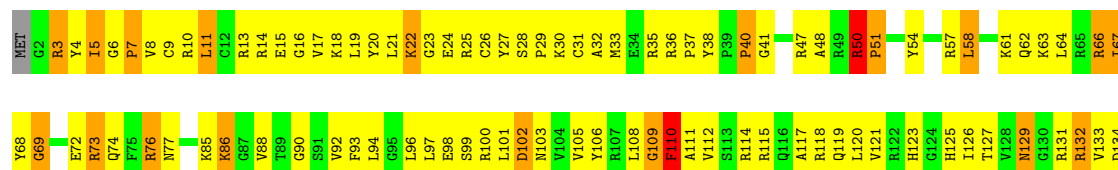
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

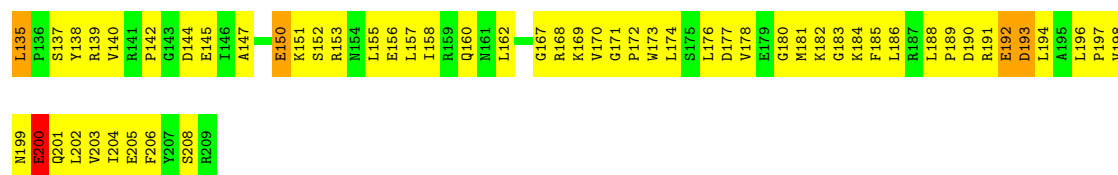
Chain CC:



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

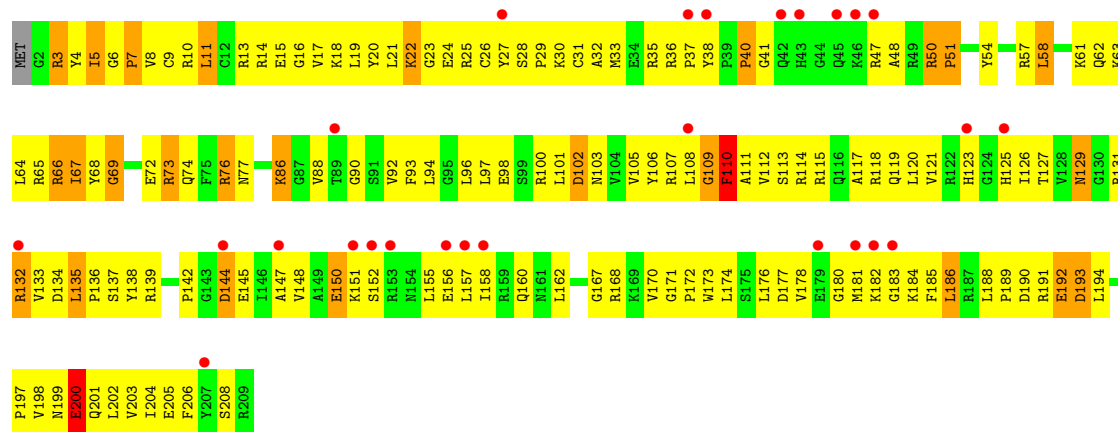
Chain AD:





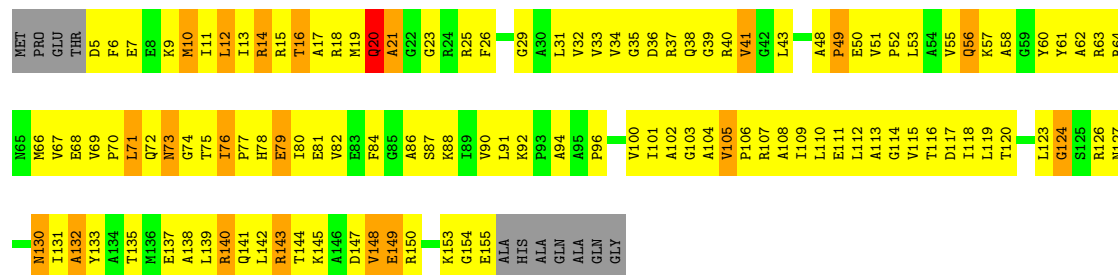
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CD:



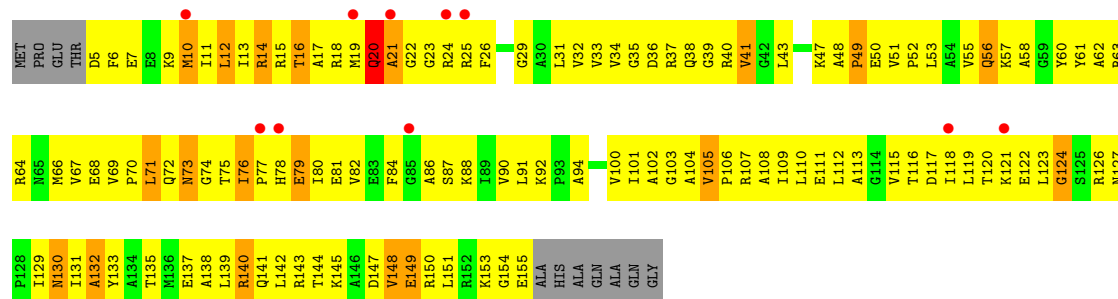
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:



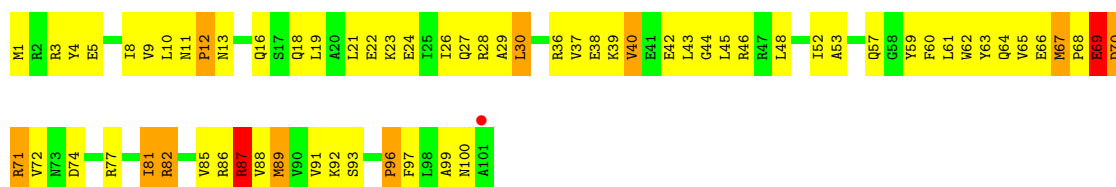
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:



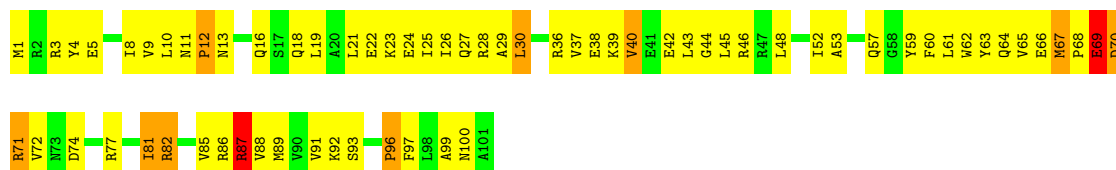
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



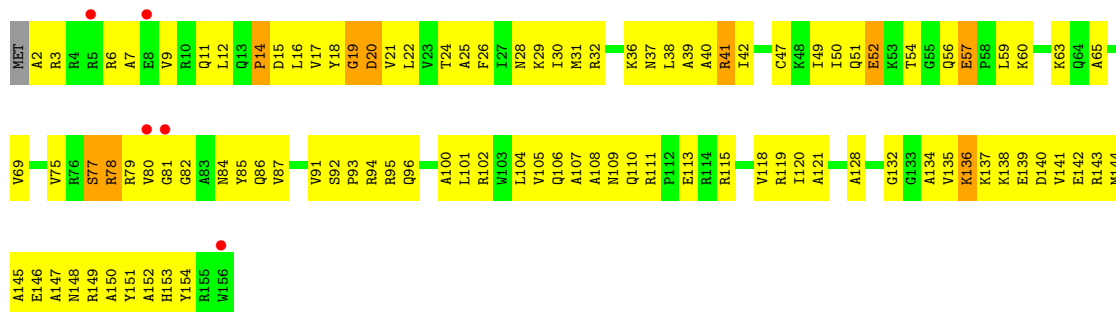
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CF:



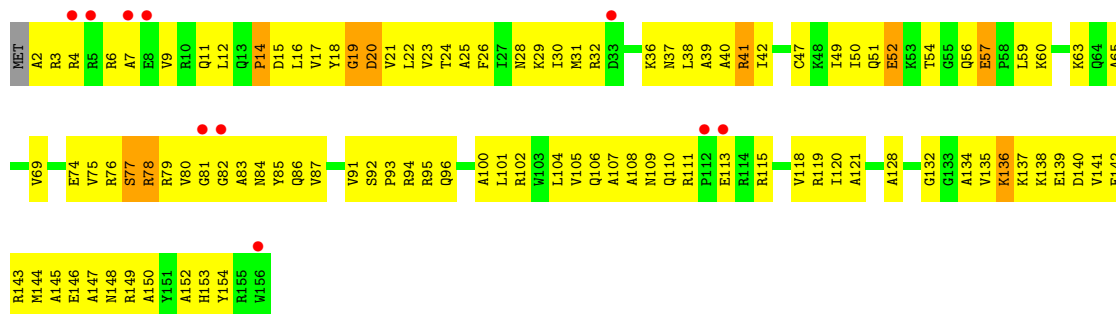
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:



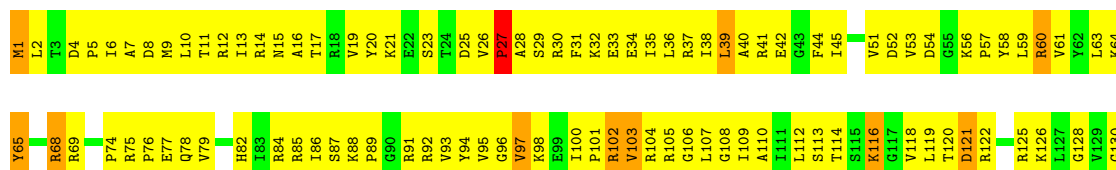
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG:



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



G131
E132
L133
I134
C135
E136
V137
W138

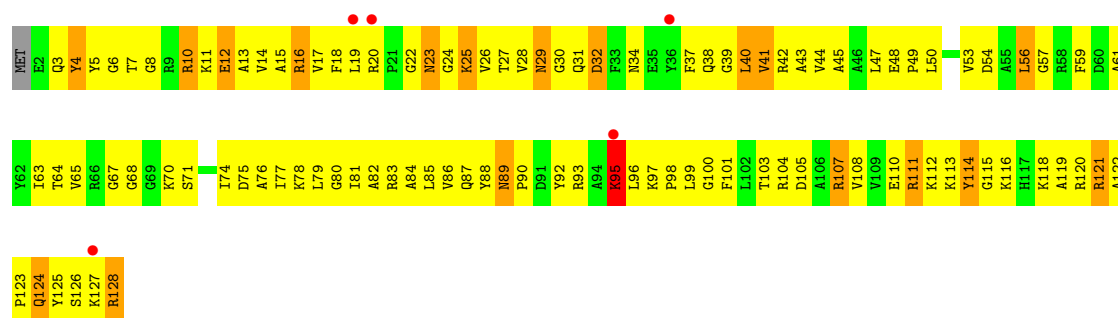
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH:



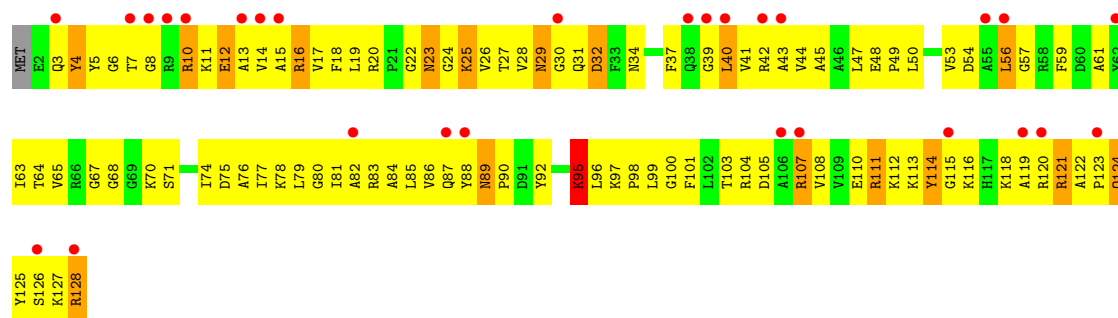
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



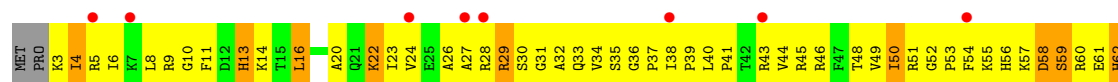
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

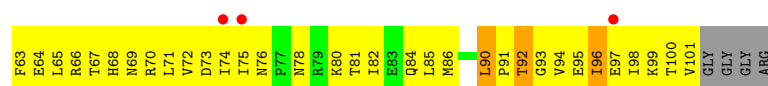
Chain CI:



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

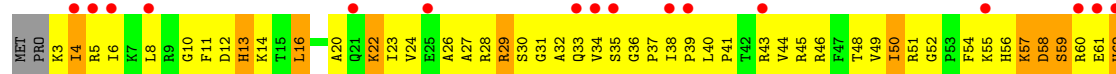
Chain AJ:





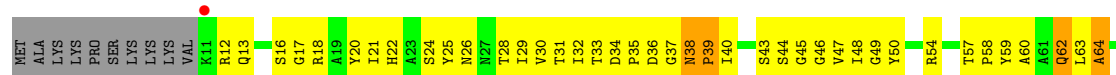
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:



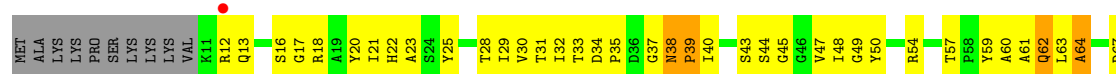
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



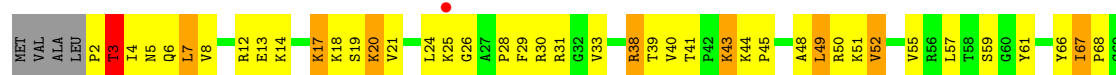
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



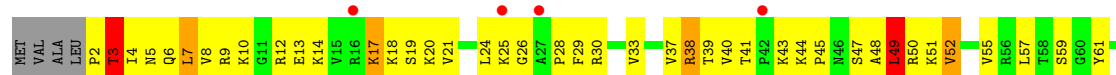
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

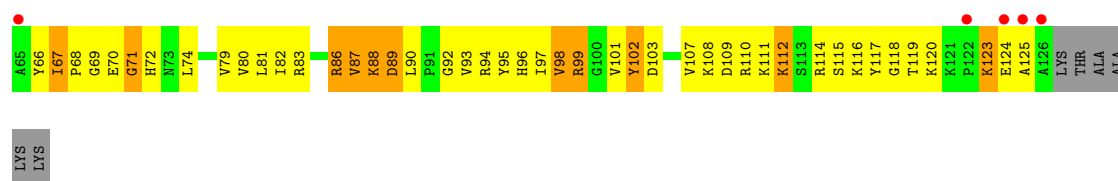
Chain AL:



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

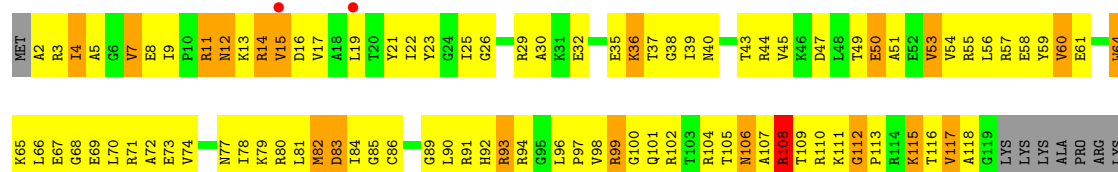
Chain CL:





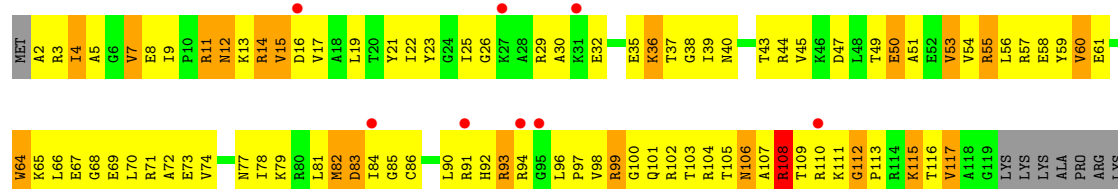
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:



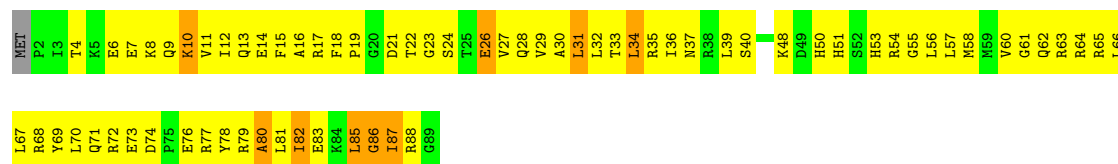
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN:



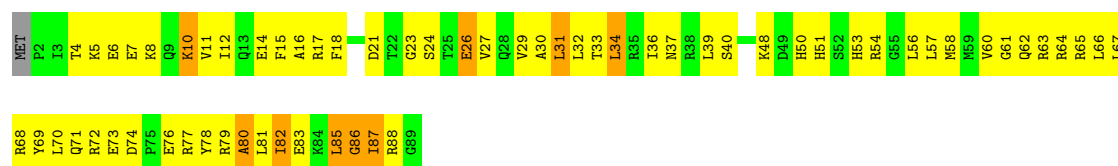
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



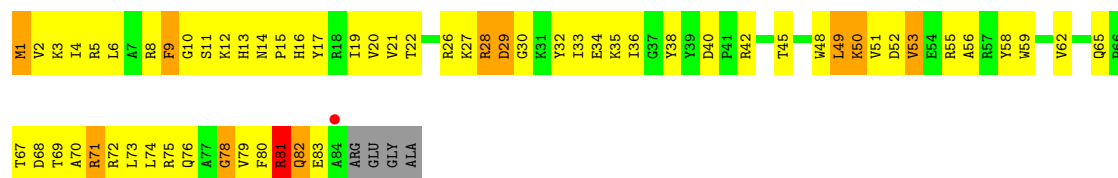
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



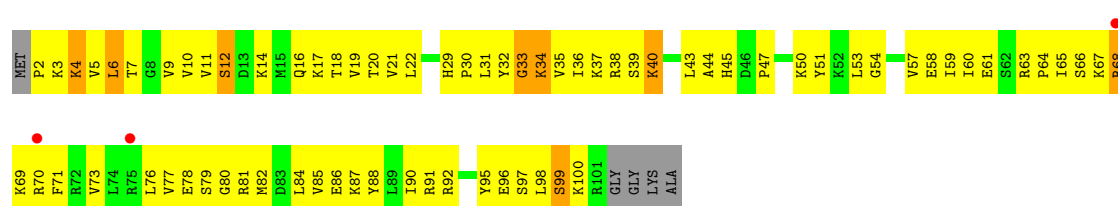
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



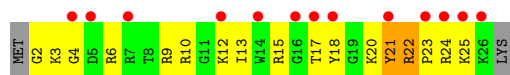
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



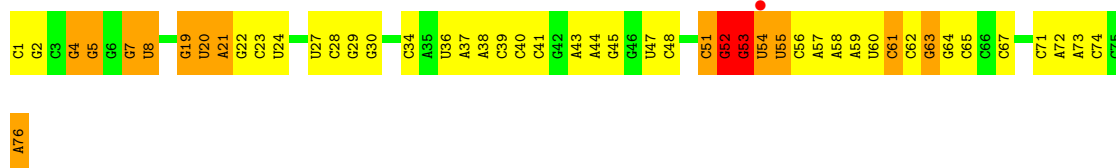
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:



- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AV:



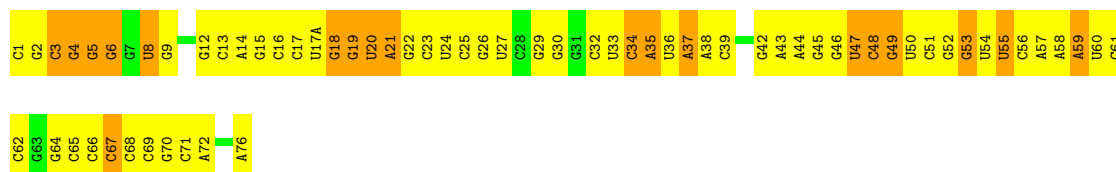
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AW:



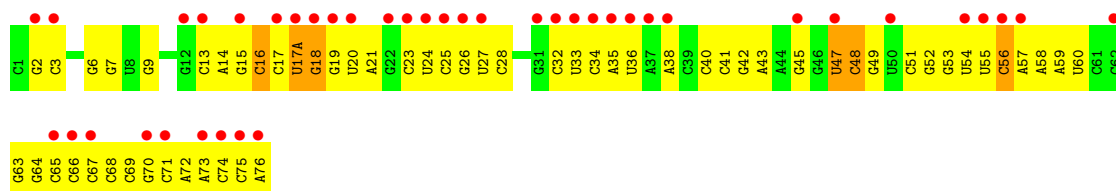
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain CV:



- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain CW:



G	G	C	A	A	G	G	A	G	G10	U11	A12	A13	A14	A15	A16	U17	G18	U19	U20	C21	A22	A23	A24	A25
---	---	---	---	---	---	---	---	---	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Category	Value
L61	10
E62	9
G63	8
F64	7
R65	6
A66	5
S67	4
D68	3
L72	2
G73	1
S74	1
F75	1
D76	1
P77	1
K78	1
T79	1
G80	1
N81	1
Q82	1
L83	1
K84	1
G85	1
P86	1
K89	1
R90	1
N91	1
I92	1
K93	1
K94	1
Y95	1
L96	1

K0	G1	F2	K3	D4	Y6	G6	H7	D8	Y9	H10	P11	A12	P13	K14	T15	GLU	ASN	ILE	LYS	GLY	LEU	GLY	ASP	LEU	LEU	LYS	PRO	PRO	GLY	ILE	PRO	LYS	THR	THR	PRO	LYS	GLN	ASN	GLY	GLY	GLY	LYS	ARG	LYS	ARG	TRP	THR	GLY	ASP	LYS	GLY	GLN	LYS	ILE	TYR	GLU	TRP	ASP	SER	GLN	ALA	CYT
----	----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

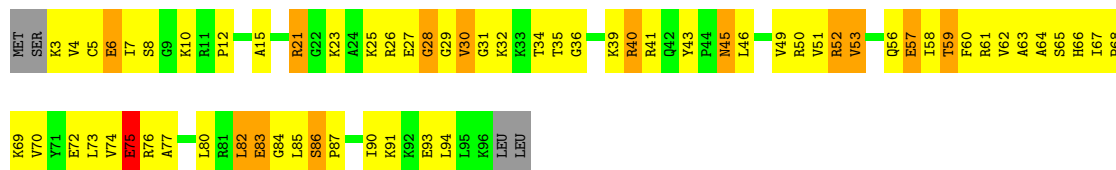
[illegible]

Met	K3	K4	K5	K6	K7	K8	K9	K10	K11	K12	K13	K14	K15	K16	K17	K18	K19	K20	K21	K22	K23	K24	K25	K26	K27	K28	K29	K30	K31	K32	K33	K34	K35	K36	K37	K38	K39	K40	K41	K42	K43	K44	K45	K46	K47	K48	K49	K50	K51	K52	K53	K54	K55	K56	K57	K58	K59	K60	K61	K62	K63	K64	K65	K66	K67	K68	K69	K70	K71	K72	K73	K74	K75	K76	K77	K78	K79	K80	K81	K82	K83	K84	K85	K86	K87	K88	K89	K90	K91	K92	K93	K94	K95	K96	K97	K98	K99	K100	K101	K102	K103	K104	K105	K106	K107	K108	K109	K110	K111	K112	K113	K114	K115	K116	K117	K118	K119	K120	K121	K122	K123	K124	K125	K126	K127	K128	K129	K130	K131	K132	K133	K134	K135	K136	K137	K138	K139	K140	K141	K142	K143	K144	K145	K146	K147	K148	K149	K150	K151	K152	K153	K154	K155	K156	K157	K158	K159	K160	K161	K162	K163	K164	K165	K166	K167	K168	K169	K170	K171	K172	K173	K174	K175	K176	K177	K178	K179	K180	K181	K182	K183	K184	K185	K186	K187	K188	K189	K190	K191	K192	K193	K194	K195	K196	K197	K198	K199	K200	K201	K202	K203	K204	K205	K206	K207	K208	K209	K210	K211	K212	K213	K214	K215	K216	K217	K218	K219	K220	K221	K222	K223	K224	K225	K226	K227	K228	K229	K230	K231	K232	K233	K234	K235	K236	K237	K238	K239	K240	K241	K242	K243	K244	K245	K246	K247	K248	K249	K250	K251	K252	K253	K254	K255	K256	K257	K258	K259	K260	K261	K262	K263	K264	K265	K266	K267	K268	K269	K270	K271	K272	K273	K274	K275	K276	K277	K278	K279	K280	K281	K282	K283	K284	K285	K286	K287	K288	K289	K290	K291	K292	K293	K294	K295	K296	K297	K298	K299	K300	K301	K302	K303	K304	K305	K306	K307	K308	K309	K310	K311	K312	K313	K314	K315	K316	K317	K318	K319	K320	K321	K322	K323	K324	K325	K326	K327	K328	K329	K330	K331	K332	K333	K334	K335	K336	K337	K338	K339	K340	K341	K342	K343	K344	K345	K346	K347	K348	K349	K350	K351	K352	K353	K354	K355	K356	K357	K358	K359	K360	K361	K362	K363	K364	K365	K366	K367	K368	K369	K370	K371	K372	K373	K374	K375	K376	K377	K378	K379	K380	K381	K382	K383	K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441	K442	K443	K444	K445	K446	K447	K448	K449	K450	K451	K452	K453	K454	K455	K456	K457	K458	K459	K460	K461	K462	K463	K464	K465	K466	K467	K468	K469	K470	K471	K472	K473	K474	K475	K476	K477	K478	K479	K480	K481	K482	K483	K484	K485	K486	K487	K488	K489	K490	K491	K492	K493	K494	K495	K496	K497	K498	K499	K500	K501	K502	K503	K504	K505	K506	K507	K508	K509	K510	K511	K512	K513	K514	K515	K516	K517	K518	K519	K520	K521	K522	K523	K524	K525
-----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



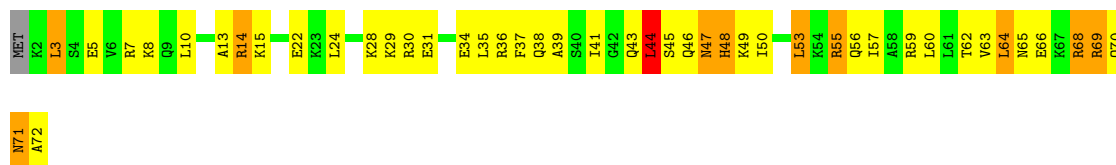
• Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain D1:



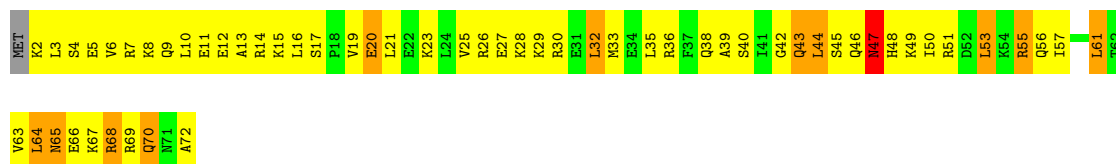
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain B2:



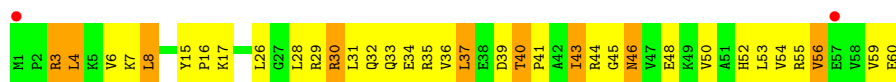
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain D2:



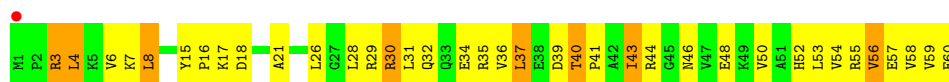
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain B3:



• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain D3:



• Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain B4:



GLY
ASP
SER
TYR
ARG
LYS
GLY
ARG

• Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain D4: 

MET LYS E3 G4 I5 H6 P7 K8 L9 V10 P11 A12 R13 I14 I15 C16 G17 C18 V21 I22 E23 T24 T25 Y26 S26 T27 K28 P29 V30 E31 V32 V33 V34 V35 C36 P41 P42 P43 T44 T45 Q46 Q47 R48 R49 V50 T52 E53 G54 R55 V56 E57 R58 PHE GLN ARG ARG TYR TYR GLY

ASP
SER
TYR
ARG
LYS
GLY
ARG

• Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain B5: 

MET A2 K3 H4 P5 V6 R16 D17 A18 R19 R20 T26 P27 C33 C36 K37 A38 R39 K40 P41 P42 H43 T44 V45 C46 G50 Y51 Y52 A53 G54 R55 K56 V57 L58 E59 V60

• Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain D5: 

MET A2 K3 H4 P5 V6 T11 R16 D17 R20 T26 P27 C33 C36 K37 A38 M39 K40 P41 P42 H43 T44 V45 C46 C49 G50 Y51 Y52 A53 G54 R55 K56 V57 L58 E59 V60

• Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain B6: 

MET ALA SER GLU VAL ARG ILE LYS L9 L10 L11 E12 C13 T14 E15 C16 R17 R18 R19 N20 Y21 A22 A23 T23 E24 K25 N26 K27 R28 N29 T30 T31 R31 R32 R33 L34 E35 L36 Y39 C40 P41 W42 C43 R44 K45 H46 T47 Y48 H49 R50 E51 V52 K53 ILE

• Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain D6: 

MET ALA SER GLU VAL ARG ILE LYS L9 L10 L11 E12 C13 T14 E15 C16 R17 R18 R19 N20 Y21 A22 A23 T23 E24 K25 N26 K27 R28 N29 T30 T31 R31 R32 R33 L34 E35 L36 R37 R38 Y39 C40 P41 W42 C43 R44 K45 H46 T47 Y48 H49 R50 E51 V52 K53 ILE

• Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain B7: 

M1 R2 R3 T4 W5 W6 P7 M8 R9 R10 K11 R12 A13 K14 R19 A20 R23 T24 G27 R28 K29 V30 R33 Q36 R39 W40 T43 P44 A45 V46 R47 R48 R49

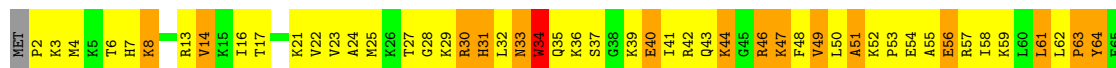
• Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain D7: 

M1 R2 R3 T4 W5 W6 P7 M8 R9 R10 K11 R12 A13 K14 R19 A20 R23 T24 G27 R28 K29 V30 R33 Q36 R39 W40 T43 P44 A45 V46 R47 R48 R49

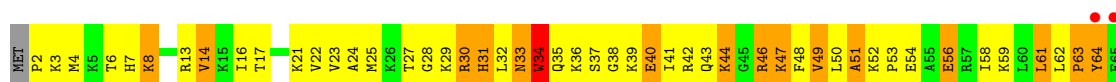
- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain B8:



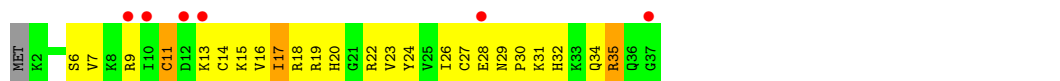
- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain D8:



- Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain B9:



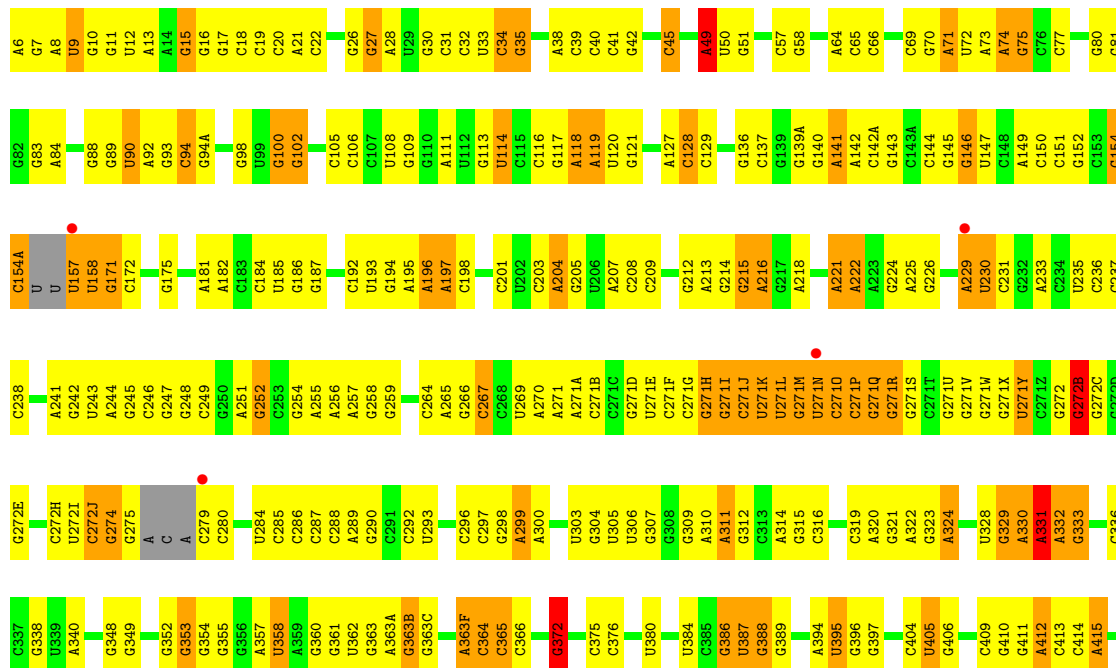
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain D9:



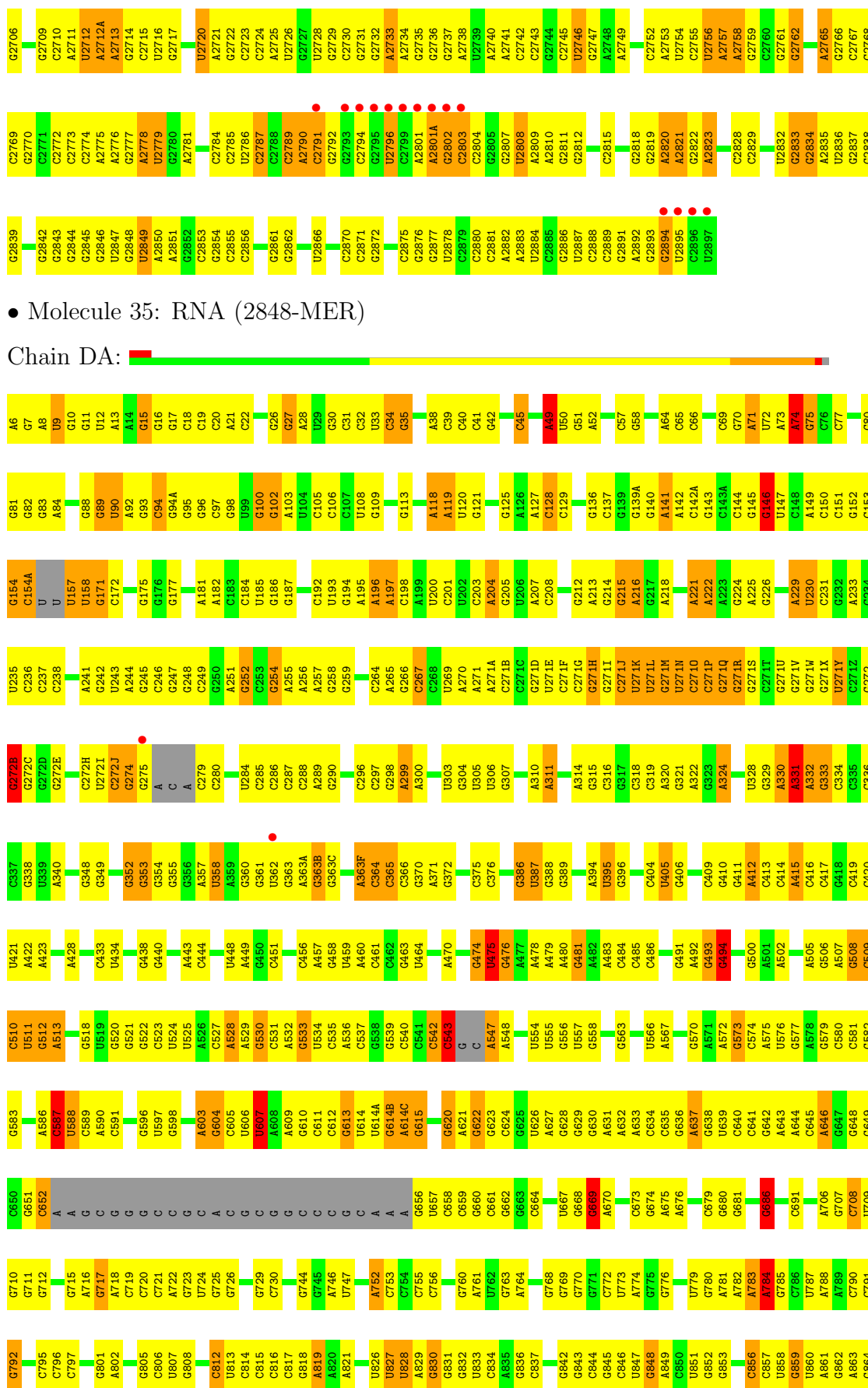
- Molecule 35: RNA (2848-MER)

Chain BA:

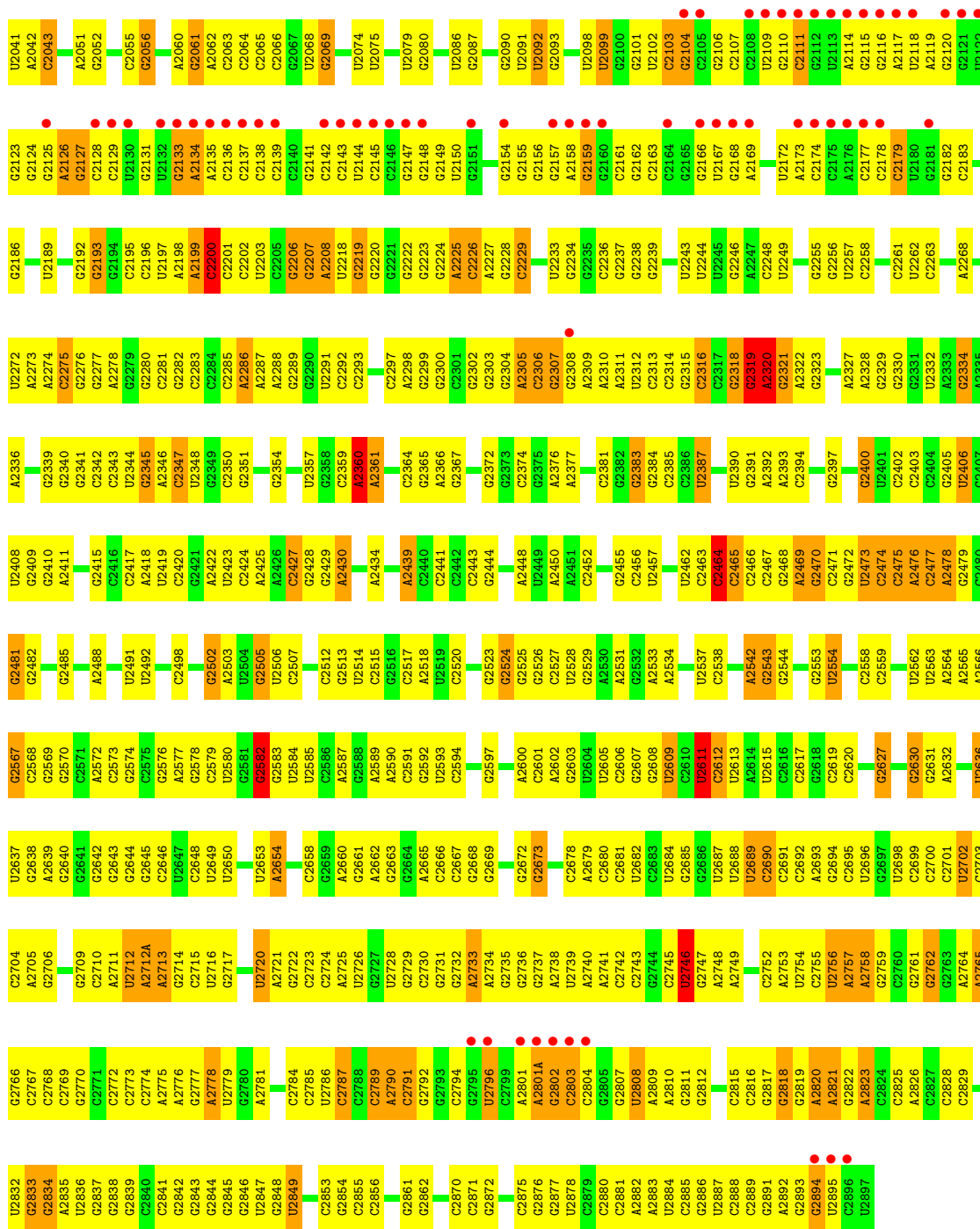


U1497	C1498	U1433	G1356	A1272	A1194	G1120	G1002	G927	A861	U787	A706	C645	G577	U499	C419
C1499	G1436	A1434	U1367	U1273	G1195	C1121	G1003	G932	G862	A788	G707	A846	A578	G500	C420
G1500	G1435	G1359	A1358	A1276	G1197	A1126	C1004	G932	A863	A789	C708	G647	G579	A501	U421
C1501	G1437	A1360	G1361	G1277	U1198	A1129	C1006	G938	G864	C790	U709	G648	C580	A502	A422
U1503	U1438	G1362	G1361	A1278	G1203	U1130	G1011	A941	A866	C791	G710	G649	C581	A505	A423
C1504	A1439	C1362	C1362	G1279	A1204	U1130	U1012	G942	G869	A793	G712	G652	G583	A428	
U1505	G1440	G1363	G1363	G1280	A1205	C1135	C1013	G943	A870	C796	G715	A	G584	G508	C433
C1506	G1441	G1364	G1364	U1281	U1205	U1142	U1013	U943	A877	C797	A716	A	G585	C509	C433
A1507	G1442	A1365	A1365	U1282	G1210	G1137	G1014	G944	G873	A717	G717	G	A586	U511	U434
U1508	G1443	G1368	G1368	G1284	A1211	G1138	G1015	A945	G874	A802	A718	G	U588	G512	G438
C1509	A1444	G1369	G1369	G1285	G1212	G1139	G1016	G946	G875	G720	C719	G	C589	A513	C440
A1509A	G1445A					G1140	U1019	G950	C876	G720	C720	G	A590	U441	
U1509B	C1446	U1288	U1288	U1288	G1215	U1141	A1020	C951	A877	G721	C721	C	C591	C517	
G1510	G1447	C1289	C1289	C1289	G1216	U1142	A1021	C952	A878	U722	A722	C	G596	G518	C444
C1511	G1448	C1375	C1375	C1290	C1217	U1143	U1022	A953	G879	G723	G723	G	U519	C445	C445
U1512	A1449	C1291	C1291	C1218	C1217	A1143	U1023	A954	G880	G733	G733	C	G597	C446	G450
C1513	G1450	U1292	U1292	G1219	G1218	G1144	G1024	C955	G881	C812	G729	A	G598	G521	A447
U1514	C1450A	C1293	C1293	G1220	G1220	C1145	G1025	G956	G882	U813	C730	G	G522	G522	U448
G1515	A1452	C1297	C1297	C1221	C1221	C1146	U1026	A957	G883	C814	G730	G	C523	C523	A449
C1516	U1453	C1298	C1298	C1221A	C1221A	C1147	A1027	U958	G886	C915	G733	C	U524	U524	C450
U1517	G1455	G1299	G1299	G1222	G1222	A1148	A1028	A959	A887	C916	A734	G	C605	U525	C451
G1518		U1300	U1300	G1223	G1223	G1149	A1029	A960	A887	C917	A735	G	U606	A526	
U1519		A1301	A1301	C1224	C1224	C1150	A1032	C961	C888	G818	G736	C	U607	C527	C456
G1520		A1302	A1302			G1151	U1033	G962	C889	A819		C	A608	A528	A457
U1523		G1309	G1309			G1154	G1034	U963	A890	A920	G744	C	A609	A529	G458
G1526		U1396	U1396			A1155	U1035	C964	G892	A821	G745	G	G610	G530	U459
U1527		U1397	U1397			A1156	G1036	C965	C893	U826	A746	C	C611	C531	A460
A1528A		U1397	U1397				G1037	C966	C895	U827	U747	A	C612	A532	C461
G1528B		C1403	C1403			C1161	C1038	C967	U895	U828	A752	A	G613	G533	C462
C1530		C1404	C1404			G1162	G1039	C968	A896	U828	C753	G	U614	U534	G463
C1531		U1405	U1405			G1163	C1040	U969	C897	A829	C754	G	U614A	C535	U464
C1532		U1406	U1406			G1164	C1041	C970	C898	G830	G755	G	G614B	A536	G465
G1533		C1407	C1407			U1165	C1042	C971	A899	G831	C756	G	A614C	C537	A466
U		C1408	C1408			C1166	U1043	G972	C902	U832	C756	G	G615	G538	C467
		C1409	C1409			U1167	A1045	A973	C903	U833		G	G616	G539	
		G1410	G1410			G1168	A1046	G974	C904	C834	G760	G		C540	A470
		C1411	C1411			G1169	G1047	C975	C905	A935	A761	G	G620	C541	
		A1412	A1412			G1170	A1048	G977	U905	G836	G621	G	G621	C542	G474
		G1413	G1413			G1171	C1049	G978	G906	C837	A764	G	G622	C543	U475
						G1172	A1050	G979	U907			G	G623	G	U476
						A1174	G1051	A980	C908	G842	G768	U667	C624	C	A477
						U1175	C1052		A909	G843	G769	G668	G625	A547	A478
						G1176	G1053	A981	A910	C844	G770	G669	G626	A548	A479
						A1177	A1106	A983	A911	G845	U773	A670	U627	A548	A479
						C1178	G1107	C986	C912	C946	U774	C673	A631	U554	A480
						C1179	U1108	G987	U913	U847	G775	G674	A632	U555	A482
						G1180	C1109	G987	C914	G848	G776	A675	A633	G556	A483
						C1181	G1110	C991	C915	A849	A777	A676	C634	U557	C484
						A1182	A1111	C992	G916	C850	A777	A676	C634	G558	C485
						G1187	G1112	G993	A917	U851	G778	A676	C634	G558	C486
						U1188	A1113	G993	G920	G852	U779	G679	A637	G563	
						A1189	G1114	A996	G921	G853	G780	G681	A637	G570	G491
						G1190	G1115	G997	U922	C856	A781	G681	A637	G570	A492
						G1191	C1116	C997	C923	C857	A783	G686	U639	G573	G493
						G1192	G1117	C998	C924	C857	A783	G686	U639	G573	G493
						G1193	C1118	U999	C925	U858	A784	G686	U639	G573	G493
							C1119	A1000	C925	U858	A784	G686	U639	G573	G493
							C1119	A1001	A926	U860	C786	C691	G642	A575	G495



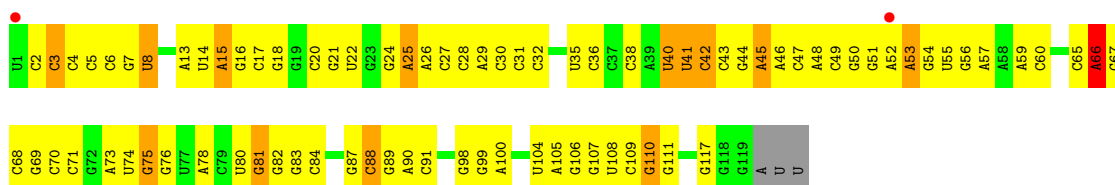




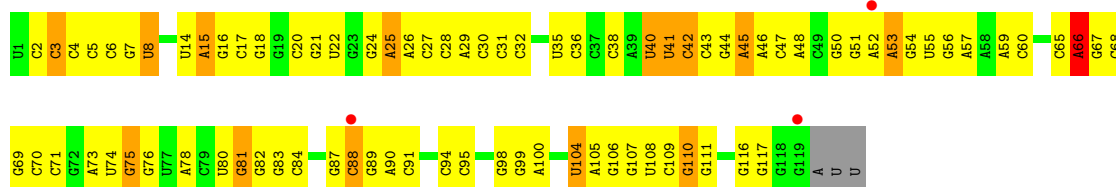


• Molecule 36: RNA (119-MER)

Chain BB:

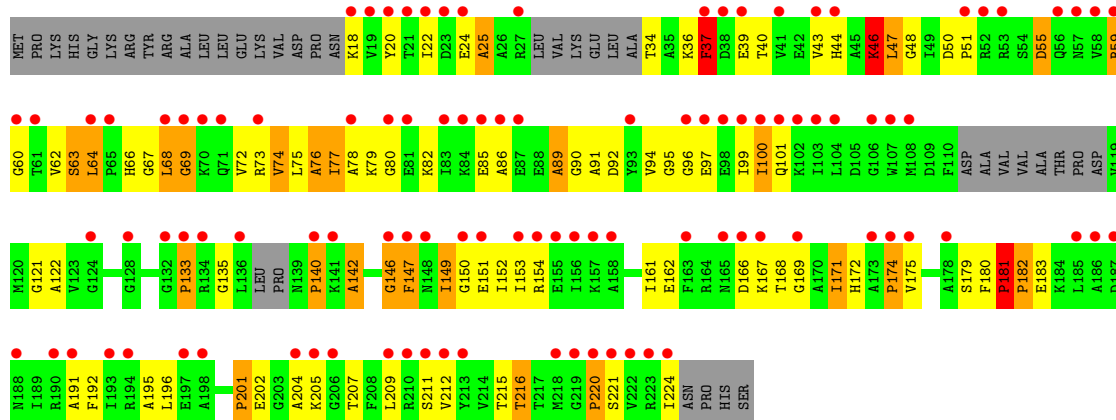


Chain DB:



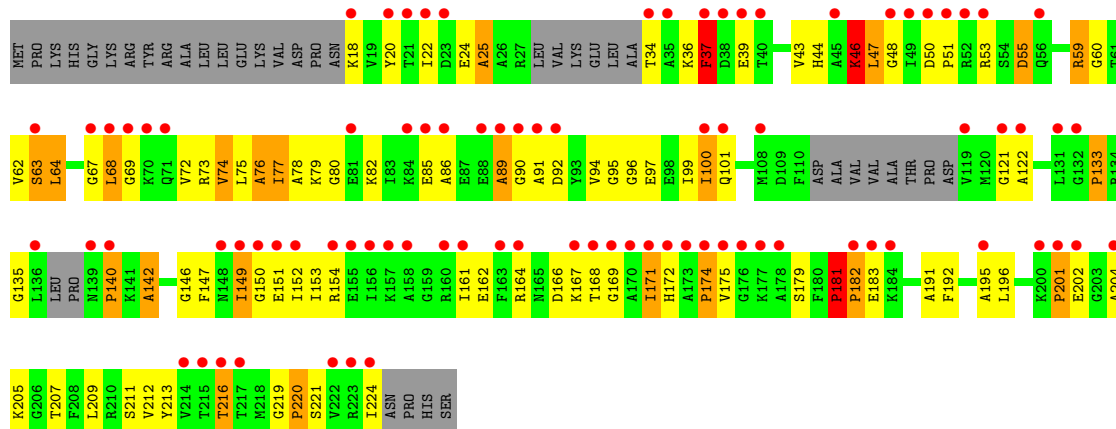
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

Chain BC:



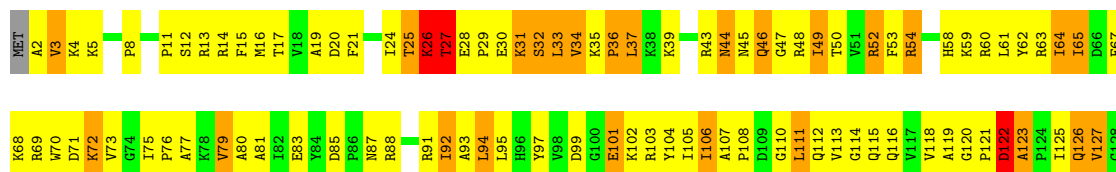
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

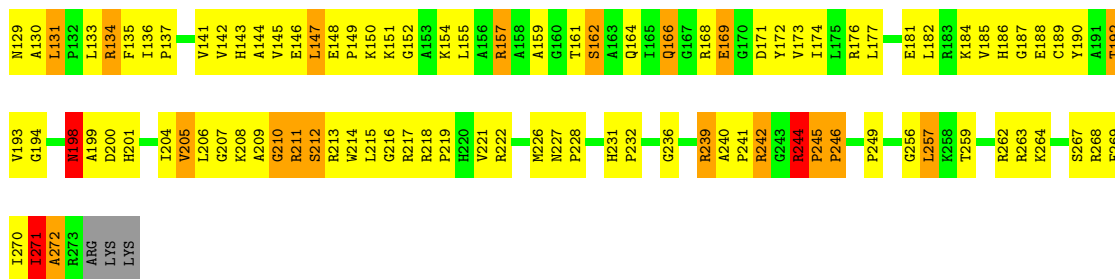
Chain DC:



• Molecule 38: 50S RIBOSOMAL PROTEIN L2

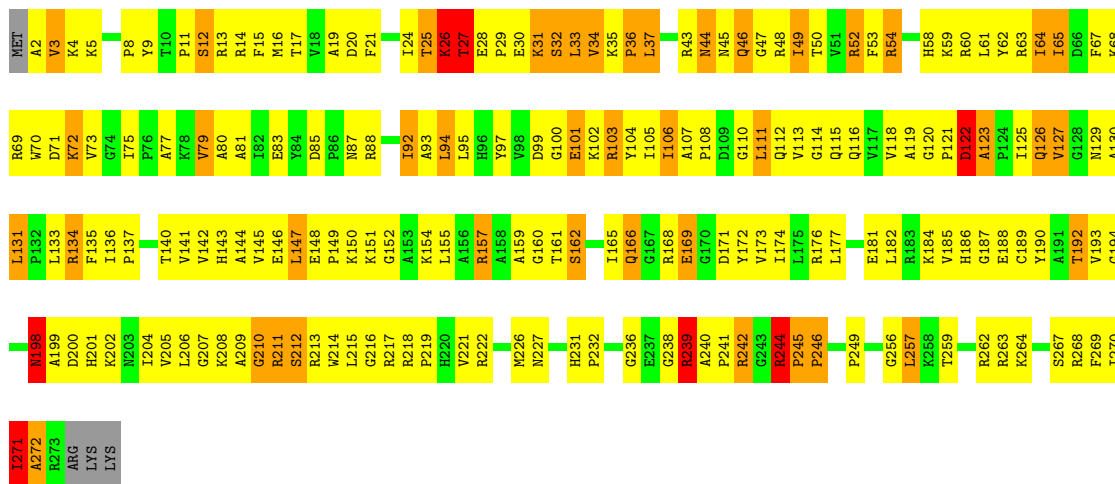
Chain BD:





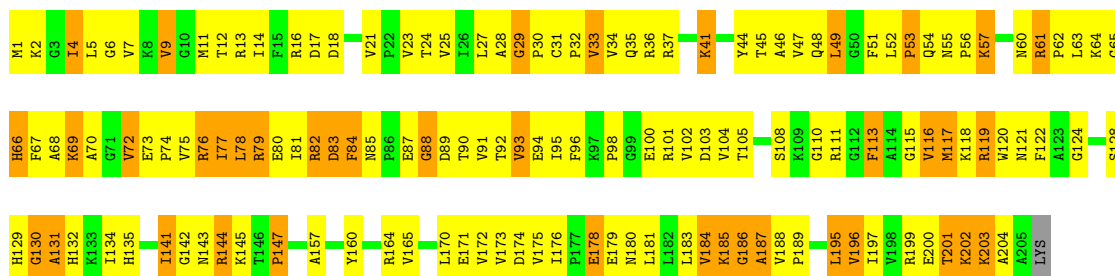
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain DD:



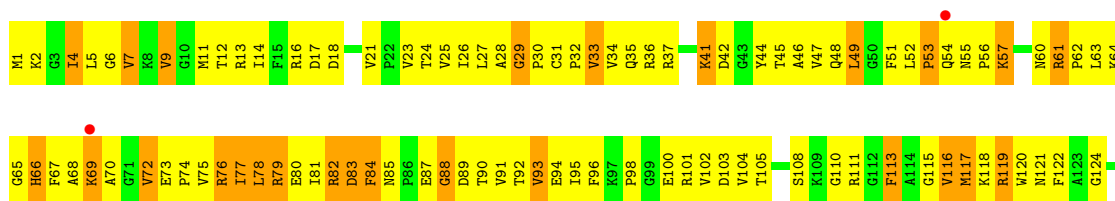
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain BE:



• Molecule 39: 50S RIBOSOMAL PROTEIN L3

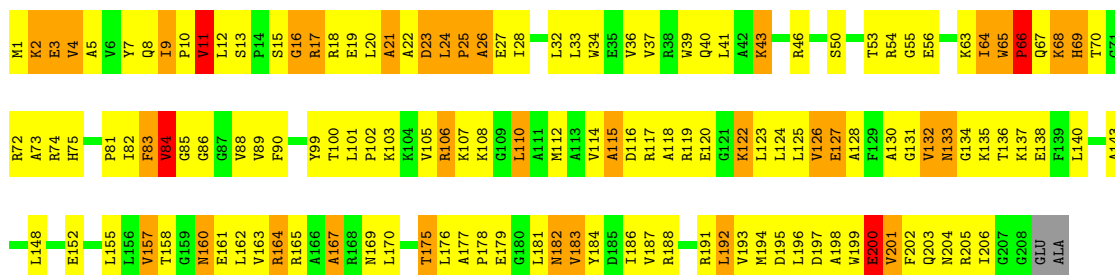
Chain DE:





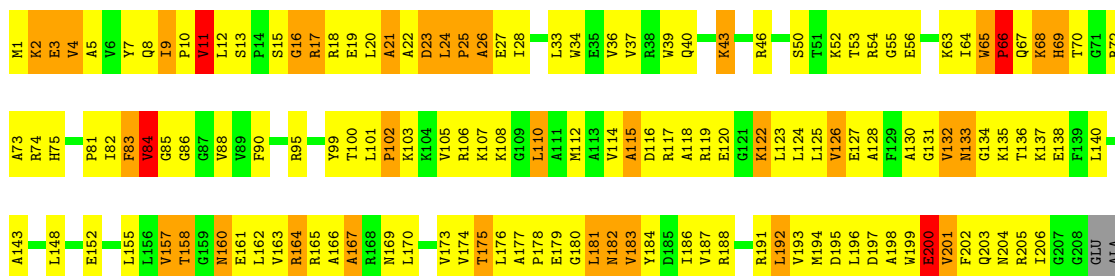
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain BF:



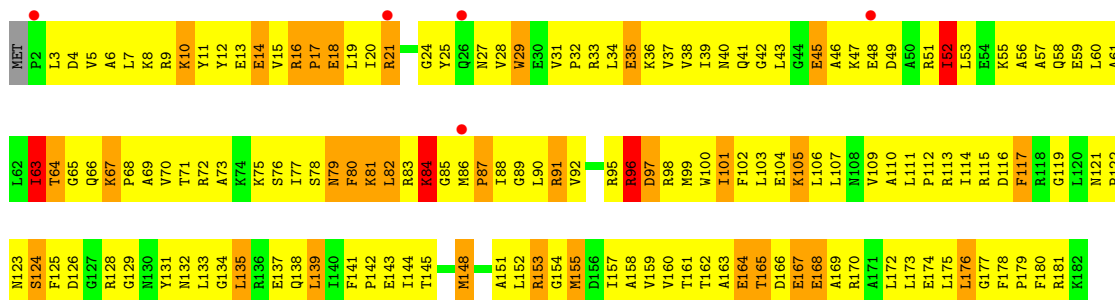
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain DF:



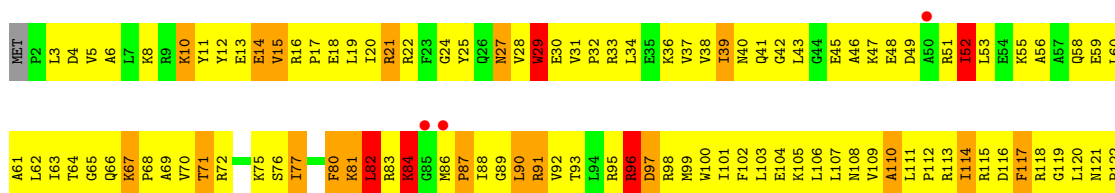
• Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain BG:



• Molecule 41: 50S RIBOSOMAL PROTEIN L5

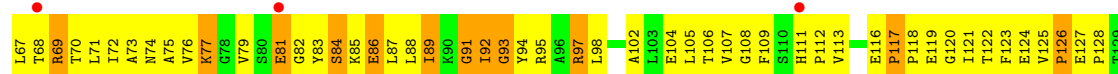
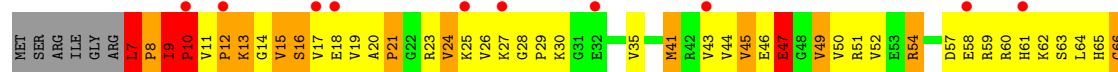
Chain DG:





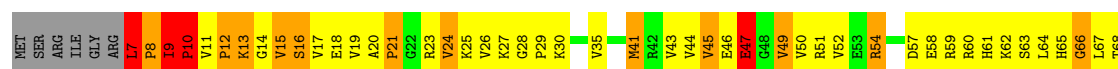
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain BH:



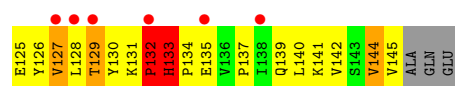
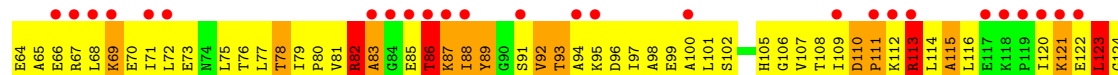
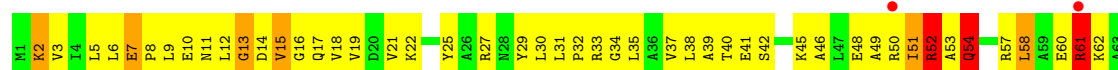
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain DH:



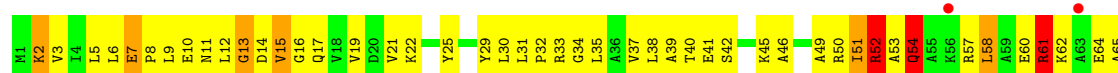
• Molecule 43: 50S RIBOSOMAL PROTEIN L9

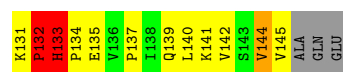
Chain BI:



• Molecule 43: 50S RIBOSOMAL PROTEIN L9

Chain DI:





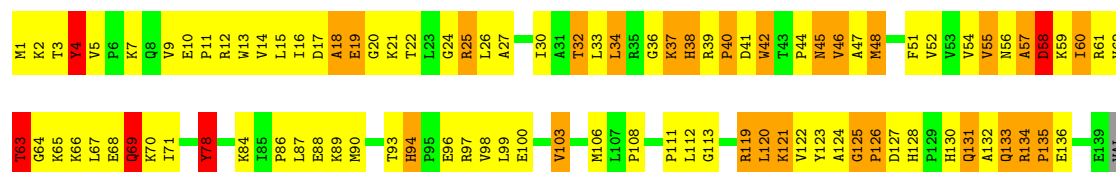
- Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



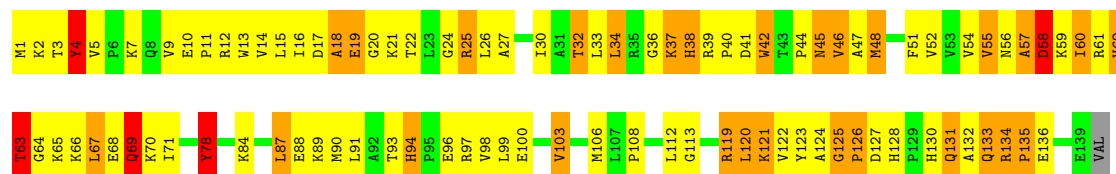
- Molecule 45: 50S RIBOSOMAL PROTEIN L13

Chain BN:



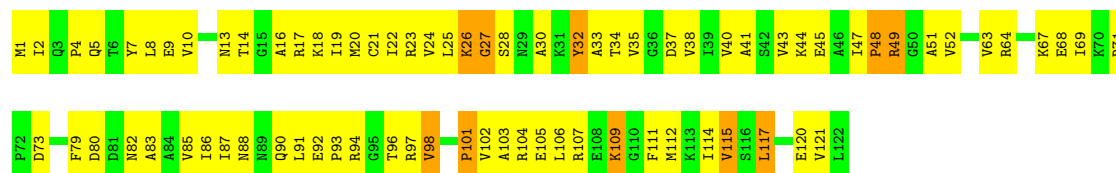
- Molecule 45: 50S RIBOSOMAL PROTEIN L13

Chain DN:



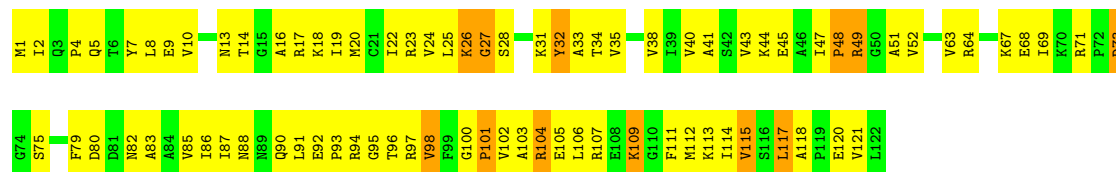
- Molecule 46: 50S RIBOSOMAL PROTEIN L14

Chain BO:



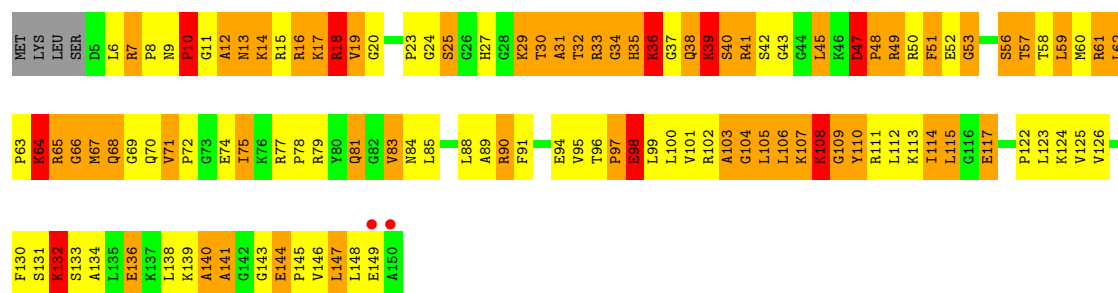
- Molecule 46: 50S RIBOSOMAL PROTEIN L14

Chain DO:



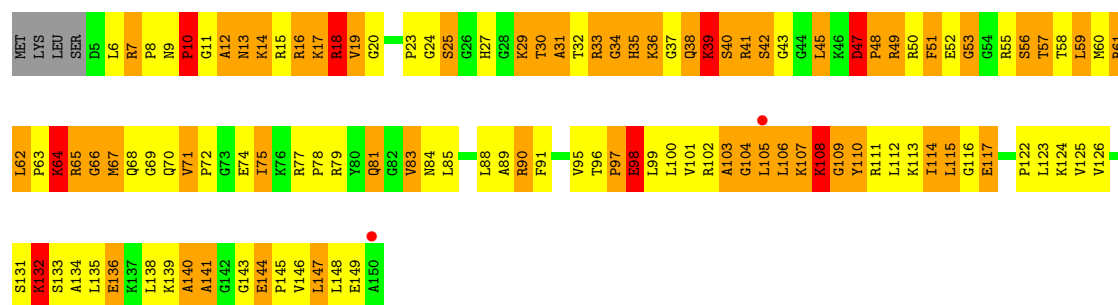
- Molecule 47: 50S RIBOSOMAL PROTEIN L15

Chain BP:



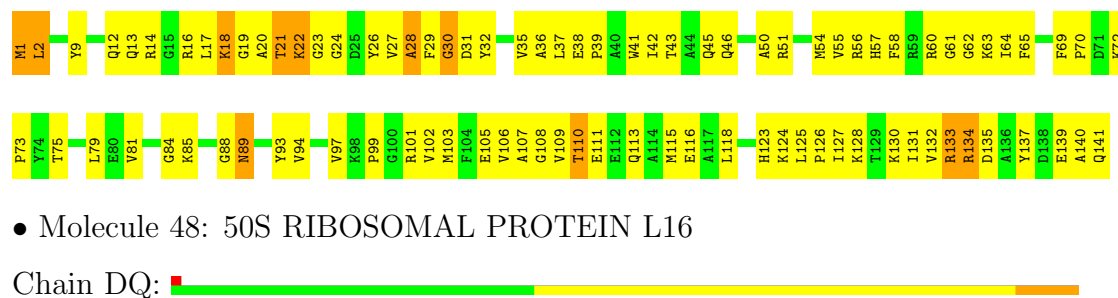
• Molecule 47: 50S RIBOSOMAL PROTEIN L15

Chain DP:



• Molecule 48: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



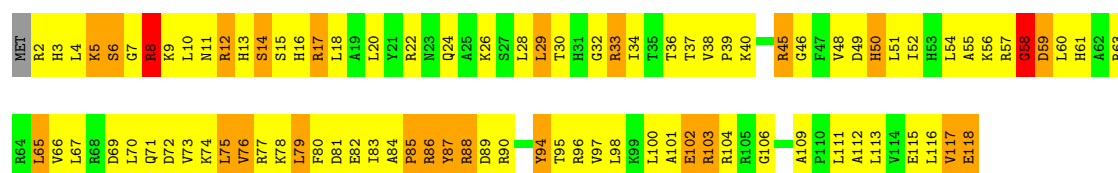
• Molecule 48: 50S RIBOSOMAL PROTEIN L16

Chain DQ:



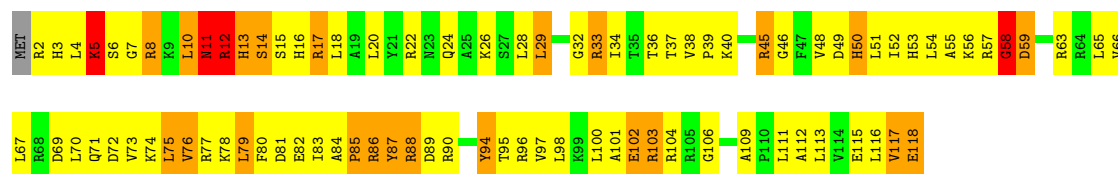
• Molecule 49: 50S RIBOSOMAL PROTEIN L17

Chain BR:



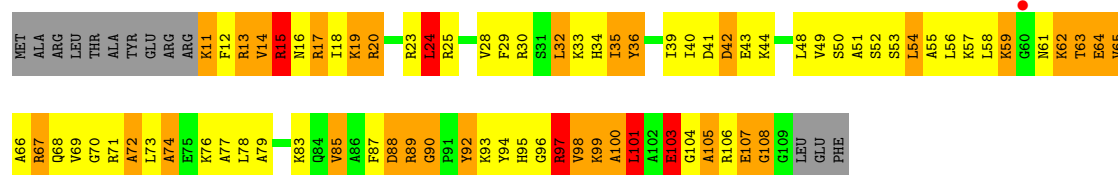
• Molecule 49: 50S RIBOSOMAL PROTEIN L17

Chain DR:



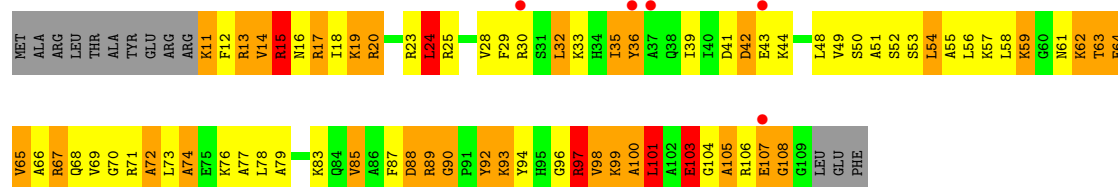
• Molecule 50: 50S RIBOSOMAL PROTEIN L18

Chain BS:



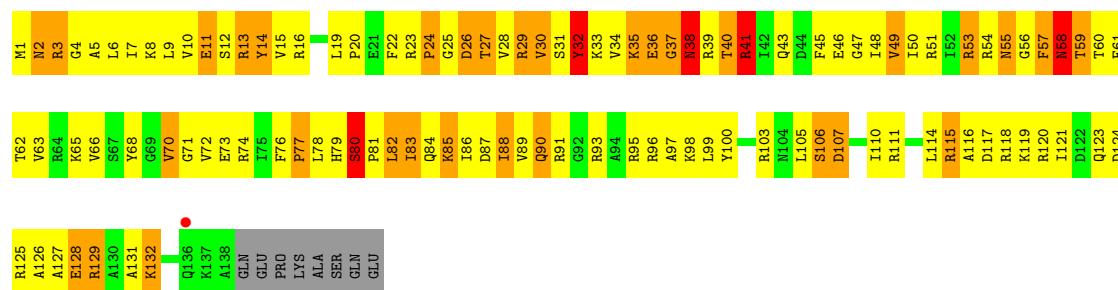
• Molecule 50: 50S RIBOSOMAL PROTEIN L18

Chain DS:



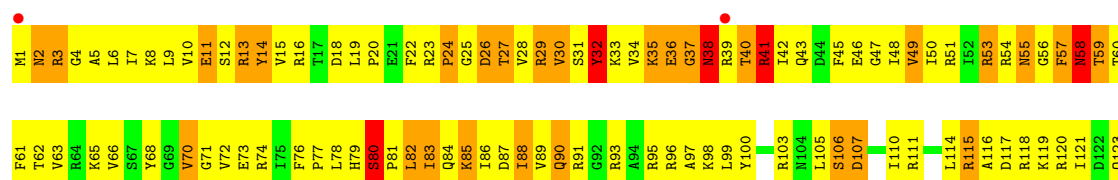
• Molecule 51: 50S RIBOSOMAL PROTEIN L19

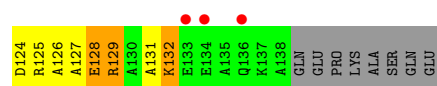
Chain BT:



• Molecule 51: 50S RIBOSOMAL PROTEIN L19

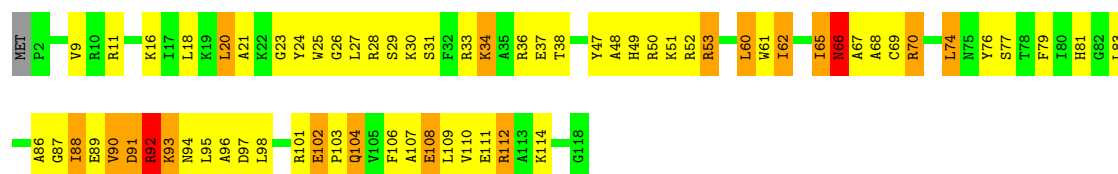
Chain DT:





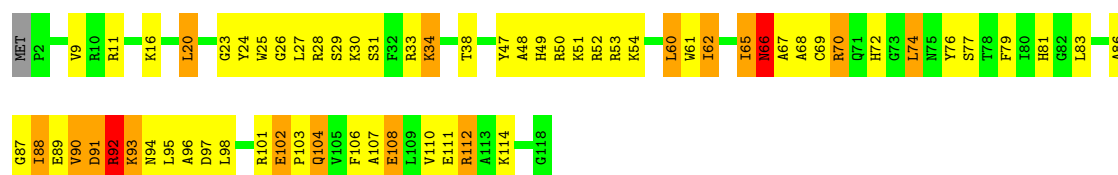
• Molecule 52: 50S RIBOSOMAL PROTEIN L20

Chain BU:



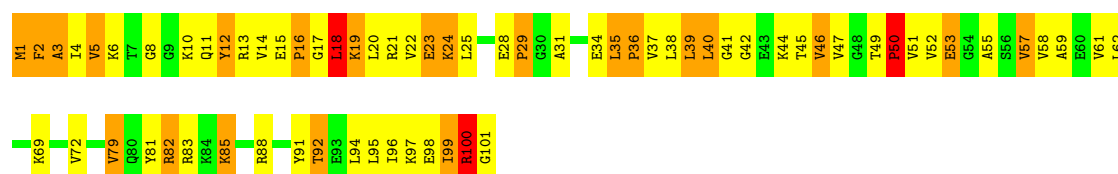
• Molecule 52: 50S RIBOSOMAL PROTEIN L20

Chain DU:



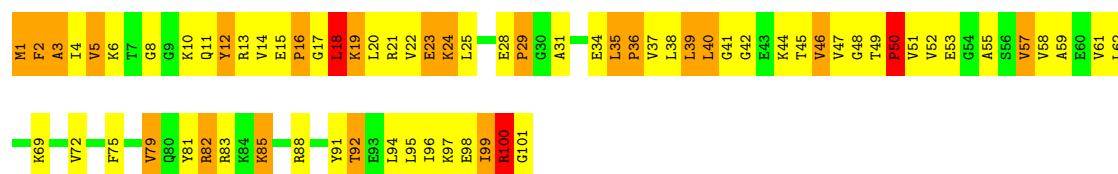
• Molecule 53: 50S RIBOSOMAL PROTEIN L21

Chain BV:



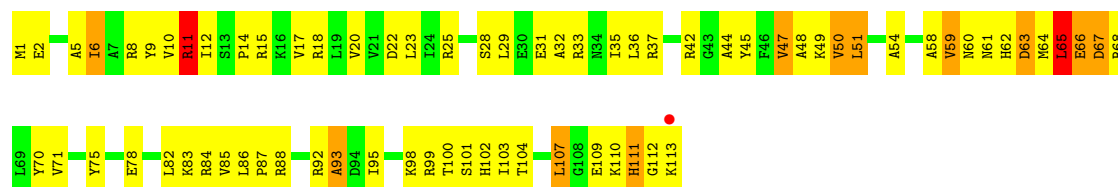
• Molecule 53: 50S RIBOSOMAL PROTEIN L21

Chain DV:



• Molecule 54: 50S RIBOSOMAL PROTEIN L22

Chain BW:



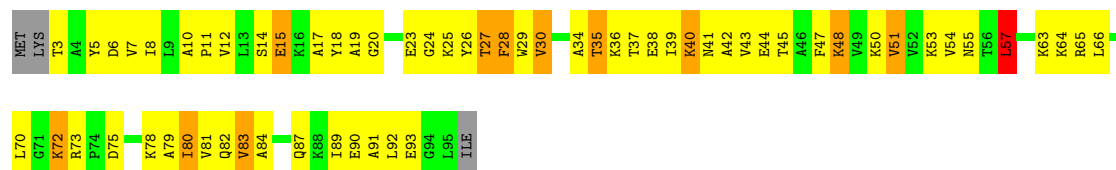
• Molecule 54: 50S RIBOSOMAL PROTEIN L22

Chain DW: 



• Molecule 55: 50S RIBOSOMAL PROTEIN L23

Chain BX: 



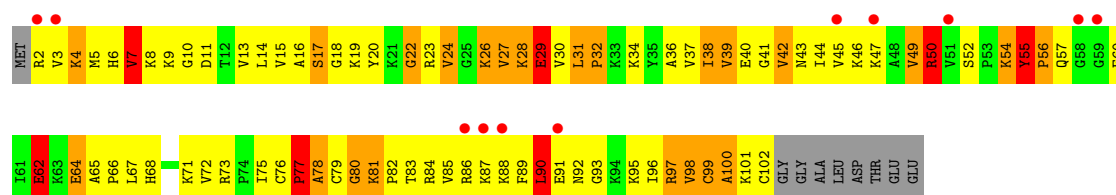
• Molecule 55: 50S RIBOSOMAL PROTEIN L23

Chain DX: 



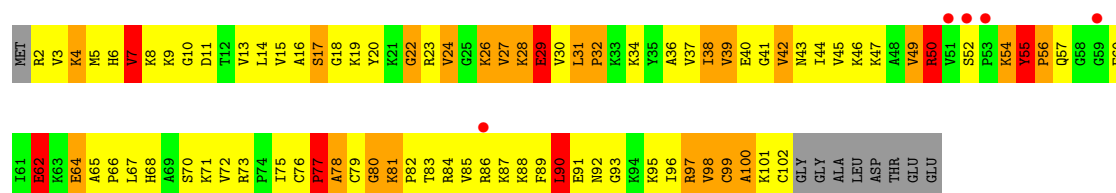
• Molecule 56: 50S RIBOSOMAL PROTEIN L24

Chain BY: 



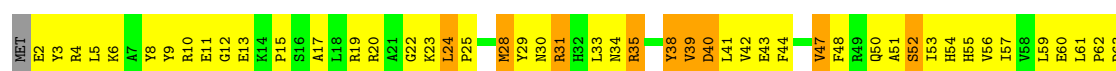
• Molecule 56: 50S RIBOSOMAL PROTEIN L24

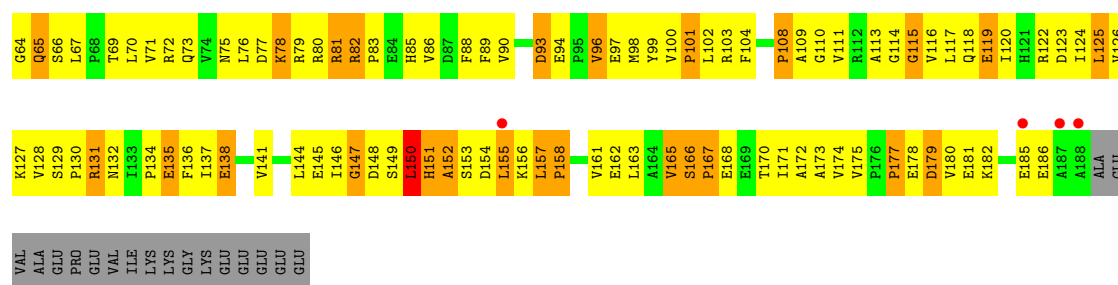
Chain DY: 



• Molecule 57: 50S RIBOSOMAL PROTEIN L25

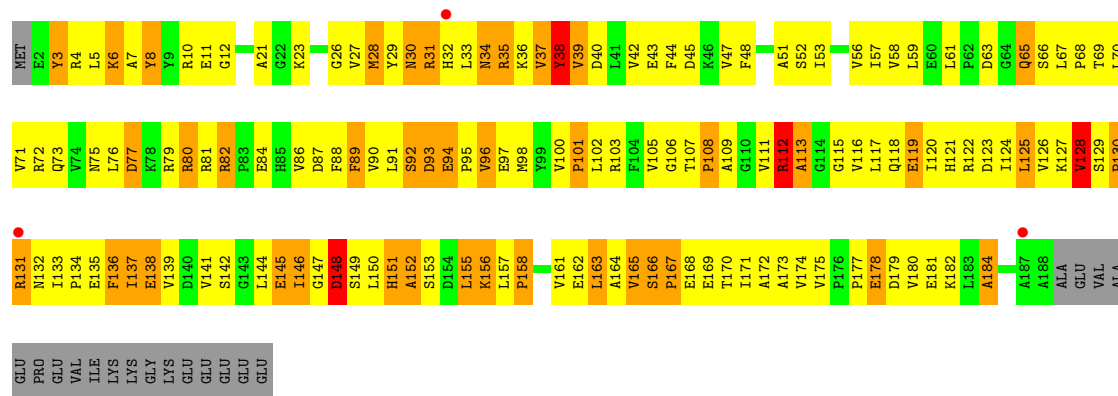
Chain BZ: 





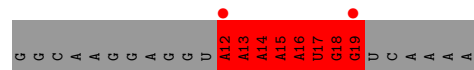
• Molecule 57: 50S RIBOSOMAL PROTEIN L25

Chain DZ:



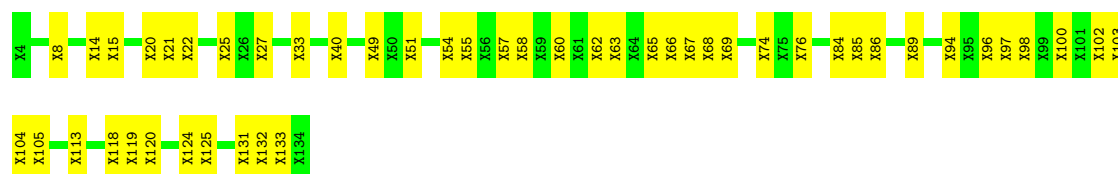
• Molecule 58: MRNA

Chain CX:



• Molecule 59: 50S RIBOSOMAL PROTEIN L10

Chain DJ:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.04Å 453.51Å 616.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.53 – 3.20 44.53 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.53-3.20) 99.5 (44.53-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.270 0.296 , 0.328	Depositor DCC
R_{free} test set	36924 reflections (3.84%)	DCC
Wilson B-factor (Å ²)	87.1	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 68.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 960332 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	296762	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A3P, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.39	0/36252	0.68	9/56580 (0.0%)
1	CA	0.37	1/36253 (0.0%)	0.70	17/56582 (0.0%)
2	AB	0.32	0/1936	0.59	0/2611
2	CB	0.32	0/1936	0.59	0/2611
3	AC	0.30	0/1637	0.55	0/2207
3	CC	0.31	0/1637	0.55	0/2207
4	AD	0.37	0/1722	0.85	6/2306 (0.3%)
4	CD	0.35	0/1722	0.85	6/2306 (0.3%)
5	AE	0.34	0/1163	0.62	0/1566
5	CE	0.34	0/1163	0.61	0/1566
6	AF	0.32	0/856	0.62	0/1154
6	CF	0.34	0/856	0.63	0/1154
7	AG	0.29	0/1276	0.52	0/1709
7	CG	0.29	0/1276	0.51	0/1709
8	AH	0.33	0/1136	0.60	0/1527
8	CH	0.31	0/1136	0.60	0/1527
9	AI	0.32	0/1027	0.57	0/1372
9	CI	0.32	0/1027	0.57	0/1372
10	AJ	0.33	0/808	0.55	0/1087
10	CJ	0.33	0/808	0.55	0/1087
11	AK	0.31	0/900	0.58	0/1213
11	CK	0.33	0/900	0.58	0/1213
12	AL	0.38	0/987	0.87	3/1322 (0.2%)
12	CL	0.37	0/987	0.89	3/1322 (0.2%)
13	AM	0.31	0/941	0.62	0/1258
13	CM	0.32	0/941	0.61	0/1258
14	AN	0.33	0/501	0.54	0/664
14	CN	0.33	0/501	0.54	0/664
15	AO	0.35	0/745	0.60	0/992
15	CO	0.34	0/745	0.60	0/992
16	AP	0.37	0/717	0.61	0/965
16	CP	0.35	0/717	0.59	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.37	0/837	0.62	0/1119
17	CQ	0.34	0/837	0.62	0/1119
18	AR	0.33	0/579	0.60	0/768
18	CR	0.33	0/579	0.59	0/768
19	AS	0.33	0/685	0.54	0/922
19	CS	0.34	0/685	0.54	0/922
20	AT	0.31	0/765	0.57	0/1007
20	CT	0.29	0/765	0.57	0/1007
21	AU	0.45	0/213	0.53	0/279
21	CU	0.45	0/213	0.54	0/279
22	AV	2.00	34/1832 (1.9%)	2.16	50/2855 (1.8%)
22	AW	0.41	0/1832	0.71	0/2855
22	CV	0.44	1/1832 (0.1%)	0.72	0/2855
22	CW	0.40	0/1832	0.71	0/2855
23	AX	2.66	24/383 (6.3%)	4.32	117/595 (19.7%)
24	AY	1.30	4/790 (0.5%)	1.44	14/1055 (1.3%)
24	CY	1.10	0/132	1.27	0/177
25	B0	0.39	0/671	0.64	0/892
25	D0	0.39	0/671	0.63	0/892
26	B1	0.47	0/741	0.75	0/986
26	D1	0.47	0/741	0.78	0/986
27	B2	0.36	0/600	0.63	0/793
27	D2	0.45	0/600	0.71	0/793
28	B3	0.42	0/473	0.68	0/636
28	D3	0.41	0/473	0.67	0/636
29	B4	0.39	0/444	0.65	0/602
29	D4	0.40	0/444	0.65	0/602
30	B5	0.48	0/473	0.76	0/639
30	D5	0.48	0/473	0.76	0/639
31	B6	0.41	0/387	0.64	0/517
31	D6	0.41	0/387	0.64	0/517
32	B7	0.52	0/427	0.68	0/563
32	D7	0.56	0/427	0.71	0/563
33	B8	0.56	0/516	0.94	1/681 (0.1%)
33	D8	0.53	0/516	0.93	1/681 (0.1%)
34	B9	0.33	0/302	0.62	0/397
34	D9	0.34	0/302	0.62	0/397
35	BA	0.60	55/67715 (0.1%)	0.77	106/105714 (0.1%)
35	DA	0.60	28/67714 (0.0%)	0.78	109/105710 (0.1%)
36	BB	0.38	0/2853	0.69	0/4451
36	DB	0.38	0/2853	0.69	0/4451
37	BC	0.33	0/1145	0.60	7/1556 (0.4%)
37	DC	0.33	0/1145	0.60	7/1556 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	BD	0.48	0/2155	0.78	1/2907 (0.0%)
38	DD	0.51	0/2155	0.80	1/2907 (0.0%)
39	BE	0.45	0/1597	0.74	0/2155
39	DE	0.44	0/1597	0.75	0/2155
40	BF	0.47	0/1659	0.75	1/2246 (0.0%)
40	DF	0.50	0/1659	0.75	0/2246
41	BG	0.33	0/1498	0.62	0/2013
41	DG	0.34	0/1498	0.64	0/2013
42	BH	0.61	1/1285 (0.1%)	0.85	3/1741 (0.2%)
42	DH	0.61	1/1285 (0.1%)	0.85	3/1741 (0.2%)
43	BI	0.38	0/1140	1.09	9/1543 (0.6%)
43	DI	0.37	0/1140	1.07	9/1543 (0.6%)
45	BN	0.41	0/1132	0.75	0/1527
45	DN	0.44	0/1132	0.76	0/1527
46	BO	0.44	0/943	0.71	0/1269
46	DO	0.41	0/943	0.69	0/1269
47	BP	0.57	0/1131	1.03	4/1504 (0.3%)
47	DP	0.56	0/1131	1.02	5/1504 (0.3%)
48	BQ	0.40	0/1143	0.63	0/1527
48	DQ	0.37	0/1143	0.63	0/1527
49	BR	0.40	0/974	0.70	1/1302 (0.1%)
49	DR	0.75	3/974 (0.3%)	0.95	6/1302 (0.5%)
50	BS	0.39	0/779	0.67	0/1038
50	DS	0.40	0/779	0.67	0/1038
51	BT	0.42	0/1156	0.74	1/1544 (0.1%)
51	DT	0.40	0/1156	0.72	1/1544 (0.1%)
52	BU	0.43	0/975	0.68	0/1297
52	DU	0.49	0/975	0.71	0/1297
53	BV	0.42	0/790	0.74	0/1057
53	DV	0.46	0/790	0.76	0/1057
54	BW	0.48	0/907	0.75	0/1216
54	DW	0.50	1/907 (0.1%)	0.76	0/1216
55	BX	0.48	0/740	0.71	1/995 (0.1%)
55	DX	0.54	0/740	0.73	1/995 (0.1%)
56	BY	0.48	0/789	0.79	1/1053 (0.1%)
56	DY	0.51	0/789	0.80	1/1053 (0.1%)
57	BZ	0.37	0/1514	0.67	0/2056
57	DZ	0.36	0/1514	0.64	0/2056
58	CX	3.13	24/195 (12.3%)	4.52	67/303 (22.1%)
All	All	0.53	177/318302 (0.1%)	0.78	572/475638 (0.1%)

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	AA	1	10
1	CA	1	9
22	AV	0	1
22	CV	0	1
24	AY	0	1
35	BA	20	57
35	DA	20	70
36	BB	0	1
36	DB	0	2
42	BH	0	1
42	DH	0	1
49	BR	0	1
49	DR	0	2
All	All	42	157

The worst 5 of 177 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AV	53	G	N3-C4	-27.79	1.16	1.35
22	AV	53	G	C2-N3	-27.03	1.11	1.32
22	AV	52	G	N7-C5	-25.47	1.24	1.39
22	AV	52	G	N9-C4	-25.25	1.17	1.38
22	AV	52	G	C5-C6	-22.33	1.20	1.42

The worst 5 of 572 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	52	G	C4-C5-N7	30.84	123.13	110.80
22	AV	53	G	N3-C2-N2	-29.82	99.03	119.90
22	AV	52	G	C5-N7-C8	-28.61	89.99	104.30
22	AV	53	G	C5'-C4'-O4'	-26.14	77.74	109.10
22	AV	53	G	N3-C4-N9	-25.89	110.46	126.00

5 of 42 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	575	G	C3'
35	BA	100	G	C1'
35	BA	474	G	C3'
35	BA	587	C	C3'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
35	BA	669	G	C4',C3',C1'

5 of 157 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	115	G	Sidechain
1	AA	120	A	Sidechain
1	AA	575	G	Sidechain
1	AA	587	G	Sidechain
1	AA	731	G	Sidechain

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	32412	0	16354	1303	0
1	CA	32413	0	16353	1699	0
2	AB	1901	0	1951	297	0
2	CB	1901	0	1951	304	0
3	AC	1613	0	1676	245	0
3	CC	1613	0	1677	238	0
4	AD	1692	0	1751	196	0
4	CD	1692	0	1753	218	0
5	AE	1147	0	1206	172	0
5	CE	1147	0	1207	191	0
6	AF	843	0	857	95	0
6	CF	843	0	857	99	0
7	AG	1257	0	1296	134	0
7	CG	1257	0	1296	146	0
8	AH	1116	0	1177	159	0
8	CH	1116	0	1177	167	0
9	AI	1011	0	1041	160	0
9	CI	1011	0	1041	161	0
10	AJ	795	0	840	156	0
10	CJ	795	0	840	157	0
11	AK	885	0	904	99	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	CK	885	0	904	95	0
12	AL	971	0	1055	117	0
12	CL	971	0	1056	116	0
13	AM	934	0	989	124	0
13	CM	934	0	987	135	0
14	AN	492	0	530	74	0
14	CN	492	0	533	78	0
15	AO	734	0	771	82	0
15	CO	734	0	771	77	0
16	AP	701	0	719	93	0
16	CP	701	0	720	105	0
17	AQ	824	0	890	88	0
17	CQ	824	0	891	91	0
18	AR	574	0	644	90	0
18	CR	574	0	644	88	0
19	AS	671	0	689	118	0
19	CS	671	0	689	112	0
20	AT	763	0	861	74	0
20	CT	763	0	861	75	0
21	AU	209	0	221	42	0
21	CU	209	0	221	39	0
22	AV	1640	0	832	85	0
22	AW	1640	0	837	60	0
22	CV	1640	0	833	134	0
22	CW	1640	0	837	71	0
23	AX	341	0	174	126	0
24	AY	769	0	763	234	0
24	CY	126	0	115	33	0
25	B0	662	0	688	60	0
25	D0	662	0	688	56	0
26	B1	734	0	808	85	0
26	D1	734	0	808	83	0
27	B2	598	0	653	65	0
27	D2	598	0	653	79	0
28	B3	468	0	523	42	0
28	D3	468	0	523	45	0
29	B4	434	0	424	92	0
29	D4	434	0	424	69	0
30	B5	459	0	480	45	0
30	D5	459	0	479	45	0
31	B6	381	0	390	61	0
31	D6	381	0	390	63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	B7	419	0	467	32	0
32	D7	419	0	467	34	0
33	B8	508	0	576	123	0
33	D8	508	0	576	122	0
34	B9	299	0	326	28	0
34	D9	299	0	326	30	0
35	BA	60459	0	30475	1946	0
35	DA	60459	0	30466	2110	1
36	BB	2551	0	1295	101	0
36	DB	2551	0	1294	90	1
37	BC	1142	0	865	72	0
37	DC	1142	0	865	71	0
38	BD	2105	0	2182	299	0
38	DD	2105	0	2182	311	0
39	BE	1564	0	1628	223	0
39	DE	1564	0	1628	233	0
40	BF	1624	0	1677	218	0
40	DF	1624	0	1676	225	0
41	BG	1474	0	1534	280	0
41	DG	1474	0	1534	306	0
42	BH	1260	0	1326	250	0
42	DH	1260	0	1326	242	0
43	BI	1125	0	1209	181	0
43	DI	1125	0	1209	169	0
44	BJ	651	0	165	21	0
45	BN	1105	0	1180	139	0
45	DN	1105	0	1180	133	0
46	BO	933	0	996	101	0
46	DO	933	0	996	114	0
47	BP	1114	0	1187	315	0
47	DP	1114	0	1187	310	0
48	BQ	1122	0	1179	113	0
48	DQ	1122	0	1179	112	0
49	BR	960	0	1021	132	0
49	DR	960	0	1019	127	0
50	BS	771	0	832	143	0
50	DS	771	0	832	132	0
51	BT	1142	0	1202	223	0
51	DT	1142	0	1201	226	0
52	BU	958	0	1015	121	0
52	DU	958	0	1015	116	0
53	BV	779	0	852	162	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	DV	779	0	852	158	0
54	BW	896	0	953	80	0
54	DW	896	0	952	77	0
55	BX	726	0	778	71	0
55	DX	726	0	778	73	0
56	BY	776	0	870	194	0
56	DY	776	0	870	192	0
57	BZ	1482	0	1503	210	0
57	DZ	1482	0	1503	244	0
58	CX	173	0	89	53	0
59	DJ	651	0	166	35	0
60	AA	373	0	0	0	0
60	AC	2	0	0	0	0
60	AD	3	0	0	0	0
60	AH	1	0	0	0	0
60	AI	3	0	0	0	0
60	AL	6	0	0	0	0
60	AN	2	0	0	0	0
60	AO	2	0	0	0	0
60	AP	1	0	0	0	0
60	AQ	3	0	0	0	0
60	AT	1	0	0	0	0
60	AV	7	0	0	0	0
60	AX	4	0	0	0	0
60	AY	3	0	0	0	0
60	B0	2	0	0	0	0
60	B1	1	0	0	0	0
60	B5	3	0	0	0	0
60	B6	1	0	0	0	0
60	B7	1	0	0	0	0
60	BA	709	0	0	0	0
60	BB	6	0	0	0	0
60	BD	5	0	0	0	0
60	BE	4	0	0	0	0
60	BF	1	0	0	0	0
60	BH	4	0	0	0	0
60	BN	1	0	0	0	0
60	BO	1	0	0	0	0
60	BP	4	0	0	5	0
60	BQ	1	0	0	0	0
60	BR	5	0	0	0	0
60	BT	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BU	2	0	0	0	0
60	BY	1	0	0	0	0
60	CA	184	0	0	0	0
60	CC	3	0	0	0	0
60	CD	1	0	0	0	0
60	CH	1	0	0	0	0
60	CJ	2	0	0	0	0
60	CM	3	0	0	0	0
60	CP	1	0	0	0	0
60	CQ	1	0	0	0	0
60	CS	2	0	0	0	0
60	CV	12	0	0	0	0
60	CY	1	0	0	0	0
60	D0	4	0	0	0	0
60	D1	2	0	0	0	0
60	D2	1	0	0	0	0
60	D3	1	0	0	0	0
60	D5	3	0	0	0	0
60	D6	2	0	0	0	0
60	D7	4	0	0	0	0
60	D8	1	0	0	0	0
60	D9	1	0	0	0	0
60	DA	897	0	0	0	0
60	DB	11	0	0	0	0
60	DD	6	0	0	0	0
60	DE	4	0	0	0	0
60	DF	3	0	0	0	0
60	DN	3	0	0	0	0
60	DO	1	0	0	0	0
60	DP	6	0	0	0	0
60	DR	2	0	0	0	0
60	DT	1	0	0	0	0
60	DU	4	0	0	0	0
60	DW	1	0	0	0	0
60	DY	1	0	0	0	0
61	AD	2	0	0	0	0
61	AN	1	0	0	0	0
61	CD	1	0	0	0	0
62	AA	2	0	0	0	0
All	All	296762	0	199834	19831	1

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 40.

The worst 5 of 19831 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:162:GLN:HB2	23:AX:23:A:C5	1.34	1.59
42:BH:11:VAL:HG22	42:BH:49:VAL:CG1	1.08	1.56
42:DH:11:VAL:HG22	42:DH:49:VAL:CG1	1.08	1.55
1:CA:644:G:C2'	1:CA:645:C:H5''	1.39	1.53
24:AY:57:GLN:HG3	35:BA:1913:A:C2	1.45	1.47

All (1) 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)
35:DA:1411:C:O3'	36:DB:53:A:O2'[1.655]	2.19	0.01

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%)	133 (57%)	67 (29%)	33 (14%)	0	2
2	CB	233/256 (91%)	133 (57%)	68 (29%)	32 (14%)	0	2
3	AC	205/239 (86%)	130 (63%)	50 (24%)	25 (12%)	1	3
3	CC	205/239 (86%)	128 (62%)	52 (25%)	25 (12%)	1	3
4	AD	206/209 (99%)	139 (68%)	45 (22%)	22 (11%)	1	5
4	CD	206/209 (99%)	138 (67%)	46 (22%)	22 (11%)	1	5
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%)	74 (75%)	13 (13%)	12 (12%)	1	4
6	CF	99/101 (98%)	74 (75%)	13 (13%)	12 (12%)	1	4
7	AG	153/156 (98%)	107 (70%)	35 (23%)	11 (7%)	2	13
7	CG	153/156 (98%)	107 (70%)	35 (23%)	11 (7%)	2	13
8	AH	136/138 (99%)	99 (73%)	31 (23%)	6 (4%)	4	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	CH	136/138 (99%)	99 (73%)	30 (22%)	7 (5%)	3	25
9	AI	121/128 (94%)	75 (62%)	31 (26%)	15 (12%)	1	3
9	CI	121/128 (94%)	74 (61%)	33 (27%)	14 (12%)	1	4
10	AJ	97/105 (92%)	64 (66%)	28 (29%)	5 (5%)	3	25
10	CJ	97/105 (92%)	64 (66%)	28 (29%)	5 (5%)	3	25
11	AK	117/129 (91%)	76 (65%)	28 (24%)	13 (11%)	1	4
11	CK	117/129 (91%)	76 (65%)	28 (24%)	13 (11%)	1	4
12	AL	123/135 (91%)	89 (72%)	21 (17%)	13 (11%)	1	5
12	CL	123/135 (91%)	87 (71%)	22 (18%)	14 (11%)	1	4
13	AM	110/126 (87%)	62 (56%)	27 (24%)	21 (19%)	0	0
13	CM	110/126 (87%)	63 (57%)	26 (24%)	21 (19%)	0	0
14	AN	58/61 (95%)	37 (64%)	14 (24%)	7 (12%)	1	4
14	CN	58/61 (95%)	36 (62%)	16 (28%)	6 (10%)	1	6
15	AO	86/89 (97%)	54 (63%)	25 (29%)	7 (8%)	1	10
15	CO	86/89 (97%)	55 (64%)	24 (28%)	7 (8%)	1	10
16	AP	82/88 (93%)	55 (67%)	18 (22%)	9 (11%)	1	5
16	CP	82/88 (93%)	55 (67%)	18 (22%)	9 (11%)	1	5
17	AQ	98/105 (93%)	65 (66%)	21 (21%)	12 (12%)	1	3
17	CQ	98/105 (93%)	66 (67%)	20 (20%)	12 (12%)	1	3
18	AR	68/88 (77%)	36 (53%)	22 (32%)	10 (15%)	0	2
18	CR	68/88 (77%)	35 (52%)	23 (34%)	10 (15%)	0	2
19	AS	83/93 (89%)	48 (58%)	18 (22%)	17 (20%)	0	0
19	CS	83/93 (89%)	48 (58%)	18 (22%)	17 (20%)	0	0
20	AT	97/106 (92%)	62 (64%)	25 (26%)	10 (10%)	1	6
20	CT	97/106 (92%)	62 (64%)	25 (26%)	10 (10%)	1	6
21	AU	23/27 (85%)	11 (48%)	10 (44%)	2 (9%)	1	8
21	CU	23/27 (85%)	11 (48%)	10 (44%)	2 (9%)	1	8
24	AY	95/97 (98%)	81 (85%)	10 (10%)	4 (4%)	4	31
24	CY	14/97 (14%)	8 (57%)	4 (29%)	2 (14%)	0	2
25	B0	82/85 (96%)	67 (82%)	10 (12%)	5 (6%)	2	19
25	D0	82/85 (96%)	66 (80%)	10 (12%)	6 (7%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	B1	92/98 (94%)	70 (76%)	16 (17%)	6 (6%)	2	17
26	D1	92/98 (94%)	74 (80%)	9 (10%)	9 (10%)	1	7
27	B2	69/72 (96%)	51 (74%)	13 (19%)	5 (7%)	2	13
27	D2	69/72 (96%)	47 (68%)	18 (26%)	4 (6%)	3	21
28	B3	58/60 (97%)	49 (84%)	8 (14%)	1 (2%)	14	62
28	D3	58/60 (97%)	50 (86%)	7 (12%)	1 (2%)	14	62
29	B4	54/71 (76%)	28 (52%)	12 (22%)	14 (26%)	0	0
29	D4	54/71 (76%)	28 (52%)	12 (22%)	14 (26%)	0	0
30	B5	57/60 (95%)	42 (74%)	9 (16%)	6 (10%)	1	5
30	D5	57/60 (95%)	41 (72%)	10 (18%)	6 (10%)	1	5
31	B6	41/54 (76%)	17 (42%)	15 (37%)	9 (22%)	0	0
31	D6	41/54 (76%)	16 (39%)	16 (39%)	9 (22%)	0	0
32	B7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	11	55
32	D7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	11	55
33	B8	62/65 (95%)	35 (56%)	15 (24%)	12 (19%)	0	0
33	D8	62/65 (95%)	34 (55%)	15 (24%)	13 (21%)	0	0
34	B9	34/37 (92%)	24 (71%)	8 (24%)	2 (6%)	2	20
34	D9	34/37 (92%)	24 (71%)	8 (24%)	2 (6%)	2	20
37	BC	183/229 (80%)	75 (41%)	67 (37%)	41 (22%)	0	0
37	DC	183/229 (80%)	76 (42%)	65 (36%)	42 (23%)	0	0
38	BD	270/276 (98%)	199 (74%)	48 (18%)	23 (8%)	1	9
38	DD	270/276 (98%)	198 (73%)	47 (17%)	25 (9%)	1	8
39	BE	203/206 (98%)	142 (70%)	37 (18%)	24 (12%)	1	4
39	DE	203/206 (98%)	143 (70%)	36 (18%)	24 (12%)	1	4
40	BF	206/210 (98%)	137 (66%)	40 (19%)	29 (14%)	0	2
40	DF	206/210 (98%)	137 (66%)	41 (20%)	28 (14%)	0	2
41	BG	177/182 (97%)	109 (62%)	44 (25%)	24 (14%)	0	2
41	DG	177/182 (97%)	107 (60%)	43 (24%)	27 (15%)	0	1
42	BH	163/180 (91%)	90 (55%)	42 (26%)	31 (19%)	0	0
42	DH	163/180 (91%)	90 (55%)	42 (26%)	31 (19%)	0	0
43	BI	143/148 (97%)	80 (56%)	36 (25%)	27 (19%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	DI	143/148 (97%)	80 (56%)	36 (25%)	27 (19%)	0	0
45	BN	137/140 (98%)	97 (71%)	20 (15%)	20 (15%)	0	2
45	DN	137/140 (98%)	96 (70%)	21 (15%)	20 (15%)	0	2
46	BO	120/122 (98%)	99 (82%)	15 (12%)	6 (5%)	3	26
46	DO	120/122 (98%)	99 (82%)	15 (12%)	6 (5%)	3	26
47	BP	144/150 (96%)	70 (49%)	34 (24%)	40 (28%)	0	0
47	DP	144/150 (96%)	70 (49%)	34 (24%)	40 (28%)	0	0
48	BQ	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	1	7
48	DQ	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	1	7
49	BR	115/118 (98%)	80 (70%)	20 (17%)	15 (13%)	0	3
49	DR	115/118 (98%)	82 (71%)	20 (17%)	13 (11%)	1	4
50	BS	97/112 (87%)	46 (47%)	20 (21%)	31 (32%)	0	0
50	DS	97/112 (87%)	46 (47%)	20 (21%)	31 (32%)	0	0
51	BT	136/146 (93%)	79 (58%)	33 (24%)	24 (18%)	0	1
51	DT	136/146 (93%)	80 (59%)	31 (23%)	25 (18%)	0	1
52	BU	115/118 (98%)	87 (76%)	18 (16%)	10 (9%)	1	8
52	DU	115/118 (98%)	88 (76%)	17 (15%)	10 (9%)	1	8
53	BV	99/101 (98%)	72 (73%)	12 (12%)	15 (15%)	0	1
53	DV	99/101 (98%)	72 (73%)	12 (12%)	15 (15%)	0	1
54	BW	111/113 (98%)	84 (76%)	17 (15%)	10 (9%)	1	8
54	DW	111/113 (98%)	85 (77%)	16 (14%)	10 (9%)	1	8
55	BX	91/96 (95%)	73 (80%)	15 (16%)	3 (3%)	6	38
55	DX	91/96 (95%)	72 (79%)	16 (18%)	3 (3%)	6	38
56	BY	99/110 (90%)	50 (50%)	23 (23%)	26 (26%)	0	0
56	DY	99/110 (90%)	50 (50%)	23 (23%)	26 (26%)	0	0
57	BZ	185/206 (90%)	123 (66%)	38 (20%)	24 (13%)	0	3
57	DZ	185/206 (90%)	101 (55%)	49 (26%)	35 (19%)	0	0
All	All	11855/12786 (93%)	7751 (65%)	2556 (22%)	1548 (13%)	0	2

5 of 1548 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	75	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	AB	83	MET
2	AB	101	MET
2	AB	150	SER
2	AB	238	LEU

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%)	185 (92%)	17 (8%)	16	53
2	CB	202/220 (92%)	185 (92%)	17 (8%)	16	53
3	AC	160/188 (85%)	151 (94%)	9 (6%)	30	75
3	CC	160/188 (85%)	151 (94%)	9 (6%)	30	75
4	AD	179/181 (99%)	165 (92%)	14 (8%)	18	59
4	CD	179/181 (99%)	164 (92%)	15 (8%)	16	53
5	AE	115/123 (94%)	105 (91%)	10 (9%)	15	51
5	CE	115/123 (94%)	105 (91%)	10 (9%)	15	51
6	AF	90/90 (100%)	87 (97%)	3 (3%)	50	87
6	CF	90/90 (100%)	87 (97%)	3 (3%)	50	87
7	AG	126/127 (99%)	124 (98%)	2 (2%)	75	94
7	CG	126/127 (99%)	124 (98%)	2 (2%)	75	94
8	AH	119/119 (100%)	110 (92%)	9 (8%)	19	60
8	CH	119/119 (100%)	110 (92%)	9 (8%)	19	60
9	AI	98/99 (99%)	88 (90%)	10 (10%)	11	40
9	CI	98/99 (99%)	88 (90%)	10 (10%)	11	40
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	8	35
10	CJ	88/92 (96%)	78 (89%)	10 (11%)	8	35
11	AK	90/99 (91%)	85 (94%)	5 (6%)	30	75
11	CK	90/99 (91%)	85 (94%)	5 (6%)	30	75
12	AL	104/111 (94%)	95 (91%)	9 (9%)	15	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	CL	104/111 (94%)	95 (91%)	9 (9%)	15	51
13	AM	94/101 (93%)	86 (92%)	8 (8%)	15	53
13	CM	94/101 (93%)	86 (92%)	8 (8%)	15	53
14	AN	49/50 (98%)	45 (92%)	4 (8%)	17	56
14	CN	49/50 (98%)	45 (92%)	4 (8%)	17	56
15	AO	79/80 (99%)	74 (94%)	5 (6%)	25	69
15	CO	79/80 (99%)	74 (94%)	5 (6%)	25	69
16	AP	72/74 (97%)	67 (93%)	5 (7%)	22	65
16	CP	72/74 (97%)	66 (92%)	6 (8%)	16	55
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	51	87
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	66	92
18	AR	61/77 (79%)	59 (97%)	2 (3%)	50	87
18	CR	61/77 (79%)	59 (97%)	2 (3%)	50	87
19	AS	72/80 (90%)	62 (86%)	10 (14%)	5	24
19	CS	72/80 (90%)	62 (86%)	10 (14%)	5	24
20	AT	76/82 (93%)	67 (88%)	9 (12%)	8	33
20	CT	76/82 (93%)	67 (88%)	9 (12%)	8	33
21	AU	19/22 (86%)	17 (90%)	2 (10%)	10	39
21	CU	19/22 (86%)	18 (95%)	1 (5%)	32	75
24	AY	78/78 (100%)	42 (54%)	36 (46%)	0	0
24	CY	12/78 (15%)	8 (67%)	4 (33%)	0	0
25	B0	66/67 (98%)	58 (88%)	8 (12%)	7	32
25	D0	66/67 (98%)	58 (88%)	8 (12%)	7	32
26	B1	78/83 (94%)	67 (86%)	11 (14%)	5	23
26	D1	78/83 (94%)	67 (86%)	11 (14%)	5	23
27	B2	66/67 (98%)	59 (89%)	7 (11%)	10	38
27	D2	66/67 (98%)	56 (85%)	10 (15%)	4	19
28	B3	51/52 (98%)	41 (80%)	10 (20%)	2	10
28	D3	51/52 (98%)	41 (80%)	10 (20%)	2	10
29	B4	49/63 (78%)	40 (82%)	9 (18%)	2	11
29	D4	49/63 (78%)	42 (86%)	7 (14%)	5	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	B5	51/52 (98%)	47 (92%)	4 (8%)	18	59
30	D5	51/52 (98%)	47 (92%)	4 (8%)	18	59
31	B6	43/52 (83%)	39 (91%)	4 (9%)	13	46
31	D6	43/52 (83%)	38 (88%)	5 (12%)	8	34
32	B7	41/42 (98%)	36 (88%)	5 (12%)	7	31
32	D7	41/42 (98%)	36 (88%)	5 (12%)	7	31
33	B8	53/55 (96%)	45 (85%)	8 (15%)	4	19
33	D8	53/55 (96%)	45 (85%)	8 (15%)	4	19
34	B9	33/34 (97%)	32 (97%)	1 (3%)	53	88
34	D9	33/34 (97%)	32 (97%)	1 (3%)	53	88
37	BC	61/181 (34%)	57 (93%)	4 (7%)	24	67
37	DC	61/181 (34%)	57 (93%)	4 (7%)	24	67
38	BD	213/218 (98%)	176 (83%)	37 (17%)	3	13
38	DD	213/218 (98%)	176 (83%)	37 (17%)	3	13
39	BE	165/166 (99%)	142 (86%)	23 (14%)	5	24
39	DE	165/166 (99%)	142 (86%)	23 (14%)	5	24
40	BF	165/166 (99%)	143 (87%)	22 (13%)	6	27
40	DF	165/166 (99%)	143 (87%)	22 (13%)	6	27
41	BG	155/156 (99%)	133 (86%)	22 (14%)	5	22
41	DG	155/156 (99%)	135 (87%)	20 (13%)	6	28
42	BH	137/148 (93%)	122 (89%)	15 (11%)	9	37
42	DH	137/148 (93%)	122 (89%)	15 (11%)	9	37
43	BI	121/124 (98%)	104 (86%)	17 (14%)	5	23
43	DI	121/124 (98%)	103 (85%)	18 (15%)	4	20
45	BN	117/119 (98%)	97 (83%)	20 (17%)	3	14
45	DN	117/119 (98%)	96 (82%)	21 (18%)	2	12
46	BO	100/100 (100%)	95 (95%)	5 (5%)	34	78
46	DO	100/100 (100%)	94 (94%)	6 (6%)	27	72
47	BP	112/116 (97%)	80 (71%)	32 (29%)	0	1
47	DP	112/116 (97%)	81 (72%)	31 (28%)	0	2
48	BQ	111/111 (100%)	104 (94%)	7 (6%)	25	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	DQ	111/111 (100%)	104 (94%)	7 (6%)	25	69
49	BR	100/101 (99%)	86 (86%)	14 (14%)	5	23
49	DR	100/101 (99%)	84 (84%)	16 (16%)	3	16
50	BS	77/88 (88%)	64 (83%)	13 (17%)	3	14
50	DS	77/88 (88%)	64 (83%)	13 (17%)	3	14
51	BT	120/127 (94%)	99 (82%)	21 (18%)	3	13
51	DT	120/127 (94%)	100 (83%)	20 (17%)	3	14
52	BU	92/94 (98%)	80 (87%)	12 (13%)	6	28
52	DU	92/94 (98%)	81 (88%)	11 (12%)	7	32
53	BV	82/82 (100%)	68 (83%)	14 (17%)	3	14
53	DV	82/82 (100%)	68 (83%)	14 (17%)	3	14
54	BW	91/92 (99%)	81 (89%)	10 (11%)	9	36
54	DW	91/92 (99%)	81 (89%)	10 (11%)	9	36
55	BX	74/78 (95%)	62 (84%)	12 (16%)	3	15
55	DX	74/78 (95%)	62 (84%)	12 (16%)	3	15
56	BY	84/91 (92%)	70 (83%)	14 (17%)	3	14
56	DY	84/91 (92%)	70 (83%)	14 (17%)	3	14
57	BZ	163/179 (91%)	147 (90%)	16 (10%)	12	43
57	DZ	163/179 (91%)	143 (88%)	20 (12%)	7	31
All	All	9806/10588 (93%)	8674 (88%)	1132 (12%)	8	35

5 of 1132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	BU	112	ARG
7	CG	57	GLU
51	DT	85	LYS
54	BW	11	ARG
57	BZ	150	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 302 such sidechains are listed below:

Mol	Chain	Res	Type
50	BS	95	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	CC	136	GLN
49	DR	71	GLN
52	BU	49	HIS
57	BZ	34	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1522 (98%)	206 (13%)	21 (1%)
1	CA	1505/1522 (98%)	235 (15%)	24 (1%)
22	AV	76/77 (98%)	18 (23%)	1 (1%)
22	AW	76/77 (98%)	14 (18%)	1 (1%)
22	CV	76/77 (98%)	20 (26%)	1 (1%)
22	CW	76/77 (98%)	8 (10%)	0
23	AX	15/25 (60%)	14 (93%)	10 (66%)
35	BA	2805/2848 (98%)	485 (17%)	58 (2%)
35	DA	2804/2848 (98%)	487 (17%)	58 (2%)
36	BB	118/122 (96%)	20 (16%)	1 (0%)
36	DB	118/122 (96%)	20 (16%)	1 (0%)
58	CX	8/25 (32%)	7 (87%)	5 (62%)
All	All	9182/9342 (98%)	1534 (16%)	181 (1%)

5 of 1534 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	31	G

5 of 181 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	2126	A
1	CA	428	G
35	DA	1992	G
35	BA	2422	A
36	BB	66	A

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	A3P	AA	1493	1	26,28,29	0.78	0	39,42,45	2.01	4 (10%)
1	A3P	CA	1493	1	26,28,29	0.82	1 (3%)	39,42,45	0.88	1 (2%)

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
1	A3P	AA	1493	1	-	0/13/30/31	0/3/3/3
1	A3P	CA	1493	1	-	0/13/30/31	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1493	A3P	P2-O4P	2.31	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1493	A3P	O2P-P1-O3'	-8.14	83.64	107.09
1	AA	1493	A3P	O3'-P1-O1P	6.43	125.27	106.80
1	AA	1493	A3P	P1-O3'-C3'	-4.98	110.27	121.77
1	CA	1493	A3P	O2P-P1-O1P	2.68	119.13	110.36
1	AA	1493	A3P	O2P-P1-O1P	2.67	119.09	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2338 ligands modelled in this entry, 2338 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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
9	AI	2
9	CI	2
41	DG	1
41	BG	1
31	D6	1
31	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	B6	46:HIS	C	47:THR	N	7.76
1	D6	46:HIS	C	47:THR	N	7.76
1	BG	112:PRO	C	113:ARG	N	4.73
1	DG	112:PRO	C	113:ARG	N	4.47
1	AM	69:GLU	C	70:LEU	N	4.25

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	1508/1522 (99%)	-0.05	29 (1%) 64 18	54, 107, 196, 201	0
1	CA	1508/1522 (99%)	0.64	128 (8%) 11 3	60, 169, 201, 201	0
2	AB	235/256 (91%)	0.17	5 (2%) 60 15	77, 152, 197, 201	0
2	CB	235/256 (91%)	0.42	12 (5%) 27 5	90, 173, 201, 201	0
3	AC	207/239 (86%)	0.17	3 (1%) 72 22	83, 149, 188, 201	0
3	CC	207/239 (86%)	0.65	18 (8%) 10 3	106, 175, 201, 201	0
4	AD	208/209 (99%)	-0.07	0 100 100	65, 105, 149, 180	0
4	CD	208/209 (99%)	0.87	26 (12%) 5 1	85, 173, 201, 201	0
5	AE	151/162 (93%)	-0.02	0 100 100	70, 107, 155, 198	0
5	CE	151/162 (93%)	0.53	10 (6%) 18 4	89, 155, 197, 201	0
6	AF	101/101 (100%)	-0.01	1 (0%) 79 29	70, 125, 163, 190	0
6	CF	101/101 (100%)	-0.11	0 100 100	65, 110, 155, 184	0
7	AG	155/156 (99%)	0.13	5 (3%) 45 9	85, 141, 184, 201	0
7	CG	155/156 (99%)	0.47	10 (6%) 18 4	86, 164, 200, 201	0
8	AH	138/138 (100%)	-0.02	0 100 100	66, 108, 151, 171	0
8	CH	138/138 (100%)	0.41	6 (4%) 34 7	79, 157, 189, 201	0
9	AI	127/128 (99%)	0.60	5 (3%) 37 7	94, 164, 200, 201	0
9	CI	127/128 (99%)	1.25	28 (22%) 1 1	115, 177, 201, 201	0
10	AJ	99/105 (94%)	0.75	11 (11%) 6 2	105, 169, 201, 201	0
10	CJ	99/105 (94%)	1.54	22 (22%) 1 1	125, 181, 201, 201	0
11	AK	119/129 (92%)	0.10	2 (1%) 67 19	60, 113, 168, 197	0
11	CK	119/129 (92%)	0.19	4 (3%) 43 9	78, 139, 188, 200	0
12	AL	125/135 (92%)	0.03	2 (1%) 68 20	59, 90, 144, 201	0
12	CL	125/135 (92%)	0.65	9 (7%) 15 3	63, 139, 187, 201	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	118/126 (93%)	0.33	2 (1%) 67 19	96, 152, 189, 201	0
13	CM	118/126 (93%)	0.63	8 (6%) 17 4	102, 165, 201, 201	0
14	AN	60/61 (98%)	0.53	3 (5%) 28 5	99, 153, 198, 201	0
14	CN	60/61 (98%)	0.92	9 (15%) 3 1	118, 171, 200, 201	0
15	AO	88/89 (98%)	-0.04	0 100 100	69, 102, 149, 171	0
15	CO	88/89 (98%)	0.07	0 100 100	75, 123, 163, 176	0
16	AP	84/88 (95%)	-0.00	1 (1%) 75 26	60, 92, 143, 195	0
16	CP	84/88 (95%)	1.01	11 (13%) 4 1	112, 172, 198, 201	0
17	AQ	100/105 (95%)	-0.12	0 100 100	63, 97, 134, 156	0
17	CQ	100/105 (95%)	0.36	3 (3%) 48 10	102, 142, 181, 195	0
18	AR	70/88 (79%)	0.13	1 (1%) 72 22	78, 116, 165, 178	0
18	CR	70/88 (79%)	0.22	2 (2%) 49 10	79, 120, 180, 196	0
19	AS	85/93 (91%)	0.62	5 (5%) 22 5	101, 164, 198, 201	0
19	CS	85/93 (91%)	0.96	9 (10%) 7 2	118, 176, 199, 201	0
20	AT	99/106 (93%)	0.08	1 (1%) 79 29	60, 104, 163, 191	0
20	CT	99/106 (93%)	0.57	6 (6%) 21 4	113, 169, 198, 201	0
21	AU	25/27 (92%)	1.53	7 (28%) 1 1	91, 151, 184, 201	0
21	CU	25/27 (92%)	2.31	13 (52%) 0 0	84, 159, 199, 201	0
22	AV	77/77 (100%)	-0.21	1 (1%) 74 24	55, 106, 161, 194	0
22	AW	77/77 (100%)	2.39	43 (55%) 0 0	125, 201, 201, 201	0
22	CV	77/77 (100%)	-0.11	0 100 100	50, 131, 175, 182	0
22	CW	77/77 (100%)	2.50	41 (53%) 0 0	146, 201, 201, 201	0
23	AX	16/25 (64%)	2.68	10 (62%) 0 0	84, 199, 201, 201	0
24	AY	97/97 (100%)	0.81	10 (10%) 7 2	99, 149, 192, 201	1 (1%)
24	CY	16/97 (16%)	1.07	3 (18%) 2 1	130, 157, 201, 201	0
25	B0	84/85 (98%)	0.32	4 (4%) 29 6	51, 90, 164, 196	0
25	D0	84/85 (98%)	0.49	7 (8%) 11 3	70, 105, 166, 191	0
26	B1	94/98 (95%)	-0.04	1 (1%) 77 27	44, 76, 145, 161	0
26	D1	94/98 (95%)	-0.17	0 100 100	41, 74, 139, 159	0
27	B2	71/72 (98%)	-0.06	0 100 100	65, 103, 150, 169	0
27	D2	71/72 (98%)	-0.20	0 100 100	42, 71, 129, 195	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	B3	60/60 (100%)	0.19	2 (3%)	44	9	42, 88, 148, 201	0
28	D3	60/60 (100%)	0.05	1 (1%)	67	19	50, 87, 142, 200	0
29	B4	56/71 (78%)	0.13	3 (5%)	25	5	96, 160, 187, 197	0
29	D4	56/71 (78%)	0.52	6 (10%)	6	2	122, 176, 201, 201	0
30	B5	59/60 (98%)	0.04	4 (6%)	17	4	37, 70, 174, 181	0
30	D5	59/60 (98%)	0.17	4 (6%)	17	4	27, 75, 177, 201	0
31	B6	45/54 (83%)	1.52	13 (28%)	1	1	97, 141, 184, 187	0
31	D6	45/54 (83%)	1.01	7 (15%)	3	1	103, 161, 195, 199	0
32	B7	49/49 (100%)	-0.13	0	100	100	38, 55, 112, 194	0
32	D7	49/49 (100%)	-0.16	0	100	100	21, 40, 108, 159	0
33	B8	64/65 (98%)	-0.06	0	100	100	32, 72, 132, 200	0
33	D8	64/65 (98%)	0.13	2 (3%)	47	10	41, 83, 148, 201	0
34	B9	36/37 (97%)	1.08	6 (16%)	2	1	83, 123, 168, 201	0
34	D9	36/37 (97%)	1.11	4 (11%)	6	2	91, 128, 167, 197	0
35	BA	2807/2848 (98%)	-0.10	88 (3%)	47	10	32, 74, 188, 201	0
35	DA	2807/2848 (98%)	-0.04	73 (2%)	53	11	29, 77, 189, 201	0
36	BB	119/122 (97%)	-0.09	2 (1%)	67	19	76, 130, 181, 201	0
36	DB	119/122 (97%)	0.13	3 (2%)	54	12	87, 151, 189, 200	0
37	BC	191/229 (83%)	2.32	104 (54%)	0	0	160, 198, 201, 201	0
37	DC	191/229 (83%)	2.15	86 (45%)	1	0	154, 197, 201, 201	0
38	BD	272/276 (98%)	-0.16	0	100	100	38, 71, 107, 184	0
38	DD	272/276 (98%)	-0.13	0	100	100	32, 68, 111, 185	0
39	BE	205/206 (99%)	-0.09	0	100	100	36, 83, 157, 201	0
39	DE	205/206 (99%)	-0.02	3 (1%)	70	21	25, 91, 157, 201	0
40	BF	208/210 (99%)	-0.21	0	100	100	30, 73, 156, 186	0
40	DF	208/210 (99%)	-0.18	0	100	100	24, 78, 165, 196	0
41	BG	181/182 (99%)	0.21	5 (2%)	50	11	79, 142, 188, 201	0
41	DG	181/182 (99%)	0.29	4 (2%)	59	14	92, 155, 193, 201	0
42	BH	165/180 (91%)	0.65	14 (8%)	11	3	90, 157, 193, 201	0
42	DH	165/180 (91%)	0.05	0	100	100	55, 112, 158, 182	0
43	BI	145/148 (97%)	1.29	34 (23%)	1	1	60, 161, 201, 201	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	DI	145/148 (97%)	0.43	10 (6%) 17 4	70, 130, 200, 201	0
44	BJ	0/130	-	-	-	-
45	BN	139/140 (99%)	-0.11	0 100 100	52, 88, 145, 201	0
45	DN	139/140 (99%)	-0.16	0 100 100	44, 79, 140, 189	0
46	BO	122/122 (100%)	-0.29	0 100 100	42, 72, 101, 178	0
46	DO	122/122 (100%)	0.11	0 100 100	59, 104, 154, 201	0
47	BP	146/150 (97%)	0.00	2 (1%) 72 22	26, 92, 150, 197	0
47	DP	146/150 (97%)	0.14	2 (1%) 72 22	35, 96, 170, 198	0
48	BQ	141/141 (100%)	-0.06	0 100 100	48, 89, 132, 201	0
48	DQ	141/141 (100%)	0.19	2 (1%) 72 22	53, 106, 159, 191	0
49	BR	117/118 (99%)	-0.19	0 100 100	39, 76, 125, 150	0
49	DR	117/118 (99%)	0.08	0 100 100	53, 90, 147, 162	0
50	BS	99/112 (88%)	0.16	1 (1%) 79 29	75, 133, 182, 189	0
50	DS	99/112 (88%)	0.46	5 (5%) 27 5	95, 145, 196, 201	0
51	BT	138/146 (94%)	-0.02	1 (0%) 84 38	51, 87, 182, 201	0
51	DT	138/146 (94%)	0.30	5 (3%) 41 8	68, 131, 194, 201	0
52	BU	117/118 (99%)	-0.18	0 100 100	37, 73, 137, 201	0
52	DU	117/118 (99%)	-0.24	0 100 100	25, 62, 114, 174	0
53	BV	101/101 (100%)	-0.05	0 100 100	35, 103, 143, 201	0
53	DV	101/101 (100%)	-0.19	0 100 100	33, 80, 126, 180	0
54	BW	113/113 (100%)	-0.15	1 (0%) 81 32	43, 70, 133, 201	0
54	DW	113/113 (100%)	-0.25	0 100 100	37, 60, 118, 187	0
55	BX	93/96 (96%)	-0.08	0 100 100	43, 89, 125, 140	0
55	DX	93/96 (96%)	-0.21	0 100 100	43, 65, 114, 153	0
56	BY	101/110 (91%)	0.52	11 (10%) 6 2	63, 109, 182, 201	0
56	DY	101/110 (91%)	0.21	5 (4%) 28 5	54, 99, 176, 201	0
57	BZ	187/206 (90%)	0.09	4 (2%) 60 15	74, 121, 171, 201	0
57	DZ	187/206 (90%)	0.10	3 (1%) 68 20	76, 133, 187, 201	0
58	CX	8/25 (32%)	1.23	2 (25%) 1 1	106, 165, 200, 201	0
59	DJ	0/131	-	-	-	-
All	All	21299/22389 (95%)	0.20	1059 (4%) 28 5	21, 111, 198, 201	1 (0%)

The worst 5 of 1059 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
43	BI	111	PRO	15.1
35	DA	2112	G	13.4
3	CC	169	ALA	11.2
1	AA	81	U	10.0
22	CW	34	C	9.8

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

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
1	A3P	CA	1493	26/27	0.46	-	191,200,203,203	0
1	A3P	AA	1493	26/27	0.18	-	151,182,188,189	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	MG	AA	1774	1/1	0.56	-	120,120,120,120	0
60	MG	DA	3553	1/1	0.70	-	68,68,68,68	0
60	MG	CA	1684	1/1	0.43	-	64,64,64,64	0
60	MG	DA	3251	1/1	0.21	-	53,53,53,53	0
60	MG	DA	3531	1/1	0.31	-	82,82,82,82	0
60	MG	DA	3718	1/1	0.72	-	92,92,92,92	0
60	MG	DA	3727	1/1	0.36	-	70,70,70,70	1
60	MG	BA	3015	1/1	0.07	-	105,105,105,105	0
60	MG	BA	3268	1/1	0.18	-	88,88,88,88	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1673	1/1	0.32	-	62,62,62,62	0
60	MG	DA	3282	1/1	0.37	-	31,31,31,31	0
60	MG	DA	3410	1/1	0.41	-	25,25,25,25	0
60	MG	DA	3226	1/1	0.68	-	54,54,54,54	0
60	MG	BA	3467	1/1	0.15	-	93,93,93,93	0
60	MG	DA	3480	1/1	0.25	-	87,87,87,87	0
60	MG	DA	3067	1/1	0.29	-	106,106,106,106	0
60	MG	DA	3563	1/1	0.48	-	68,68,68,68	1
60	MG	AA	1694	1/1	0.24	-	56,56,56,56	1
60	MG	DA	2921	1/1	1.62	-	114,114,114,114	0
60	MG	DA	3669	1/1	0.38	-	39,39,39,39	0
60	MG	CA	1665	1/1	0.13	-	79,79,79,79	0
60	MG	DA	3715	1/1	0.22	-	64,64,64,64	0
60	MG	BA	3439	1/1	0.25	-	37,37,37,37	0
60	MG	BA	2930	1/1	0.23	-	85,85,85,85	0
60	MG	BA	3580	1/1	0.20	-	135,135,135,135	0
60	MG	B6	101	1/1	0.39	-	111,111,111,111	0
60	MG	AA	1899	1/1	0.41	-	63,63,63,63	0
60	MG	BA	3531	1/1	0.53	-	53,53,53,53	0
60	MG	BA	2959	1/1	0.26	-	65,65,65,65	0
60	MG	CA	1695	1/1	0.54	-	110,110,110,110	0
60	MG	AA	1704	1/1	0.30	-	84,84,84,84	0
60	MG	AV	104	1/1	0.26	-	133,133,133,133	0
60	MG	AA	1914	1/1	0.22	-	56,56,56,56	0
60	MG	DA	3393	1/1	0.21	-	6,6,6,6	1
60	MG	BA	2970	1/1	1.51	-	101,101,101,101	0
60	MG	DA	3029	1/1	0.17	-	30,30,30,30	0
60	MG	BA	3048	1/1	0.17	-	90,90,90,90	0
60	MG	DA	3131	1/1	0.58	-	154,154,154,154	0
60	MG	DA	3136	1/1	0.47	-	97,97,97,97	0
60	MG	DP	201	1/1	0.11	-	36,36,36,36	1
61	ZN	AN	101	1/1	0.13	-	153,153,153,153	0
60	MG	BA	3010	1/1	0.75	-	95,95,95,95	0
60	MG	BA	3411	1/1	0.45	-	76,76,76,76	0
60	MG	AA	1741	1/1	0.17	-	54,54,54,54	0
60	MG	DA	3171	1/1	0.24	-	71,71,71,71	0
60	MG	DA	3009	1/1	1.61	-	83,83,83,83	0
60	MG	BA	3364	1/1	0.78	-	66,66,66,66	1
60	MG	CA	1708	1/1	0.21	-	64,64,64,64	1
60	MG	AA	1737	1/1	0.51	-	69,69,69,69	0
60	MG	DA	3537	1/1	0.47	-	56,56,56,56	0
60	MG	AA	1923	1/1	0.42	-	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3483	1/1	0.55	-	55,55,55,55	0
60	MG	DN	201	1/1	0.21	-	19,19,19,19	1
60	MG	DA	3620	1/1	0.12	-	70,70,70,70	0
60	MG	DA	3594	1/1	0.22	-	63,63,63,63	1
60	MG	AA	1624	1/1	0.68	-	98,98,98,98	0
60	MG	AA	1746	1/1	0.38	-	66,66,66,66	0
60	MG	BA	3485	1/1	0.54	-	103,103,103,103	0
60	MG	DA	3783	1/1	0.95	-	90,90,90,90	0
60	MG	DA	3485	1/1	1.69	-	8,8,8,8	1
60	MG	BA	3487	1/1	0.30	-	64,64,64,64	0
60	MG	AA	1783	1/1	0.56	-	73,73,73,73	0
60	MG	B5	103	1/1	0.32	-	36,36,36,36	0
60	MG	DA	3211	1/1	0.23	-	65,65,65,65	0
60	MG	DA	3213	1/1	0.63	-	67,67,67,67	0
60	MG	DA	3796	1/1	0.27	-	95,95,95,95	1
60	MG	CA	1637	1/1	0.15	-	114,114,114,114	0
60	MG	CA	1667	1/1	0.06	-	66,66,66,66	0
60	MG	CA	1729	1/1	0.25	-	88,88,88,88	0
60	MG	DA	2923	1/1	0.14	-	94,94,94,94	0
60	MG	BA	2969	1/1	0.26	-	41,41,41,41	0
60	MG	BA	3216	1/1	0.42	-	73,73,73,73	0
60	MG	DA	2969	1/1	1.06	-	98,98,98,98	0
60	MG	DA	2973	1/1	0.40	-	21,21,21,21	0
60	MG	DA	3309	1/1	0.59	-	76,76,76,76	0
60	MG	BA	2948	1/1	0.21	-	64,64,64,64	0
60	MG	BA	3042	1/1	0.33	-	103,103,103,103	0
60	MG	AA	1777	1/1	0.36	-	115,115,115,115	0
60	MG	DD	306	1/1	0.11	-	60,60,60,60	0
60	MG	BA	3590	1/1	0.17	-	90,90,90,90	0
60	MG	BA	3575	1/1	0.45	-	92,92,92,92	0
60	MG	AA	1633	1/1	1.33	-	72,72,72,72	1
60	MG	DP	205	1/1	0.38	-	63,63,63,63	0
60	MG	AV	103	1/1	0.08	-	72,72,72,72	0
60	MG	DA	3696	1/1	0.65	-	80,80,80,80	0
60	MG	AA	1725	1/1	0.49	-	70,70,70,70	1
60	MG	BA	3570	1/1	0.60	-	115,115,115,115	0
60	MG	DA	3792	1/1	0.41	-	77,77,77,77	0
60	MG	BA	3393	1/1	0.21	-	104,104,104,104	0
60	MG	DA	3060	1/1	0.58	-	77,77,77,77	0
60	MG	AA	1622	1/1	0.36	-	70,70,70,70	0
60	MG	BA	3387	1/1	0.41	-	87,87,87,87	0
60	MG	DA	3786	1/1	0.37	-	144,144,144,144	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3217	1/1	0.67	-	69,69,69,69	0
60	MG	BA	3449	1/1	0.14	-	69,69,69,69	0
60	MG	DA	3624	1/1	0.40	-	71,71,71,71	0
60	MG	DA	3638	1/1	0.31	-	21,21,21,21	0
60	MG	DA	3297	1/1	0.60	-	53,53,53,53	0
60	MG	DA	3717	1/1	0.31	-	155,155,155,155	0
60	MG	BA	3138	1/1	0.14	-	60,60,60,60	0
60	MG	DA	3341	1/1	0.52	-	62,62,62,62	0
60	MG	CD	302	1/1	0.27	-	68,68,68,68	0
60	MG	BA	3518	1/1	0.33	-	64,64,64,64	0
60	MG	DA	3234	1/1	0.41	-	118,118,118,118	0
60	MG	BA	3004	1/1	1.42	-	84,84,84,84	0
60	MG	CA	1745	1/1	0.22	-	112,112,112,112	0
60	MG	DA	3327	1/1	0.09	-	39,39,39,39	1
60	MG	BA	3115	1/1	0.40	-	93,93,93,93	0
60	MG	BA	3002	1/1	1.67	-	83,83,83,83	0
60	MG	BA	3283	1/1	0.32	-	58,58,58,58	0
60	MG	DA	3701	1/1	0.12	-	55,55,55,55	0
60	MG	BA	3333	1/1	0.35	-	72,72,72,72	0
60	MG	DA	3560	1/1	0.17	-	58,58,58,58	0
60	MG	DA	3141	1/1	0.28	-	99,99,99,99	0
60	MG	AA	1691	1/1	0.58	-	90,90,90,90	0
60	MG	CA	1681	1/1	0.31	-	95,95,95,95	0
60	MG	BA	3331	1/1	1.40	-	92,92,92,92	0
60	MG	DE	302	1/1	0.13	-	39,39,39,39	1
60	MG	BA	3444	1/1	0.77	-	69,69,69,69	0
60	MG	BA	3392	1/1	0.89	-	87,87,87,87	0
60	MG	DA	3509	1/1	0.47	-	39,39,39,39	0
60	MG	DA	3529	1/1	0.09	-	42,42,42,42	0
60	MG	BA	3249	1/1	0.82	-	79,79,79,79	0
60	MG	AA	1897	1/1	0.19	-	68,68,68,68	0
60	MG	DA	3266	1/1	0.37	-	57,57,57,57	0
60	MG	BA	3577	1/1	0.42	-	38,38,38,38	0
60	MG	BA	3154	1/1	0.35	-	54,54,54,54	0
60	MG	DU	203	1/1	0.46	-	36,36,36,36	0
60	MG	DA	3222	1/1	0.32	-	79,79,79,79	0
60	MG	BA	3589	1/1	0.09	-	41,41,41,41	0
60	MG	BA	3493	1/1	0.43	-	101,101,101,101	0
60	MG	DA	3146	1/1	0.59	-	85,85,85,85	0
60	MG	BA	3416	1/1	0.68	-	58,58,58,58	0
60	MG	AA	1638	1/1	0.38	-	119,119,119,119	0
60	MG	BA	3275	1/1	0.18	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3331	1/1	0.10	-	45,45,45,45	1
60	MG	BA	2977	1/1	1.02	-	93,93,93,93	0
60	MG	AA	1693	1/1	0.13	-	56,56,56,56	1
60	MG	BE	301	1/1	0.39	-	88,88,88,88	0
60	MG	AA	1650	1/1	0.32	-	73,73,73,73	0
60	MG	DD	304	1/1	0.40	-	97,97,97,97	0
60	MG	DA	3471	1/1	0.57	-	63,63,63,63	0
60	MG	BA	3535	1/1	0.17	-	81,81,81,81	0
60	MG	DA	3755	1/1	0.15	-	128,128,128,128	0
60	MG	DA	3603	1/1	0.20	-	60,60,60,60	0
60	MG	BA	2992	1/1	0.29	-	50,50,50,50	1
60	MG	DA	3103	1/1	0.25	-	60,60,60,60	0
60	MG	BA	3382	1/1	0.12	-	77,77,77,77	0
60	MG	DA	2943	1/1	0.07	-	71,71,71,71	1
60	MG	BA	2949	1/1	0.50	-	102,102,102,102	0
60	MG	BA	3075	1/1	0.42	-	87,87,87,87	0
60	MG	DA	3172	1/1	1.01	-	102,102,102,102	0
60	MG	AA	1825	1/1	0.75	-	71,71,71,71	0
60	MG	AA	1771	1/1	0.55	-	95,95,95,95	0
60	MG	DA	3478	1/1	0.77	-	112,112,112,112	0
60	MG	BA	3136	1/1	0.19	-	34,34,34,34	0
60	MG	DA	3322	1/1	0.52	-	89,89,89,89	0
60	MG	DA	3789	1/1	0.40	-	68,68,68,68	0
60	MG	DA	3463	1/1	0.54	-	83,83,83,83	0
60	MG	DA	3010	1/1	0.24	-	49,49,49,49	0
60	MG	CA	1693	1/1	0.67	-	73,73,73,73	0
60	MG	CA	1703	1/1	1.03	-	82,82,82,82	0
60	MG	DA	3283	1/1	0.12	-	65,65,65,65	0
60	MG	CA	1662	1/1	0.11	-	79,79,79,79	0
60	MG	BA	3460	1/1	0.54	-	40,40,40,40	0
60	MG	AT	201	1/1	0.20	-	76,76,76,76	1
60	MG	AA	1655	1/1	0.05	-	101,101,101,101	0
60	MG	BA	3180	1/1	0.27	-	42,42,42,42	0
60	MG	DA	3651	1/1	0.35	-	93,93,93,93	0
60	MG	CV	111	1/1	0.12	-	71,71,71,71	0
60	MG	DA	3777	1/1	0.29	-	70,70,70,70	0
60	MG	AA	1911	1/1	0.13	-	55,55,55,55	0
60	MG	BA	3129	1/1	0.43	-	42,42,42,42	0
60	MG	DA	3636	1/1	0.14	-	50,50,50,50	0
60	MG	DA	3108	1/1	0.21	-	81,81,81,81	0
60	MG	BA	2981	1/1	0.22	-	80,80,80,80	0
60	MG	AA	1762	1/1	0.23	-	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1610	1/1	1.90	-	143,143,143,143	0
60	MG	BA	2953	1/1	0.55	-	84,84,84,84	0
60	MG	DA	3565	1/1	0.16	-	54,54,54,54	0
60	MG	BA	3373	1/1	0.21	-	56,56,56,56	0
60	MG	AA	1710	1/1	0.24	-	77,77,77,77	0
60	MG	BA	3526	1/1	1.17	-	76,76,76,76	0
60	MG	AA	1717	1/1	0.37	-	120,120,120,120	0
60	MG	DA	3061	1/1	0.28	-	67,67,67,67	0
60	MG	AA	1807	1/1	0.33	-	61,61,61,61	0
60	MG	DA	2998	1/1	0.29	-	49,49,49,49	0
60	MG	BA	3054	1/1	0.29	-	100,100,100,100	0
60	MG	DA	3617	1/1	0.43	-	111,111,111,111	0
60	MG	DA	3640	1/1	0.46	-	81,81,81,81	1
60	MG	AA	1644	1/1	0.31	-	84,84,84,84	0
60	MG	BA	3453	1/1	0.07	-	120,120,120,120	0
60	MG	DA	3682	1/1	0.25	-	103,103,103,103	0
60	MG	DA	3089	1/1	0.15	-	81,81,81,81	0
60	MG	BA	3367	1/1	1.61	-	96,96,96,96	0
60	MG	BF	301	1/1	0.34	-	60,60,60,60	0
60	MG	BA	3599	1/1	0.08	-	83,83,83,83	0
60	MG	DA	3732	1/1	0.29	-	67,67,67,67	0
60	MG	BA	3322	1/1	0.68	-	24,24,24,24	0
60	MG	DA	3404	1/1	0.40	-	87,87,87,87	0
60	MG	AA	1813	1/1	0.41	-	134,134,134,134	0
60	MG	DA	3372	1/1	0.25	-	82,82,82,82	0
60	MG	DA	3551	1/1	0.55	-	53,53,53,53	0
60	MG	BA	3272	1/1	1.20	-	126,126,126,126	0
60	MG	CA	1764	1/1	0.17	-	82,82,82,82	0
60	MG	BA	3551	1/1	0.92	-	82,82,82,82	0
60	MG	BA	3269	1/1	0.16	-	63,63,63,63	0
60	MG	DA	3271	1/1	0.67	-	96,96,96,96	0
60	MG	DA	3760	1/1	0.31	-	52,52,52,52	0
60	MG	AA	1631	1/1	0.86	-	85,85,85,85	0
60	MG	BA	3509	1/1	0.51	-	58,58,58,58	0
60	MG	BO	201	1/1	0.25	-	88,88,88,88	0
60	MG	BA	3236	1/1	0.84	-	86,86,86,86	0
60	MG	DA	3365	1/1	0.40	-	92,92,92,92	0
60	MG	DA	3586	1/1	0.54	-	34,34,34,34	0
60	MG	BA	2901	1/1	1.19	-	113,113,113,113	0
60	MG	DA	3194	1/1	0.23	-	92,92,92,92	0
60	MG	DA	3318	1/1	0.10	-	59,59,59,59	0
60	MG	BA	3151	1/1	0.18	-	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3325	1/1	0.29	-	109,109,109,109	0
60	MG	AA	1763	1/1	0.26	-	88,88,88,88	0
60	MG	BA	3116	1/1	0.56	-	81,81,81,81	0
60	MG	CA	1627	1/1	0.17	-	71,71,71,71	0
60	MG	AA	1800	1/1	0.74	-	114,114,114,114	0
60	MG	DA	3542	1/1	0.14	-	74,74,74,74	0
60	MG	BA	3332	1/1	0.44	-	19,19,19,19	0
60	MG	DA	3078	1/1	0.66	-	73,73,73,73	0
60	MG	DA	2975	1/1	0.30	-	56,56,56,56	0
60	MG	BA	3458	1/1	1.15	-	104,104,104,104	0
60	MG	BA	3521	1/1	0.28	-	119,119,119,119	0
60	MG	DA	2908	1/1	1.25	-	97,97,97,97	0
60	MG	DA	3227	1/1	0.43	-	73,73,73,73	0
60	MG	BA	2915	1/1	0.35	-	70,70,70,70	0
60	MG	DA	3762	1/1	0.13	-	99,99,99,99	0
60	MG	DA	3772	1/1	0.12	-	69,69,69,69	0
60	MG	DA	3459	1/1	0.60	-	92,92,92,92	0
60	MG	BA	3074	1/1	0.48	-	36,36,36,36	0
60	MG	AA	1862	1/1	0.39	-	65,65,65,65	0
60	MG	DA	3530	1/1	0.38	-	122,122,122,122	0
60	MG	BA	3058	1/1	0.27	-	74,74,74,74	0
60	MG	AA	1772	1/1	0.43	-	85,85,85,85	0
60	MG	DA	3017	1/1	0.40	-	70,70,70,70	0
60	MG	DA	2958	1/1	0.18	-	59,59,59,59	1
60	MG	B5	101	1/1	0.56	-	83,83,83,83	0
60	MG	AA	1727	1/1	0.12	-	84,84,84,84	1
60	MG	BA	3409	1/1	0.58	-	104,104,104,104	0
60	MG	DA	3629	1/1	0.31	-	45,45,45,45	0
60	MG	BA	2993	1/1	0.91	-	86,86,86,86	0
60	MG	BA	2944	1/1	0.26	-	43,43,43,43	0
60	MG	DA	3757	1/1	0.62	-	86,86,86,86	0
60	MG	DA	3045	1/1	0.12	-	47,47,47,47	0
60	MG	DA	2982	1/1	0.34	-	97,97,97,97	0
60	MG	CA	1671	1/1	0.41	-	99,99,99,99	0
60	MG	CA	1713	1/1	0.28	-	65,65,65,65	1
60	MG	DA	2971	1/1	0.19	-	20,20,20,20	0
60	MG	BA	3281	1/1	0.45	-	94,94,94,94	0
60	MG	BA	3374	1/1	0.80	-	74,74,74,74	0
60	MG	BA	3299	1/1	0.37	-	66,66,66,66	0
60	MG	BA	3442	1/1	0.23	-	65,65,65,65	0
60	MG	AA	1810	1/1	0.24	-	71,71,71,71	0
60	MG	AA	1761	1/1	1.21	-	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3143	1/1	0.70	-	113,113,113,113	0
60	MG	BD	302	1/1	0.30	-	52,52,52,52	0
60	MG	DA	2993	1/1	0.64	-	96,96,96,96	0
60	MG	DW	201	1/1	0.32	-	36,36,36,36	1
60	MG	DA	3723	1/1	0.52	-	101,101,101,101	0
60	MG	BA	3041	1/1	0.42	-	37,37,37,37	0
60	MG	AA	1788	1/1	0.25	-	80,80,80,80	0
60	MG	DA	3447	1/1	0.69	-	70,70,70,70	0
60	MG	BA	3161	1/1	0.26	-	39,39,39,39	0
60	MG	DA	2930	1/1	1.29	-	1,1,1,1	1
60	MG	DA	2976	1/1	0.64	-	1,1,1,1	1
60	MG	BA	2913	1/1	0.69	-	51,51,51,51	0
60	MG	BA	3200	1/1	0.11	-	31,31,31,31	0
60	MG	AA	1797	1/1	0.29	-	76,76,76,76	0
60	MG	AA	1646	1/1	0.54	-	106,106,106,106	0
60	MG	BA	3034	1/1	0.22	-	51,51,51,51	0
60	MG	CA	1660	1/1	0.32	-	99,99,99,99	0
60	MG	D0	103	1/1	0.31	-	74,74,74,74	0
60	MG	BA	3007	1/1	0.29	-	93,93,93,93	0
60	MG	DA	2959	1/1	0.36	-	61,61,61,61	0
60	MG	BA	3607	1/1	0.77	-	95,95,95,95	0
60	MG	DA	2939	1/1	0.82	-	1,1,1,1	1
60	MG	DA	2995	1/1	0.13	-	44,44,44,44	0
60	MG	DA	3496	1/1	0.27	-	83,83,83,83	0
60	MG	CA	1755	1/1	0.32	-	100,100,100,100	0
60	MG	AA	1827	1/1	0.21	-	85,85,85,85	0
60	MG	AA	1833	1/1	0.30	-	87,87,87,87	0
60	MG	BA	3024	1/1	0.32	-	79,79,79,79	0
60	MG	DU	204	1/1	0.27	-	19,19,19,19	0
60	MG	DA	3377	1/1	0.24	-	16,16,16,16	0
60	MG	DA	3430	1/1	0.25	-	25,25,25,25	0
60	MG	AA	1856	1/1	0.47	-	80,80,80,80	0
60	MG	DA	2951	1/1	0.45	-	102,102,102,102	0
60	MG	BA	3391	1/1	1.31	-	91,91,91,91	1
60	MG	DA	3256	1/1	0.55	-	42,42,42,42	0
60	MG	DA	3081	1/1	0.26	-	75,75,75,75	0
60	MG	BA	3561	1/1	1.12	-	122,122,122,122	0
60	MG	DA	3639	1/1	0.33	-	37,37,37,37	0
60	MG	AA	1971	1/1	0.67	-	125,125,125,125	0
60	MG	CA	1644	1/1	0.33	-	92,92,92,92	0
60	MG	BA	3539	1/1	0.28	-	97,97,97,97	1
60	MG	BA	3252	1/1	0.14	-	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3539	1/1	0.58	-	70,70,70,70	0
60	MG	DO	201	1/1	0.17	-	117,117,117,117	0
60	MG	DA	3720	1/1	0.10	-	66,66,66,66	0
60	MG	BA	3063	1/1	0.31	-	59,59,59,59	0
60	MG	BA	3389	1/1	0.42	-	56,56,56,56	0
60	MG	BH	203	1/1	0.47	-	75,75,75,75	0
60	MG	BA	3174	1/1	0.25	-	83,83,83,83	0
60	MG	DA	3044	1/1	0.20	-	78,78,78,78	0
60	MG	DA	3267	1/1	0.34	-	62,62,62,62	0
60	MG	CC	302	1/1	0.59	-	114,114,114,114	0
60	MG	AA	1941	1/1	0.56	-	63,63,63,63	0
60	MG	DA	3549	1/1	0.55	-	97,97,97,97	0
60	MG	AA	1649	1/1	0.15	-	63,63,63,63	0
60	MG	CA	1780	1/1	0.68	-	47,47,47,47	1
60	MG	DA	3646	1/1	0.77	-	57,57,57,57	0
60	MG	BA	3078	1/1	0.20	-	18,18,18,18	0
60	MG	BA	3327	1/1	0.56	-	59,59,59,59	0
60	MG	AA	1712	1/1	0.81	-	188,188,188,188	0
60	MG	DA	3105	1/1	0.86	-	92,92,92,92	0
60	MG	AA	1926	1/1	0.16	-	59,59,59,59	0
60	MG	AA	1961	1/1	0.25	-	87,87,87,87	0
60	MG	DA	3513	1/1	0.13	-	95,95,95,95	0
60	MG	BA	2997	1/1	0.40	-	82,82,82,82	0
60	MG	DA	3126	1/1	0.26	-	60,60,60,60	0
60	MG	CA	1699	1/1	0.21	-	64,64,64,64	0
60	MG	DA	3764	1/1	0.27	-	75,75,75,75	0
60	MG	DA	3527	1/1	0.07	-	46,46,46,46	0
60	MG	CA	1707	1/1	0.10	-	79,79,79,79	0
60	MG	DA	3036	1/1	0.45	-	76,76,76,76	0
60	MG	DA	2913	1/1	0.35	-	15,15,15,15	1
60	MG	BA	3308	1/1	0.29	-	53,53,53,53	1
60	MG	DA	3023	1/1	0.39	-	41,41,41,41	0
60	MG	BA	2931	1/1	0.18	-	44,44,44,44	0
60	MG	CA	1701	1/1	0.21	-	83,83,83,83	0
60	MG	BA	3294	1/1	0.33	-	73,73,73,73	0
60	MG	BA	3059	1/1	0.24	-	98,98,98,98	0
60	MG	BA	3284	1/1	0.57	-	97,97,97,97	0
60	MG	DA	3285	1/1	0.33	-	37,37,37,37	0
60	MG	BA	3600	1/1	0.54	-	63,63,63,63	0
60	MG	DA	3455	1/1	0.42	-	71,71,71,71	0
60	MG	AA	1889	1/1	0.40	-	115,115,115,115	0
60	MG	CA	1716	1/1	0.52	-	110,110,110,110	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3160	1/1	0.31	-	68,68,68,68	0
60	MG	DA	3369	1/1	0.27	-	95,95,95,95	0
60	MG	DA	3661	1/1	0.33	-	100,100,100,100	0
60	MG	CA	1664	1/1	0.19	-	91,91,91,91	0
60	MG	DA	2961	1/1	0.43	-	126,126,126,126	0
60	MG	CA	1670	1/1	0.29	-	66,66,66,66	0
60	MG	D5	101	1/1	0.29	-	48,48,48,48	0
60	MG	DA	3130	1/1	1.31	-	108,108,108,108	0
60	MG	BA	3349	1/1	0.34	-	68,68,68,68	0
60	MG	BA	3062	1/1	0.21	-	61,61,61,61	0
60	MG	BD	305	1/1	0.13	-	168,168,168,168	0
60	MG	BA	3194	1/1	0.12	-	67,67,67,67	0
60	MG	DA	2910	1/1	0.68	-	68,68,68,68	0
60	MG	DA	3189	1/1	0.22	-	80,80,80,80	0
60	MG	BA	3359	1/1	0.83	-	101,101,101,101	0
60	MG	AA	1643	1/1	0.17	-	92,92,92,92	0
60	MG	AA	1790	1/1	0.43	-	96,96,96,96	0
60	MG	BA	2983	1/1	0.20	-	63,63,63,63	0
60	MG	CA	1657	1/1	0.50	-	85,85,85,85	0
60	MG	DA	3748	1/1	0.61	-	125,125,125,125	0
60	MG	BA	3226	1/1	0.51	-	78,78,78,78	0
60	MG	DA	3216	1/1	0.36	-	36,36,36,36	0
60	MG	DA	3434	1/1	0.51	-	44,44,44,44	0
60	MG	DA	3168	1/1	1.12	-	100,100,100,100	0
60	MG	AA	1670	1/1	0.20	-	28,28,28,28	1
60	MG	DA	3260	1/1	0.68	-	33,33,33,33	0
60	MG	DA	3784	1/1	0.39	-	123,123,123,123	0
60	MG	BA	3486	1/1	0.28	-	54,54,54,54	0
60	MG	BR	203	1/1	0.39	-	83,83,83,83	0
60	MG	DA	3147	1/1	0.17	-	90,90,90,90	0
60	MG	DA	3593	1/1	0.29	-	61,61,61,61	0
60	MG	DB	210	1/1	0.39	-	56,56,56,56	0
60	MG	BA	3368	1/1	0.38	-	62,62,62,62	0
60	MG	AA	1959	1/1	0.74	-	146,146,146,146	0
60	MG	DA	3421	1/1	0.19	-	71,71,71,71	0
60	MG	DA	3148	1/1	1.07	-	120,120,120,120	0
60	MG	DA	3735	1/1	0.13	-	90,90,90,90	0
60	MG	DA	3501	1/1	0.53	-	59,59,59,59	0
60	MG	DA	2912	1/1	0.31	-	68,68,68,68	0
60	MG	AA	1780	1/1	0.46	-	154,154,154,154	0
60	MG	DA	3378	1/1	0.38	-	96,96,96,96	0
60	MG	BA	3434	1/1	0.42	-	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3165	1/1	0.28	-	121,121,121,121	0
60	MG	BA	3538	1/1	0.09	-	37,37,37,37	0
60	MG	AA	1668	1/1	0.61	-	78,78,78,78	0
60	MG	DA	3291	1/1	0.36	-	88,88,88,88	0
60	MG	BA	3436	1/1	0.13	-	62,62,62,62	0
60	MG	CA	1634	1/1	0.15	-	97,97,97,97	0
60	MG	CA	1629	1/1	0.28	-	98,98,98,98	0
60	MG	BA	2939	1/1	0.32	-	80,80,80,80	0
60	MG	BA	3030	1/1	0.54	-	79,79,79,79	0
60	MG	DA	2940	1/1	0.42	-	106,106,106,106	0
60	MG	BA	2926	1/1	0.21	-	20,20,20,20	0
60	MG	CA	1742	1/1	0.11	-	81,81,81,81	0
60	MG	DA	3725	1/1	0.36	-	71,71,71,71	0
60	MG	BA	2950	1/1	0.33	-	55,55,55,55	1
60	MG	BA	2920	1/1	0.28	-	42,42,42,42	0
60	MG	BB	202	1/1	0.49	-	62,62,62,62	0
60	MG	DA	3250	1/1	0.27	-	69,69,69,69	0
60	MG	DA	3281	1/1	0.44	-	31,31,31,31	0
60	MG	DA	3218	1/1	0.42	-	130,130,130,130	0
60	MG	BA	3207	1/1	0.43	-	43,43,43,43	0
60	MG	BR	205	1/1	0.17	-	76,76,76,76	0
60	MG	BA	3065	1/1	0.40	-	50,50,50,50	0
60	MG	AA	1749	1/1	0.22	-	74,74,74,74	1
60	MG	DA	2962	1/1	0.62	-	84,84,84,84	0
60	MG	DA	3201	1/1	0.34	-	62,62,62,62	0
60	MG	DA	3176	1/1	0.44	-	37,37,37,37	0
60	MG	BA	3025	1/1	0.22	-	83,83,83,83	0
60	MG	DA	3203	1/1	0.71	-	112,112,112,112	0
60	MG	BA	2937	1/1	0.33	-	40,40,40,40	0
60	MG	DA	3053	1/1	0.35	-	33,33,33,33	0
60	MG	DA	3242	1/1	0.35	-	31,31,31,31	0
60	MG	DA	3550	1/1	0.48	-	86,86,86,86	0
60	MG	CA	1623	1/1	0.07	-	81,81,81,81	0
60	MG	DA	3616	1/1	0.35	-	51,51,51,51	0
60	MG	DA	3671	1/1	0.88	-	103,103,103,103	0
60	MG	BA	3320	1/1	0.31	-	92,92,92,92	0
60	MG	DA	3557	1/1	0.14	-	64,64,64,64	0
60	MG	DA	3510	1/1	0.10	-	59,59,59,59	0
60	MG	BA	3086	1/1	0.15	-	123,123,123,123	0
60	MG	DA	3494	1/1	0.37	-	41,41,41,41	0
60	MG	DA	3491	1/1	1.03	-	107,107,107,107	0
60	MG	BA	2988	1/1	0.14	-	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1724	1/1	0.47	-	102,102,102,102	0
60	MG	AA	1680	1/1	0.27	-	75,75,75,75	0
60	MG	DA	3057	1/1	0.22	-	32,32,32,32	0
60	MG	BA	3088	1/1	0.79	-	62,62,62,62	0
60	MG	DA	3383	1/1	0.57	-	135,135,135,135	0
60	MG	BA	3067	1/1	0.19	-	34,34,34,34	0
60	MG	BA	3189	1/1	0.33	-	62,62,62,62	0
60	MG	DA	3192	1/1	0.99	-	70,70,70,70	0
60	MG	BA	3182	1/1	0.25	-	60,60,60,60	0
60	MG	AA	1616	1/1	0.53	-	61,61,61,61	0
60	MG	AA	1776	1/1	0.77	-	119,119,119,119	0
60	MG	BA	3355	1/1	0.25	-	26,26,26,26	0
60	MG	DA	3104	1/1	0.10	-	63,63,63,63	0
60	MG	DA	3210	1/1	0.28	-	71,71,71,71	0
60	MG	BA	2934	1/1	0.34	-	57,57,57,57	0
60	MG	BE	302	1/1	0.12	-	30,30,30,30	0
60	MG	AA	1906	1/1	0.28	-	65,65,65,65	1
60	MG	BA	3003	1/1	0.35	-	75,75,75,75	0
60	MG	BA	3499	1/1	0.32	-	43,43,43,43	0
60	MG	DA	3379	1/1	0.39	-	72,72,72,72	0
60	MG	BA	3090	1/1	0.14	-	27,27,27,27	0
60	MG	BA	3097	1/1	0.40	-	89,89,89,89	0
60	MG	AA	1879	1/1	0.48	-	74,74,74,74	0
60	MG	BA	3405	1/1	0.46	-	44,44,44,44	0
60	MG	DA	3679	1/1	0.28	-	51,51,51,51	0
60	MG	AA	1795	1/1	0.14	-	96,96,96,96	0
60	MG	AA	1626	1/1	0.64	-	89,89,89,89	0
60	MG	DA	3334	1/1	0.17	-	56,56,56,56	0
60	MG	BA	3334	1/1	0.17	-	60,60,60,60	0
60	MG	BA	3302	1/1	1.19	-	69,69,69,69	0
60	MG	CP	101	1/1	0.06	-	81,81,81,81	0
60	MG	DA	2950	1/1	0.17	-	80,80,80,80	1
60	MG	DA	3302	1/1	0.60	-	57,57,57,57	0
60	MG	DA	3235	1/1	0.38	-	110,110,110,110	0
60	MG	DA	3135	1/1	0.30	-	51,51,51,51	0
60	MG	AA	1964	1/1	1.12	-	106,106,106,106	0
60	MG	DA	3576	1/1	0.34	-	87,87,87,87	0
60	MG	CV	109	1/1	0.11	-	95,95,95,95	0
60	MG	BA	3588	1/1	1.35	-	90,90,90,90	0
60	MG	DA	3767	1/1	0.61	-	67,67,67,67	0
60	MG	DA	3169	1/1	1.32	-	67,67,67,67	0
60	MG	AL	205	1/1	0.29	-	47,47,47,47	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3206	1/1	0.51	-	59,59,59,59	0
60	MG	DD	301	1/1	0.35	-	57,57,57,57	0
60	MG	CA	1749	1/1	0.58	-	16,16,16,16	1
60	MG	AA	1816	1/1	0.31	-	64,64,64,64	0
60	MG	AA	1742	1/1	0.24	-	63,63,63,63	1
60	MG	DA	3591	1/1	0.62	-	19,19,19,19	1
60	MG	BT	201	1/1	0.37	-	117,117,117,117	0
60	MG	CA	1728	1/1	0.19	-	88,88,88,88	0
60	MG	BA	3070	1/1	0.46	-	108,108,108,108	0
60	MG	BA	3413	1/1	0.66	-	73,73,73,73	0
60	MG	BA	3602	1/1	1.42	-	122,122,122,122	1
60	MG	CA	1652	1/1	0.51	-	78,78,78,78	0
60	MG	DA	3436	1/1	0.29	-	104,104,104,104	0
60	MG	DA	3099	1/1	0.37	-	67,67,67,67	0
60	MG	BA	3205	1/1	0.56	-	78,78,78,78	0
60	MG	DA	3462	1/1	0.87	-	78,78,78,78	0
60	MG	AA	1730	1/1	0.26	-	77,77,77,77	1
60	MG	CA	1636	1/1	0.54	-	77,77,77,77	0
60	MG	DA	3294	1/1	0.10	-	80,80,80,80	1
60	MG	BA	3229	1/1	1.07	-	88,88,88,88	0
60	MG	DA	3428	1/1	0.30	-	65,65,65,65	0
60	MG	BA	3500	1/1	0.37	-	79,79,79,79	0
60	MG	CA	1700	1/1	0.38	-	104,104,104,104	0
60	MG	BA	3126	1/1	0.13	-	36,36,36,36	0
60	MG	BB	205	1/1	0.12	-	69,69,69,69	1
60	MG	DA	3524	1/1	0.55	-	61,61,61,61	0
60	MG	D0	104	1/1	0.66	-	98,98,98,98	0
60	MG	BA	3559	1/1	0.20	-	45,45,45,45	0
60	MG	DA	3599	1/1	0.21	-	39,39,39,39	0
60	MG	AA	1721	1/1	0.14	-	111,111,111,111	0
60	MG	BA	3512	1/1	0.28	-	51,51,51,51	0
60	MG	BA	3335	1/1	1.60	-	113,113,113,113	0
60	MG	BA	3231	1/1	0.38	-	28,28,28,28	0
60	MG	BA	3549	1/1	0.62	-	84,84,84,84	0
60	MG	BA	3199	1/1	1.82	-	110,110,110,110	0
60	MG	BA	2908	1/1	0.18	-	84,84,84,84	0
60	MG	DA	3751	1/1	0.53	-	82,82,82,82	0
60	MG	DA	3237	1/1	0.35	-	37,37,37,37	0
60	MG	BA	3144	1/1	0.34	-	73,73,73,73	0
60	MG	CA	1650	1/1	0.75	-	79,79,79,79	0
60	MG	BA	3241	1/1	0.25	-	44,44,44,44	0
60	MG	AA	1629	1/1	0.33	-	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3390	1/1	0.17	-	65,65,65,65	0
60	MG	AA	1769	1/1	0.44	-	101,101,101,101	0
60	MG	BA	2906	1/1	0.34	-	92,92,92,92	0
60	MG	DA	3269	1/1	0.44	-	44,44,44,44	0
60	MG	AA	1948	1/1	0.56	-	114,114,114,114	0
60	MG	DA	3349	1/1	1.10	-	141,141,141,141	0
60	MG	DA	3676	1/1	0.65	-	96,96,96,96	0
60	MG	DA	2901	1/1	0.33	-	51,51,51,51	0
60	MG	CA	1630	1/1	0.17	-	68,68,68,68	0
60	MG	BA	3139	1/1	0.32	-	27,27,27,27	0
60	MG	DA	2974	1/1	0.61	-	47,47,47,47	1
60	MG	DA	3007	1/1	0.33	-	57,57,57,57	0
60	MG	DA	3782	1/1	0.27	-	51,51,51,51	0
60	MG	AA	1945	1/1	1.08	-	94,94,94,94	1
60	MG	CM	203	1/1	0.13	-	123,123,123,123	0
60	MG	DA	3695	1/1	0.43	-	81,81,81,81	0
60	MG	DA	3119	1/1	0.17	-	66,66,66,66	0
60	MG	AA	1759	1/1	0.37	-	51,51,51,51	0
60	MG	DA	3588	1/1	0.36	-	83,83,83,83	0
60	MG	DA	2946	1/1	0.31	-	96,96,96,96	0
60	MG	DA	3288	1/1	0.13	-	60,60,60,60	0
60	MG	BA	3366	1/1	0.59	-	71,71,71,71	0
60	MG	BA	3077	1/1	0.39	-	71,71,71,71	0
60	MG	DA	3229	1/1	0.07	-	51,51,51,51	0
60	MG	AA	1773	1/1	0.14	-	50,50,50,50	0
60	MG	AA	1652	1/1	0.18	-	95,95,95,95	0
60	MG	AN	102	1/1	0.11	-	141,141,141,141	0
60	MG	AA	1895	1/1	0.24	-	72,72,72,72	0
60	MG	DA	3303	1/1	0.31	-	54,54,54,54	0
60	MG	BA	3583	1/1	0.58	-	81,81,81,81	1
60	MG	CA	1741	1/1	1.79	-	106,106,106,106	0
60	MG	BA	3300	1/1	0.42	-	71,71,71,71	0
60	MG	BA	3576	1/1	0.18	-	97,97,97,97	0
60	MG	AA	1850	1/1	0.83	-	89,89,89,89	0
60	MG	DA	3445	1/1	0.25	-	55,55,55,55	0
60	MG	DA	3674	1/1	0.67	-	55,55,55,55	0
60	MG	CS	102	1/1	0.10	-	102,102,102,102	0
60	MG	DA	3386	1/1	0.37	-	99,99,99,99	0
60	MG	DA	3353	1/1	0.15	-	84,84,84,84	0
60	MG	DA	3062	1/1	0.32	-	88,88,88,88	0
60	MG	BA	3471	1/1	0.53	-	96,96,96,96	0
60	MG	AA	1881	1/1	0.51	-	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1973	1/1	0.25	-	69,69,69,69	0
60	MG	BA	3093	1/1	0.21	-	52,52,52,52	0
60	MG	AA	1842	1/1	0.14	-	58,58,58,58	0
60	MG	D6	102	1/1	0.92	-	97,97,97,97	0
60	MG	CA	1604	1/1	0.17	-	63,63,63,63	0
60	MG	AA	1603	1/1	0.20	-	74,74,74,74	0
60	MG	BA	3456	1/1	0.57	-	33,33,33,33	0
60	MG	DA	3518	1/1	0.38	-	62,62,62,62	1
60	MG	BA	3196	1/1	0.47	-	64,64,64,64	0
60	MG	BA	3177	1/1	0.38	-	45,45,45,45	0
60	MG	BA	3262	1/1	0.24	-	50,50,50,50	0
60	MG	BA	3137	1/1	0.23	-	43,43,43,43	0
60	MG	DA	2985	1/1	0.40	-	39,39,39,39	0
60	MG	DA	3230	1/1	0.38	-	94,94,94,94	0
60	MG	DA	3033	1/1	0.13	-	50,50,50,50	0
60	MG	BA	3354	1/1	0.58	-	76,76,76,76	0
60	MG	CA	1675	1/1	0.58	-	93,93,93,93	0
60	MG	DA	3228	1/1	0.27	-	79,79,79,79	0
60	MG	DA	3295	1/1	0.80	-	99,99,99,99	0
60	MG	CV	110	1/1	0.44	-	105,105,105,105	0
60	MG	DA	2903	1/1	0.46	-	43,43,43,43	0
60	MG	DA	3449	1/1	0.45	-	71,71,71,71	0
60	MG	BA	3338	1/1	0.41	-	97,97,97,97	0
60	MG	AA	1752	1/1	0.29	-	51,51,51,51	1
60	MG	DA	3464	1/1	0.62	-	62,62,62,62	1
60	MG	CM	202	1/1	0.15	-	151,151,151,151	0
60	MG	DA	3319	1/1	0.12	-	47,47,47,47	0
60	MG	BA	3218	1/1	0.30	-	111,111,111,111	0
60	MG	AA	1848	1/1	0.20	-	117,117,117,117	0
60	MG	DA	3500	1/1	0.40	-	84,84,84,84	0
60	MG	BA	3295	1/1	0.56	-	51,51,51,51	0
60	MG	BA	3586	1/1	0.81	-	86,86,86,86	0
60	MG	DA	3693	1/1	0.45	-	33,33,33,33	1
60	MG	DA	3443	1/1	0.41	-	133,133,133,133	0
60	MG	BB	203	1/1	0.35	-	59,59,59,59	0
60	MG	BA	3289	1/1	0.34	-	39,39,39,39	0
60	MG	AA	1960	1/1	0.20	-	72,72,72,72	0
60	MG	BA	3091	1/1	0.28	-	62,62,62,62	0
60	MG	BA	3555	1/1	0.67	-	60,60,60,60	0
60	MG	AQ	203	1/1	1.06	-	130,130,130,130	0
60	MG	DA	3145	1/1	1.05	-	120,120,120,120	0
60	MG	BA	3545	1/1	0.42	-	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3144	1/1	0.38	-	131,131,131,131	0
60	MG	BA	2965	1/1	0.93	-	84,84,84,84	0
60	MG	DA	3702	1/1	0.48	-	80,80,80,80	0
60	MG	DA	3385	1/1	0.22	-	43,43,43,43	0
60	MG	BA	3430	1/1	0.35	-	68,68,68,68	0
60	MG	DA	3460	1/1	0.15	-	73,73,73,73	0
60	MG	CA	1775	1/1	0.12	-	70,70,70,70	1
60	MG	AA	1743	1/1	0.22	-	87,87,87,87	0
60	MG	BE	303	1/1	0.32	-	22,22,22,22	0
60	MG	DA	3467	1/1	0.30	-	109,109,109,109	0
60	MG	DA	3300	1/1	0.25	-	67,67,67,67	0
60	MG	DA	3354	1/1	0.23	-	52,52,52,52	0
60	MG	DA	3450	1/1	0.19	-	100,100,100,100	0
60	MG	BA	3435	1/1	0.64	-	70,70,70,70	0
60	MG	BA	3527	1/1	0.60	-	86,86,86,86	0
60	MG	DF	303	1/1	0.20	-	22,22,22,22	1
60	MG	BA	3131	1/1	0.35	-	43,43,43,43	0
60	MG	BA	3397	1/1	0.34	-	75,75,75,75	0
60	MG	AL	204	1/1	0.05	-	90,90,90,90	0
60	MG	AA	1915	1/1	0.45	-	75,75,75,75	0
60	MG	AA	1671	1/1	1.38	-	107,107,107,107	0
60	MG	AA	1757	1/1	1.82	-	111,111,111,111	0
60	MG	DA	3248	1/1	0.28	-	62,62,62,62	0
60	MG	DA	2933	1/1	0.28	-	51,51,51,51	0
60	MG	DA	3140	1/1	0.60	-	77,77,77,77	0
60	MG	DA	3243	1/1	0.78	-	64,64,64,64	0
60	MG	CA	1611	1/1	0.34	-	86,86,86,86	0
60	MG	AA	1814	1/1	1.06	-	77,77,77,77	0
60	MG	DA	3232	1/1	0.34	-	59,59,59,59	0
60	MG	DA	3155	1/1	0.87	-	78,78,78,78	0
60	MG	AO	102	1/1	1.06	-	77,77,77,77	0
60	MG	AA	1822	1/1	0.34	-	60,60,60,60	0
60	MG	BA	3584	1/1	0.23	-	65,65,65,65	0
60	MG	DA	3112	1/1	0.09	-	87,87,87,87	0
60	MG	AA	1847	1/1	0.47	-	76,76,76,76	0
60	MG	BA	3472	1/1	0.94	-	100,100,100,100	0
60	MG	AA	1811	1/1	0.23	-	49,49,49,49	0
60	MG	DA	3665	1/1	0.58	-	96,96,96,96	0
60	MG	AA	1724	1/1	0.17	-	86,86,86,86	1
60	MG	AA	1859	1/1	0.17	-	44,44,44,44	0
60	MG	BA	3503	1/1	0.32	-	65,65,65,65	1
60	MG	DA	3697	1/1	0.28	-	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	2982	1/1	0.11	-	58,58,58,58	1
60	MG	DN	203	1/1	0.85	-	64,64,64,64	1
60	MG	DA	3158	1/1	0.47	-	130,130,130,130	0
60	MG	DA	3761	1/1	0.58	-	96,96,96,96	0
60	MG	DA	3364	1/1	0.34	-	59,59,59,59	0
60	MG	CA	1726	1/1	1.04	-	107,107,107,107	0
60	MG	BA	3245	1/1	0.20	-	116,116,116,116	0
60	MG	DA	3178	1/1	0.34	-	29,29,29,29	0
60	MG	AA	1611	1/1	0.36	-	66,66,66,66	0
60	MG	BA	3166	1/1	0.45	-	89,89,89,89	0
60	MG	DA	3059	1/1	0.58	-	77,77,77,77	0
60	MG	BA	3340	1/1	0.94	-	99,99,99,99	0
60	MG	BA	2957	1/1	0.44	-	81,81,81,81	0
60	MG	DA	3507	1/1	0.27	-	5,5,5,5	1
60	MG	DA	3444	1/1	0.40	-	31,31,31,31	0
60	MG	AA	1681	1/1	0.20	-	106,106,106,106	0
60	MG	DA	3592	1/1	0.47	-	58,58,58,58	0
60	MG	AA	1604	1/1	0.34	-	118,118,118,118	0
60	MG	DA	2960	1/1	0.63	-	57,57,57,57	1
60	MG	DA	3753	1/1	0.77	-	83,83,83,83	0
60	MG	DA	3245	1/1	0.34	-	78,78,78,78	0
60	MG	DA	3590	1/1	0.41	-	67,67,67,67	0
60	MG	AA	1917	1/1	0.34	-	78,78,78,78	0
60	MG	CA	1603	1/1	0.31	-	112,112,112,112	0
60	MG	CA	1763	1/1	0.59	-	105,105,105,105	0
60	MG	DA	3475	1/1	0.47	-	115,115,115,115	0
60	MG	DA	3653	1/1	0.55	-	82,82,82,82	0
60	MG	AA	1824	1/1	0.14	-	83,83,83,83	0
60	MG	DA	3191	1/1	0.20	-	83,83,83,83	0
60	MG	DA	3511	1/1	1.27	-	83,83,83,83	0
60	MG	DA	3630	1/1	0.29	-	99,99,99,99	0
60	MG	AA	1950	1/1	0.38	-	81,81,81,81	0
60	MG	BA	3504	1/1	0.22	-	59,59,59,59	0
60	MG	AY	101	1/1	1.16	-	6,6,6,6	1
60	MG	BA	3114	1/1	0.10	-	80,80,80,80	0
60	MG	AA	1747	1/1	0.63	-	119,119,119,119	0
60	MG	BA	3303	1/1	0.15	-	88,88,88,88	0
60	MG	BA	3347	1/1	0.50	-	30,30,30,30	0
60	MG	DA	3152	1/1	0.42	-	108,108,108,108	0
60	MG	BA	3422	1/1	0.15	-	68,68,68,68	0
60	MG	AA	1955	1/1	0.22	-	64,64,64,64	1
60	MG	DA	3361	1/1	0.35	-	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	B0	102	1/1	0.28	-	91,91,91,91	0
60	MG	CA	1683	1/1	0.37	-	60,60,60,60	0
60	MG	DA	3746	1/1	0.68	-	71,71,71,71	0
60	MG	DA	3567	1/1	1.06	-	98,98,98,98	0
60	MG	BA	3542	1/1	0.37	-	102,102,102,102	0
60	MG	CA	1746	1/1	0.63	-	85,85,85,85	0
60	MG	DA	3778	1/1	0.24	-	115,115,115,115	0
60	MG	BA	3158	1/1	0.21	-	33,33,33,33	0
60	MG	DA	3214	1/1	0.49	-	102,102,102,102	0
60	MG	BA	2940	1/1	0.43	-	63,63,63,63	0
60	MG	DA	3013	1/1	0.45	-	68,68,68,68	0
60	MG	DA	3028	1/1	0.40	-	79,79,79,79	0
60	MG	DA	3070	1/1	0.12	-	59,59,59,59	0
60	MG	DA	3660	1/1	0.71	-	78,78,78,78	0
60	MG	BA	3346	1/1	0.58	-	71,71,71,71	0
60	MG	DA	3683	1/1	0.66	-	46,46,46,46	0
60	MG	AA	1863	1/1	0.32	-	80,80,80,80	0
60	MG	BA	2946	1/1	0.38	-	49,49,49,49	0
60	MG	AA	1754	1/1	0.15	-	124,124,124,124	0
60	MG	DA	3263	1/1	0.30	-	125,125,125,125	0
60	MG	DA	3008	1/1	0.31	-	70,70,70,70	0
60	MG	BA	3386	1/1	0.34	-	72,72,72,72	0
60	MG	CA	1762	1/1	0.22	-	95,95,95,95	0
60	MG	DA	3770	1/1	0.27	-	85,85,85,85	1
60	MG	DA	3546	1/1	0.88	-	11,11,11,11	1
60	MG	DD	303	1/1	0.38	-	64,64,64,64	0
60	MG	BA	3495	1/1	0.23	-	69,69,69,69	0
60	MG	AA	1625	1/1	0.56	-	73,73,73,73	1
60	MG	DA	3577	1/1	0.16	-	92,92,92,92	0
60	MG	BA	2960	1/1	0.57	-	84,84,84,84	0
60	MG	DA	3650	1/1	0.34	-	106,106,106,106	0
60	MG	DA	3122	1/1	0.68	-	38,38,38,38	0
60	MG	BU	201	1/1	0.48	-	46,46,46,46	0
60	MG	DA	3707	1/1	0.41	-	55,55,55,55	1
60	MG	BA	2907	1/1	0.34	-	108,108,108,108	0
60	MG	DA	3188	1/1	0.29	-	31,31,31,31	0
60	MG	DA	3747	1/1	0.58	-	38,38,38,38	1
60	MG	DA	3694	1/1	0.25	-	107,107,107,107	0
60	MG	DA	3479	1/1	0.55	-	127,127,127,127	0
60	MG	BA	3157	1/1	0.54	-	60,60,60,60	0
60	MG	BA	3201	1/1	0.21	-	50,50,50,50	0
60	MG	AA	1952	1/1	0.90	-	97,97,97,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3710	1/1	0.58	-	92,92,92,92	0
60	MG	DA	3328	1/1	0.26	-	34,34,34,34	0
60	MG	AA	1678	1/1	0.32	-	76,76,76,76	0
60	MG	CA	1680	1/1	0.89	-	102,102,102,102	0
60	MG	CA	1606	1/1	0.10	-	60,60,60,60	0
60	MG	CA	1782	1/1	0.21	-	52,52,52,52	0
60	MG	BA	3378	1/1	0.42	-	79,79,79,79	0
60	MG	AA	1723	1/1	0.14	-	91,91,91,91	0
60	MG	BA	3514	1/1	0.40	-	76,76,76,76	0
60	MG	DA	3016	1/1	0.29	-	51,51,51,51	0
60	MG	AA	1766	1/1	0.68	-	74,74,74,74	0
60	MG	CA	1730	1/1	0.16	-	106,106,106,106	0
60	MG	BA	3258	1/1	0.49	-	69,69,69,69	0
60	MG	AA	1606	1/1	0.25	-	77,77,77,77	0
60	MG	D7	103	1/1	1.91	-	69,69,69,69	0
60	MG	CA	1738	1/1	0.17	-	80,80,80,80	0
60	MG	DA	3268	1/1	0.29	-	35,35,35,35	0
60	MG	BA	3375	1/1	1.10	-	74,74,74,74	0
60	MG	BP	203	1/1	0.21	-	88,88,88,88	0
60	MG	DA	2972	1/1	0.92	-	97,97,97,97	0
60	MG	DA	3794	1/1	0.18	-	79,79,79,79	0
60	MG	BA	3104	1/1	0.44	-	78,78,78,78	0
60	MG	BA	3548	1/1	0.38	-	92,92,92,92	0
60	MG	AA	1831	1/1	0.82	-	89,89,89,89	0
60	MG	DA	3034	1/1	0.34	-	98,98,98,98	0
60	MG	DA	3368	1/1	0.54	-	104,104,104,104	0
60	MG	DA	3721	1/1	0.18	-	171,171,171,171	0
60	MG	CA	1677	1/1	0.99	-	88,88,88,88	1
60	MG	BA	3469	1/1	0.20	-	102,102,102,102	0
60	MG	BA	3357	1/1	0.35	-	78,78,78,78	1
60	MG	BA	3501	1/1	0.28	-	112,112,112,112	0
60	MG	DA	2919	1/1	0.22	-	57,57,57,57	0
60	MG	AA	1642	1/1	0.17	-	108,108,108,108	0
60	MG	DA	3255	1/1	0.42	-	51,51,51,51	0
60	MG	CA	1691	1/1	0.08	-	103,103,103,103	0
60	MG	DA	3202	1/1	0.17	-	70,70,70,70	0
60	MG	DA	3357	1/1	0.32	-	64,64,64,64	0
60	MG	DA	2965	1/1	0.61	-	52,52,52,52	0
60	MG	BA	3279	1/1	0.38	-	59,59,59,59	0
60	MG	BA	3445	1/1	0.59	-	111,111,111,111	0
60	MG	BA	3571	1/1	0.42	-	77,77,77,77	0
60	MG	BA	3341	1/1	0.40	-	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1705	1/1	0.44	-	62,62,62,62	0
60	MG	BA	3149	1/1	0.29	-	86,86,86,86	0
60	MG	DA	2980	1/1	0.21	-	69,69,69,69	0
60	MG	BA	2985	1/1	0.67	-	84,84,84,84	0
60	MG	AA	1865	1/1	0.39	-	96,96,96,96	0
60	MG	AA	1839	1/1	0.36	-	74,74,74,74	0
60	MG	BA	2936	1/1	0.29	-	43,43,43,43	0
60	MG	AD	303	1/1	0.34	-	134,134,134,134	0
60	MG	DA	3675	1/1	0.39	-	39,39,39,39	0
60	MG	BA	3348	1/1	0.26	-	61,61,61,61	0
60	MG	DA	3330	1/1	0.35	-	1,1,1,1	1
60	MG	DA	3238	1/1	0.33	-	134,134,134,134	0
60	MG	AA	1819	1/1	0.08	-	75,75,75,75	0
60	MG	BA	2979	1/1	0.41	-	66,66,66,66	0
60	MG	BA	3291	1/1	0.54	-	41,41,41,41	0
60	MG	BA	3483	1/1	0.51	-	60,60,60,60	0
60	MG	DA	3314	1/1	0.15	-	71,71,71,71	0
60	MG	DA	3050	1/1	0.53	-	40,40,40,40	0
60	MG	DA	3344	1/1	0.28	-	75,75,75,75	0
60	MG	DA	3763	1/1	0.36	-	62,62,62,62	1
60	MG	DA	2989	1/1	0.26	-	83,83,83,83	0
60	MG	BA	3361	1/1	1.63	-	105,105,105,105	0
60	MG	DA	3298	1/1	0.34	-	65,65,65,65	0
60	MG	DA	3040	1/1	0.55	-	81,81,81,81	0
60	MG	AA	1866	1/1	0.33	-	74,74,74,74	0
60	MG	AA	1733	1/1	0.15	-	71,71,71,71	0
60	MG	BA	3585	1/1	1.72	-	143,143,143,143	0
60	MG	BA	3046	1/1	0.10	-	90,90,90,90	0
60	MG	BA	3012	1/1	0.45	-	34,34,34,34	0
60	MG	BA	2924	1/1	0.42	-	73,73,73,73	0
60	MG	AA	1932	1/1	0.34	-	82,82,82,82	0
60	MG	DA	3734	1/1	0.17	-	74,74,74,74	0
60	MG	DA	3758	1/1	0.81	-	95,95,95,95	0
60	MG	BA	3558	1/1	0.40	-	78,78,78,78	0
60	MG	BA	3089	1/1	0.32	-	33,33,33,33	0
60	MG	BA	3329	1/1	0.44	-	1,1,1,1	1
60	MG	DA	3221	1/1	0.70	-	77,77,77,77	0
60	MG	DA	3335	1/1	0.49	-	48,48,48,48	0
60	MG	BA	3124	1/1	0.42	-	62,62,62,62	0
60	MG	CA	1737	1/1	0.13	-	120,120,120,120	0
60	MG	BA	3029	1/1	0.28	-	92,92,92,92	0
60	MG	BA	3112	1/1	0.42	-	101,101,101,101	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3285	1/1	0.18	-	96,96,96,96	0
60	MG	BA	3519	1/1	0.83	-	88,88,88,88	0
60	MG	DA	3109	1/1	0.38	-	90,90,90,90	0
60	MG	AA	1938	1/1	1.21	-	124,124,124,124	0
60	MG	BA	3036	1/1	0.32	-	98,98,98,98	0
60	MG	AY	103	1/1	0.59	-	108,108,108,108	0
60	MG	BA	3593	1/1	0.09	-	41,41,41,41	0
60	MG	AA	1667	1/1	0.25	-	49,49,49,49	0
60	MG	DA	3628	1/1	1.20	-	93,93,93,93	0
60	MG	AA	1947	1/1	0.64	-	79,79,79,79	0
60	MG	BA	3534	1/1	0.58	-	56,56,56,56	0
60	MG	BA	3193	1/1	0.63	-	109,109,109,109	0
60	MG	DA	3503	1/1	0.26	-	59,59,59,59	0
60	MG	BA	3111	1/1	0.50	-	79,79,79,79	0
60	MG	BA	3296	1/1	0.54	-	27,27,27,27	0
60	MG	DA	3219	1/1	0.39	-	62,62,62,62	0
60	MG	AA	1796	1/1	0.12	-	61,61,61,61	0
60	MG	DA	2936	1/1	0.55	-	81,81,81,81	0
60	MG	BA	2958	1/1	0.27	-	46,46,46,46	0
60	MG	CA	1751	1/1	0.29	-	69,69,69,69	1
60	MG	AA	1905	1/1	0.68	-	71,71,71,71	1
60	MG	BA	3187	1/1	0.55	-	37,37,37,37	0
60	MG	AA	1828	1/1	0.26	-	86,86,86,86	0
60	MG	DA	3077	1/1	0.69	-	68,68,68,68	0
60	MG	BA	3053	1/1	0.89	-	62,62,62,62	0
60	MG	BA	2943	1/1	0.20	-	92,92,92,92	1
60	MG	AA	1834	1/1	0.34	-	94,94,94,94	0
60	MG	AA	1794	1/1	0.51	-	106,106,106,106	0
60	MG	DA	3304	1/1	0.49	-	84,84,84,84	0
60	MG	AA	1692	1/1	0.35	-	89,89,89,89	0
60	MG	BA	2990	1/1	0.23	-	77,77,77,77	0
60	MG	BA	2980	1/1	0.31	-	47,47,47,47	0
60	MG	AA	1820	1/1	0.30	-	97,97,97,97	0
60	MG	AA	1750	1/1	0.19	-	54,54,54,54	1
60	MG	BA	3437	1/1	0.30	-	60,60,60,60	0
60	MG	DA	3084	1/1	0.35	-	57,57,57,57	0
60	MG	DA	3239	1/1	0.15	-	96,96,96,96	0
60	MG	BR	201	1/1	0.43	-	47,47,47,47	1
60	MG	CA	1711	1/1	0.07	-	65,65,65,65	1
60	MG	DA	3350	1/1	0.46	-	34,34,34,34	0
60	MG	DA	3780	1/1	0.47	-	77,77,77,77	0
60	MG	D0	102	1/1	0.38	-	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	2989	1/1	0.27	-	82,82,82,82	0
60	MG	AA	1683	1/1	0.54	-	47,47,47,47	1
60	MG	BH	204	1/1	0.22	-	57,57,57,57	1
60	MG	DA	3525	1/1	0.96	-	63,63,63,63	0
60	MG	DA	3286	1/1	0.39	-	112,112,112,112	0
60	MG	AA	1716	1/1	0.28	-	82,82,82,82	0
60	MG	DA	3521	1/1	0.25	-	99,99,99,99	0
60	MG	DA	3558	1/1	0.45	-	88,88,88,88	0
60	MG	BA	3286	1/1	0.24	-	57,57,57,57	0
60	MG	DA	3662	1/1	0.26	-	59,59,59,59	0
60	MG	DA	2977	1/1	0.47	-	60,60,60,60	0
60	MG	BA	3488	1/1	0.62	-	66,66,66,66	1
60	MG	DA	3499	1/1	0.34	-	90,90,90,90	0
60	MG	AA	1697	1/1	0.83	-	76,76,76,76	0
60	MG	DA	3306	1/1	0.12	-	56,56,56,56	0
60	MG	AI	201	1/1	0.22	-	163,163,163,163	0
60	MG	AA	1695	1/1	0.19	-	65,65,65,65	0
60	MG	DA	3019	1/1	0.60	-	92,92,92,92	0
60	MG	BA	2968	1/1	0.54	-	72,72,72,72	0
60	MG	DF	301	1/1	0.32	-	17,17,17,17	1
60	MG	BA	3418	1/1	1.17	-	69,69,69,69	0
60	MG	BA	3121	1/1	1.09	-	125,125,125,125	0
60	MG	BA	3350	1/1	1.12	-	118,118,118,118	0
60	MG	DA	3399	1/1	0.23	-	62,62,62,62	0
60	MG	DA	3596	1/1	0.48	-	54,54,54,54	1
60	MG	BA	2996	1/1	0.26	-	68,68,68,68	0
60	MG	DA	3520	1/1	0.46	-	103,103,103,103	0
60	MG	BA	2928	1/1	0.75	-	116,116,116,116	0
60	MG	DA	3371	1/1	0.11	-	59,59,59,59	1
60	MG	BA	3076	1/1	0.19	-	30,30,30,30	0
60	MG	DA	3205	1/1	0.43	-	130,130,130,130	0
60	MG	AV	106	1/1	0.24	-	87,87,87,87	1
60	MG	DA	3439	1/1	0.25	-	54,54,54,54	1
60	MG	DA	3293	1/1	0.72	-	70,70,70,70	0
60	MG	BA	3128	1/1	0.51	-	92,92,92,92	0
60	MG	AA	1884	1/1	0.13	-	89,89,89,89	0
60	MG	DA	3064	1/1	0.21	-	51,51,51,51	0
60	MG	BA	3309	1/1	0.19	-	58,58,58,58	0
60	MG	BA	3315	1/1	0.65	-	74,74,74,74	0
60	MG	BA	3490	1/1	0.59	-	19,19,19,19	0
60	MG	DA	3345	1/1	1.34	-	25,25,25,25	1
60	MG	CA	1697	1/1	0.56	-	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1602	1/1	0.15	-	76,76,76,76	0
60	MG	CA	1722	1/1	0.34	-	73,73,73,73	0
60	MG	AA	1734	1/1	0.21	-	9,9,9,9	1
60	MG	BA	3273	1/1	0.56	-	31,31,31,31	0
60	MG	BA	3468	1/1	0.40	-	36,36,36,36	0
60	MG	BA	3330	1/1	0.38	-	88,88,88,88	0
60	MG	DA	3391	1/1	0.42	-	73,73,73,73	0
60	MG	DA	3744	1/1	0.27	-	93,93,93,93	1
60	MG	BA	3228	1/1	0.60	-	99,99,99,99	0
60	MG	DA	3052	1/1	0.28	-	68,68,68,68	0
60	MG	AA	1684	1/1	0.20	-	87,87,87,87	0
60	MG	CA	1614	1/1	0.39	-	72,72,72,72	0
60	MG	BA	3071	1/1	0.73	-	110,110,110,110	0
60	MG	DA	3535	1/1	0.53	-	52,52,52,52	0
60	MG	BA	3051	1/1	0.22	-	68,68,68,68	0
60	MG	DA	3648	1/1	0.52	-	100,100,100,100	0
60	MG	AA	1713	1/1	0.12	-	70,70,70,70	0
60	MG	DA	3635	1/1	0.43	-	31,31,31,31	0
60	MG	AA	1702	1/1	0.27	-	64,64,64,64	0
60	MG	AI	202	1/1	0.11	-	117,117,117,117	0
60	MG	DA	3058	1/1	0.28	-	32,32,32,32	0
60	MG	BA	3523	1/1	1.15	-	122,122,122,122	0
60	MG	DA	3776	1/1	0.41	-	58,58,58,58	0
60	MG	DA	3731	1/1	0.25	-	45,45,45,45	1
60	MG	DA	3054	1/1	0.07	-	69,69,69,69	0
60	MG	BA	2902	1/1	0.30	-	79,79,79,79	0
60	MG	BA	3109	1/1	0.30	-	35,35,35,35	0
60	MG	BA	3431	1/1	0.53	-	79,79,79,79	0
60	MG	BA	3267	1/1	1.04	-	94,94,94,94	0
60	MG	DA	3465	1/1	0.43	-	26,26,26,26	0
60	MG	BA	3417	1/1	0.45	-	68,68,68,68	0
60	MG	CA	1666	1/1	0.07	-	63,63,63,63	0
60	MG	AA	1687	1/1	0.10	-	101,101,101,101	0
60	MG	CA	1661	1/1	0.16	-	65,65,65,65	0
60	MG	CA	1712	1/1	0.52	-	88,88,88,88	1
60	MG	CA	1648	1/1	0.52	-	90,90,90,90	0
60	MG	DA	3290	1/1	0.36	-	32,32,32,32	0
60	MG	BA	3240	1/1	0.57	-	55,55,55,55	0
60	MG	BA	3032	1/1	0.33	-	88,88,88,88	0
60	MG	CA	1621	1/1	0.42	-	89,89,89,89	0
60	MG	BA	3083	1/1	0.27	-	80,80,80,80	0
60	MG	DA	3714	1/1	1.02	-	109,109,109,109	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
60	MG	AA	1605	1/1	0.35	-	152,152,152,152	0
60	MG	DA	3627	1/1	0.33	-	70,70,70,70	0
60	MG	DA	3568	1/1	0.66	-	73,73,73,73	0
60	MG	AA	1698	1/1	0.76	-	103,103,103,103	0
60	MG	BA	3160	1/1	0.34	-	49,49,49,49	0
60	MG	DA	2928	1/1	0.32	-	61,61,61,61	1
60	MG	AA	1775	1/1	0.27	-	92,92,92,92	0
60	MG	CA	1632	1/1	0.35	-	94,94,94,94	0
60	MG	DA	2970	1/1	0.36	-	41,41,41,41	1
60	MG	DA	3356	1/1	0.56	-	32,32,32,32	0
60	MG	AA	1770	1/1	0.34	-	76,76,76,76	0
60	MG	BA	3536	1/1	0.80	-	73,73,73,73	0
60	MG	AA	1767	1/1	0.36	-	77,77,77,77	0
60	MG	DA	3389	1/1	1.11	-	145,145,145,145	0
60	MG	DA	3311	1/1	0.88	-	96,96,96,96	0
60	MG	BA	3016	1/1	0.34	-	66,66,66,66	0
60	MG	CM	201	1/1	0.12	-	131,131,131,131	0
60	MG	DA	3098	1/1	0.81	-	86,86,86,86	0
60	MG	DA	3575	1/1	0.72	-	89,89,89,89	0
60	MG	CA	1769	1/1	0.23	-	68,68,68,68	0
60	MG	D9	101	1/1	0.30	-	92,92,92,92	1
60	MG	BA	3073	1/1	0.41	-	52,52,52,52	0
60	MG	AA	1700	1/1	0.63	-	90,90,90,90	0
60	MG	DA	3544	1/1	0.16	-	62,62,62,62	0
60	MG	DA	2931	1/1	0.74	-	151,151,151,151	1
60	MG	DA	3774	1/1	0.63	-	84,84,84,84	0
60	MG	CA	1640	1/1	0.32	-	76,76,76,76	0
60	MG	AA	1614	1/1	0.39	-	113,113,113,113	0
60	MG	BA	3475	1/1	0.17	-	59,59,59,59	0
60	MG	DA	3244	1/1	0.31	-	29,29,29,29	0
60	MG	DA	3181	1/1	0.37	-	49,49,49,49	0
60	MG	DA	3204	1/1	0.15	-	70,70,70,70	0
60	MG	AA	1904	1/1	0.49	-	81,81,81,81	0
60	MG	AA	1918	1/1	0.34	-	64,64,64,64	0
60	MG	DA	2902	1/1	0.41	-	42,42,42,42	0
60	MG	BA	3130	1/1	0.17	-	62,62,62,62	0
60	MG	BA	3006	1/1	0.92	-	68,68,68,68	0
60	MG	DA	3142	1/1	0.28	-	90,90,90,90	0
60	MG	AA	1958	1/1	0.14	-	106,106,106,106	0
60	MG	BA	3574	1/1	0.29	-	53,53,53,53	0
60	MG	DA	3750	1/1	0.70	-	84,84,84,84	0
60	MG	BA	3369	1/1	0.27	-	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CV	101	1/1	0.34	-	93,93,93,93	1
60	MG	DA	3556	1/1	0.53	-	97,97,97,97	0
60	MG	DA	3726	1/1	0.22	-	65,65,65,65	0
60	MG	CA	1748	1/1	0.11	-	102,102,102,102	0
60	MG	DA	3032	1/1	0.36	-	34,34,34,34	0
60	MG	BA	3563	1/1	0.41	-	80,80,80,80	0
60	MG	DA	3579	1/1	0.33	-	110,110,110,110	0
60	MG	DA	2981	1/1	0.35	-	127,127,127,127	0
60	MG	AA	1696	1/1	0.20	-	90,90,90,90	0
60	MG	DA	3049	1/1	1.41	-	96,96,96,96	0
60	MG	B1	101	1/1	0.18	-	50,50,50,50	1
60	MG	BA	3401	1/1	0.08	-	75,75,75,75	0
60	MG	AA	1601	1/1	0.13	-	74,74,74,74	0
60	MG	BA	3567	1/1	0.28	-	76,76,76,76	0
60	MG	DA	3362	1/1	0.41	-	39,39,39,39	0
60	MG	AA	1666	1/1	2.42	-	127,127,127,127	0
60	MG	DA	3600	1/1	0.31	-	30,30,30,30	0
60	MG	CA	1641	1/1	0.32	-	84,84,84,84	0
60	MG	BA	3304	1/1	1.06	-	90,90,90,90	0
60	MG	DA	3481	1/1	0.52	-	73,73,73,73	0
60	MG	AA	1943	1/1	0.83	-	60,60,60,60	1
60	MG	BA	3084	1/1	0.27	-	88,88,88,88	0
60	MG	AV	105	1/1	0.13	-	80,80,80,80	0
60	MG	DA	3681	1/1	0.10	-	28,28,28,28	0
60	MG	BA	3463	1/1	0.67	-	66,66,66,66	0
60	MG	BA	3360	1/1	0.35	-	80,80,80,80	0
60	MG	DA	2964	1/1	0.47	-	54,54,54,54	0
60	MG	DY	201	1/1	2.75	-	168,168,168,168	0
60	MG	CA	1731	1/1	0.19	-	76,76,76,76	0
60	MG	DA	3652	1/1	0.15	-	74,74,74,74	0
60	MG	DA	3403	1/1	0.24	-	109,109,109,109	0
60	MG	CA	1747	1/1	0.18	-	79,79,79,79	0
60	MG	DA	3209	1/1	0.45	-	50,50,50,50	0
60	MG	B0	101	1/1	0.85	-	73,73,73,73	0
60	MG	DA	3195	1/1	0.49	-	96,96,96,96	0
60	MG	DA	3536	1/1	0.19	-	37,37,37,37	1
60	MG	DA	3021	1/1	1.30	-	87,87,87,87	0
60	MG	DA	3622	1/1	0.06	-	58,58,58,58	0
60	MG	AA	1801	1/1	0.20	-	130,130,130,130	0
60	MG	BA	3195	1/1	0.39	-	85,85,85,85	0
60	MG	BA	3470	1/1	0.36	-	35,35,35,35	0
60	MG	BA	2966	1/1	0.53	-	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	2933	1/1	0.24	-	36,36,36,36	0
60	MG	BA	3113	1/1	0.12	-	95,95,95,95	0
60	MG	DA	3581	1/1	0.30	-	88,88,88,88	1
60	MG	DA	3585	1/1	0.27	-	78,78,78,78	0
60	MG	DA	3414	1/1	0.76	-	121,121,121,121	0
60	MG	DA	2934	1/1	0.18	-	48,48,48,48	1
60	MG	BA	3013	1/1	0.44	-	60,60,60,60	0
60	MG	DA	3020	1/1	0.29	-	52,52,52,52	0
60	MG	DA	3127	1/1	0.30	-	93,93,93,93	0
60	MG	CA	1654	1/1	0.63	-	77,77,77,77	0
60	MG	DA	3025	1/1	0.33	-	108,108,108,108	0
60	MG	AA	1636	1/1	0.24	-	53,53,53,53	0
60	MG	D8	101	1/1	0.17	-	74,74,74,74	0
60	MG	DA	3684	1/1	0.28	-	82,82,82,82	0
60	MG	DD	302	1/1	0.19	-	53,53,53,53	0
60	MG	DA	3668	1/1	0.22	-	93,93,93,93	0
60	MG	BA	2912	1/1	0.50	-	57,57,57,57	0
60	MG	DA	2941	1/1	0.08	-	27,27,27,27	1
60	MG	DA	3340	1/1	0.33	-	96,96,96,96	0
60	MG	DA	2994	1/1	0.61	-	60,60,60,60	0
60	MG	AA	1789	1/1	0.31	-	108,108,108,108	0
60	MG	BA	3142	1/1	0.17	-	67,67,67,67	0
60	MG	CV	112	1/1	0.20	-	69,69,69,69	0
60	MG	DA	3506	1/1	1.01	-	73,73,73,73	1
60	MG	AA	1679	1/1	0.28	-	53,53,53,53	1
60	MG	BA	2995	1/1	0.32	-	84,84,84,84	0
60	MG	DA	3426	1/1	0.40	-	28,28,28,28	0
60	MG	DA	3405	1/1	0.15	-	63,63,63,63	0
60	MG	DA	3339	1/1	0.49	-	37,37,37,37	0
60	MG	AA	1916	1/1	0.11	-	70,70,70,70	0
60	MG	DA	3027	1/1	0.41	-	69,69,69,69	0
60	MG	DA	3514	1/1	0.35	-	82,82,82,82	0
60	MG	BA	3280	1/1	0.41	-	38,38,38,38	0
60	MG	BA	3484	1/1	0.32	-	94,94,94,94	0
60	MG	DA	3633	1/1	0.58	-	75,75,75,75	0
60	MG	CA	1628	1/1	0.18	-	88,88,88,88	0
60	MG	AA	1726	1/1	0.30	-	70,70,70,70	1
60	MG	DA	3690	1/1	0.34	-	62,62,62,62	0
60	MG	DA	3533	1/1	0.19	-	100,100,100,100	0
60	MG	BA	3163	1/1	0.41	-	35,35,35,35	0
60	MG	DA	3562	1/1	0.13	-	25,25,25,25	1
60	MG	AA	1782	1/1	0.34	-	103,103,103,103	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1754	1/1	0.30	-	78,78,78,78	1
60	MG	DA	3374	1/1	0.38	-	91,91,91,91	0
60	MG	CA	1740	1/1	0.71	-	85,85,85,85	0
60	MG	BA	3524	1/1	0.40	-	103,103,103,103	0
60	MG	BA	3270	1/1	0.27	-	60,60,60,60	0
61	ZN	AD	305	1/1	0.22	-	88,88,88,88	0
60	MG	DA	3001	1/1	0.07	-	79,79,79,79	0
60	MG	BA	3045	1/1	0.18	-	75,75,75,75	0
60	MG	DA	3752	1/1	0.39	-	96,96,96,96	0
60	MG	AA	1647	1/1	0.15	-	35,35,35,35	0
60	MG	BB	206	1/1	0.52	-	90,90,90,90	1
60	MG	CA	1759	1/1	0.72	-	98,98,98,98	0
60	MG	BA	3459	1/1	0.32	-	44,44,44,44	0
60	MG	D7	102	1/1	0.27	-	75,75,75,75	0
60	MG	AA	1641	1/1	0.13	-	68,68,68,68	1
60	MG	DA	3113	1/1	1.25	-	109,109,109,109	0
60	MG	AA	1930	1/1	0.16	-	64,64,64,64	0
60	MG	DA	3048	1/1	0.68	-	63,63,63,63	0
60	MG	BH	202	1/1	0.12	-	95,95,95,95	0
60	MG	AA	1876	1/1	0.27	-	92,92,92,92	1
60	MG	BA	3173	1/1	0.28	-	102,102,102,102	1
60	MG	DA	3440	1/1	0.17	-	50,50,50,50	1
60	MG	BA	3492	1/1	0.15	-	31,31,31,31	1
60	MG	DA	3419	1/1	0.82	-	122,122,122,122	0
60	MG	DB	204	1/1	0.17	-	110,110,110,110	0
60	MG	DA	3719	1/1	0.48	-	73,73,73,73	0
60	MG	CA	1685	1/1	0.36	-	92,92,92,92	0
60	MG	DA	3745	1/1	0.52	-	56,56,56,56	0
60	MG	CV	108	1/1	0.23	-	101,101,101,101	0
60	MG	DA	3754	1/1	0.53	-	34,34,34,34	1
60	MG	BA	3420	1/1	0.32	-	71,71,71,71	0
60	MG	CA	1601	1/1	0.27	-	96,96,96,96	0
60	MG	BA	3057	1/1	0.36	-	68,68,68,68	0
60	MG	DA	3100	1/1	0.50	-	67,67,67,67	0
60	MG	DA	3011	1/1	0.26	-	40,40,40,40	0
60	MG	AA	1875	1/1	0.21	-	62,62,62,62	0
60	MG	CA	1647	1/1	0.40	-	77,77,77,77	0
60	MG	BA	3263	1/1	0.98	-	76,76,76,76	0
60	MG	DA	3413	1/1	1.11	-	84,84,84,84	0
60	MG	DA	3515	1/1	1.27	-	108,108,108,108	0
60	MG	DA	3363	1/1	0.36	-	69,69,69,69	0
60	MG	BA	3400	1/1	0.10	-	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1798	1/1	0.28	-	114,114,114,114	0
60	MG	BA	3608	1/1	0.43	-	31,31,31,31	0
60	MG	DA	3759	1/1	0.50	-	49,49,49,49	0
60	MG	BA	3064	1/1	0.40	-	45,45,45,45	0
60	MG	BA	3203	1/1	0.35	-	75,75,75,75	0
60	MG	AA	1672	1/1	0.12	-	77,77,77,77	0
60	MG	AA	1925	1/1	0.14	-	72,72,72,72	0
60	MG	BA	3100	1/1	0.21	-	47,47,47,47	0
60	MG	AA	1953	1/1	0.48	-	120,120,120,120	0
60	MG	BA	3336	1/1	0.20	-	99,99,99,99	0
60	MG	CA	1659	1/1	1.48	-	100,100,100,100	0
60	MG	DA	3107	1/1	0.52	-	103,103,103,103	0
60	MG	BA	3102	1/1	0.64	-	64,64,64,64	0
60	MG	BA	3198	1/1	0.33	-	102,102,102,102	0
61	ZN	AD	301	1/1	0.22	-	106,106,106,106	0
60	MG	BA	3217	1/1	0.15	-	72,72,72,72	0
60	MG	DA	3522	1/1	0.50	-	56,56,56,56	0
60	MG	DA	2956	1/1	0.26	-	38,38,38,38	0
60	MG	BA	3324	1/1	0.37	-	63,63,63,63	0
60	MG	DA	3073	1/1	0.32	-	64,64,64,64	0
60	MG	DA	2955	1/1	0.31	-	34,34,34,34	1
60	MG	CS	101	1/1	0.12	-	97,97,97,97	1
60	MG	BA	2903	1/1	0.44	-	37,37,37,37	0
60	MG	DA	3125	1/1	0.42	-	118,118,118,118	0
60	MG	DA	3716	1/1	0.50	-	103,103,103,103	0
60	MG	AA	1966	1/1	0.34	-	99,99,99,99	0
60	MG	DA	3574	1/1	0.74	-	70,70,70,70	1
60	MG	CJ	202	1/1	0.11	-	130,130,130,130	0
60	MG	AA	1921	1/1	0.46	-	86,86,86,86	0
60	MG	DA	3606	1/1	0.10	-	88,88,88,88	1
60	MG	DA	3689	1/1	0.13	-	123,123,123,123	0
60	MG	BA	3170	1/1	0.17	-	56,56,56,56	0
60	MG	DA	3678	1/1	0.40	-	100,100,100,100	0
60	MG	BA	3190	1/1	1.47	-	117,117,117,117	0
60	MG	DA	3569	1/1	0.65	-	102,102,102,102	0
60	MG	DA	3400	1/1	0.59	-	63,63,63,63	1
60	MG	CA	1624	1/1	0.31	-	86,86,86,86	0
60	MG	DA	3791	1/1	0.61	-	76,76,76,76	0
60	MG	D6	101	1/1	0.58	-	95,95,95,95	0
60	MG	BA	2935	1/1	0.41	-	102,102,102,102	0
60	MG	DA	3006	1/1	0.46	-	107,107,107,107	0
60	MG	AX	101	1/1	0.44	-	113,113,113,113	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3162	1/1	0.67	-	41,41,41,41	0
60	MG	BA	3259	1/1	0.23	-	59,59,59,59	0
60	MG	BA	3603	1/1	0.24	-	74,74,74,74	0
60	MG	DA	3654	1/1	0.36	-	78,78,78,78	0
60	MG	CV	103	1/1	0.16	-	67,67,67,67	0
60	MG	AA	1935	1/1	0.21	-	96,96,96,96	0
60	MG	DA	3047	1/1	0.81	-	88,88,88,88	0
60	MG	AA	1677	1/1	0.27	-	76,76,76,76	1
60	MG	AA	1823	1/1	0.28	-	68,68,68,68	0
60	MG	AA	1630	1/1	0.30	-	57,57,57,57	0
60	MG	DA	3004	1/1	1.10	-	122,122,122,122	0
60	MG	DA	3523	1/1	0.17	-	34,34,34,34	0
60	MG	DA	3587	1/1	0.71	-	74,74,74,74	0
60	MG	DA	3246	1/1	0.30	-	32,32,32,32	0
60	MG	DA	3161	1/1	0.62	-	61,61,61,61	0
60	MG	DA	3738	1/1	0.21	-	89,89,89,89	0
60	MG	DA	3094	1/1	0.51	-	87,87,87,87	0
60	MG	BA	2991	1/1	0.90	-	60,60,60,60	1
60	MG	DA	3493	1/1	0.30	-	90,90,90,90	0
60	MG	BA	3011	1/1	0.94	-	107,107,107,107	0
60	MG	BA	3145	1/1	0.29	-	89,89,89,89	0
60	MG	BA	3508	1/1	0.52	-	39,39,39,39	0
60	MG	DA	3769	1/1	0.20	-	142,142,142,142	0
60	MG	AA	1919	1/1	0.15	-	78,78,78,78	0
60	MG	BA	2932	1/1	0.46	-	63,63,63,63	0
60	MG	AA	1818	1/1	0.13	-	60,60,60,60	0
60	MG	BA	3429	1/1	0.94	-	67,67,67,67	0
60	MG	DA	3742	1/1	0.52	-	51,51,51,51	0
60	MG	DA	3673	1/1	0.85	-	116,116,116,116	0
60	MG	BA	3606	1/1	0.50	-	65,65,65,65	0
60	MG	DA	3215	1/1	0.41	-	69,69,69,69	0
60	MG	DA	3042	1/1	0.39	-	60,60,60,60	0
60	MG	BA	3107	1/1	0.60	-	87,87,87,87	0
60	MG	DA	3433	1/1	0.66	-	1,1,1,1	1
60	MG	BA	3572	1/1	0.88	-	68,68,68,68	0
60	MG	AA	1845	1/1	0.30	-	53,53,53,53	0
60	MG	BA	3282	1/1	0.41	-	47,47,47,47	0
60	MG	DD	305	1/1	0.30	-	1,1,1,1	1
60	MG	CC	301	1/1	0.69	-	117,117,117,117	0
60	MG	AA	1663	1/1	0.50	-	95,95,95,95	0
60	MG	DA	3277	1/1	0.35	-	42,42,42,42	0
60	MG	AA	1869	1/1	0.58	-	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1675	1/1	0.32	-	52,52,52,52	1
60	MG	BA	3343	1/1	0.47	-	32,32,32,32	0
60	MG	BA	3155	1/1	0.49	-	29,29,29,29	0
60	MG	DA	3018	1/1	0.11	-	76,76,76,76	0
60	MG	DA	3380	1/1	0.29	-	43,43,43,43	0
60	MG	BA	3321	1/1	0.32	-	58,58,58,58	0
60	MG	CA	1668	1/1	0.30	-	94,94,94,94	0
60	MG	DA	3552	1/1	0.47	-	120,120,120,120	0
60	MG	BA	3001	1/1	0.36	-	117,117,117,117	0
60	MG	BA	3287	1/1	0.16	-	104,104,104,104	0
60	MG	CA	1625	1/1	0.15	-	62,62,62,62	0
60	MG	BP	202	1/1	0.12	-	69,69,69,69	1
60	MG	BA	3502	1/1	1.79	-	132,132,132,132	0
60	MG	DA	2954	1/1	0.52	-	47,47,47,47	1
60	MG	CA	1776	1/1	0.82	-	83,83,83,83	0
60	MG	BA	3497	1/1	1.22	-	85,85,85,85	0
60	MG	DA	3162	1/1	0.30	-	122,122,122,122	0
60	MG	CA	1736	1/1	0.12	-	60,60,60,60	0
60	MG	BA	3235	1/1	0.18	-	40,40,40,40	0
60	MG	BA	3037	1/1	0.67	-	64,64,64,64	0
60	MG	DA	3342	1/1	0.30	-	58,58,58,58	0
60	MG	DA	3254	1/1	0.09	-	59,59,59,59	0
60	MG	DA	3347	1/1	0.21	-	71,71,71,71	0
60	MG	BA	3152	1/1	0.34	-	34,34,34,34	0
60	MG	CA	1626	1/1	0.48	-	112,112,112,112	0
60	MG	DA	3655	1/1	0.74	-	91,91,91,91	0
60	MG	AA	1883	1/1	0.86	-	58,58,58,58	0
60	MG	DA	2992	1/1	0.70	-	103,103,103,103	0
60	MG	AA	1804	1/1	0.45	-	90,90,90,90	0
60	MG	BA	3156	1/1	0.33	-	27,27,27,27	0
60	MG	DA	3292	1/1	0.46	-	106,106,106,106	0
60	MG	AA	1832	1/1	0.32	-	140,140,140,140	0
60	MG	BA	3183	1/1	0.15	-	54,54,54,54	0
60	MG	DA	3649	1/1	0.48	-	66,66,66,66	0
60	MG	BA	2918	1/1	0.64	-	76,76,76,76	1
60	MG	BA	3530	1/1	0.22	-	33,33,33,33	0
60	MG	BA	3197	1/1	0.30	-	54,54,54,54	0
60	MG	AA	1837	1/1	0.21	-	75,75,75,75	0
60	MG	BA	2927	1/1	0.35	-	83,83,83,83	1
60	MG	AA	1787	1/1	0.19	-	109,109,109,109	0
60	MG	DA	3097	1/1	0.32	-	69,69,69,69	0
60	MG	CV	104	1/1	0.15	-	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3691	1/1	0.10	-	59,59,59,59	0
60	MG	DA	3276	1/1	0.26	-	58,58,58,58	0
60	MG	AA	1885	1/1	0.37	-	57,57,57,57	0
60	MG	DA	3338	1/1	0.23	-	68,68,68,68	0
60	MG	DA	2983	1/1	0.50	-	79,79,79,79	1
60	MG	BA	3110	1/1	0.21	-	55,55,55,55	0
60	MG	AX	104	1/1	0.46	-	43,43,43,43	0
60	MG	DA	3659	1/1	0.46	-	88,88,88,88	0
60	MG	BA	3597	1/1	0.75	-	53,53,53,53	1
60	MG	AA	1892	1/1	0.18	-	75,75,75,75	0
60	MG	BA	3479	1/1	0.39	-	133,133,133,133	0
60	MG	DA	3206	1/1	0.31	-	66,66,66,66	0
60	MG	DA	3705	1/1	0.53	-	58,58,58,58	0
60	MG	BA	3018	1/1	0.16	-	38,38,38,38	0
60	MG	BA	3148	1/1	0.70	-	106,106,106,106	0
60	MG	AA	1888	1/1	0.22	-	58,58,58,58	0
60	MG	CQ	201	1/1	0.07	-	98,98,98,98	1
60	MG	DA	2927	1/1	0.36	-	1,1,1,1	1
60	MG	CA	1715	1/1	0.17	-	80,80,80,80	0
60	MG	DA	3698	1/1	0.18	-	25,25,25,25	0
60	MG	DA	2997	1/1	0.52	-	43,43,43,43	0
60	MG	CA	1620	1/1	0.77	-	87,87,87,87	0
60	MG	BA	3140	1/1	0.77	-	113,113,113,113	0
60	MG	CV	106	1/1	0.39	-	101,101,101,101	0
60	MG	BA	3605	1/1	0.65	-	79,79,79,79	0
60	MG	AA	1809	1/1	1.16	-	92,92,92,92	0
60	MG	DA	3711	1/1	0.41	-	55,55,55,55	1
60	MG	BA	2909	1/1	0.17	-	50,50,50,50	0
60	MG	AA	1740	1/1	0.41	-	94,94,94,94	0
60	MG	CA	1753	1/1	0.08	-	103,103,103,103	0
60	MG	DA	3779	1/1	0.78	-	122,122,122,122	0
60	MG	BA	3533	1/1	0.44	-	83,83,83,83	0
60	MG	BA	3026	1/1	0.36	-	105,105,105,105	0
60	MG	BA	3451	1/1	0.17	-	55,55,55,55	0
60	MG	DA	3604	1/1	0.50	-	39,39,39,39	0
60	MG	BA	3587	1/1	0.54	-	47,47,47,47	0
60	MG	CA	1784	1/1	0.62	-	76,76,76,76	0
60	MG	BA	3169	1/1	0.36	-	24,24,24,24	0
60	MG	BA	2999	1/1	0.11	-	86,86,86,86	0
60	MG	DA	3382	1/1	0.12	-	101,101,101,101	0
60	MG	CA	1778	1/1	0.32	-	88,88,88,88	0
60	MG	AA	1711	1/1	0.28	-	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1936	1/1	0.21	-	135,135,135,135	0
60	MG	BA	3208	1/1	0.36	-	27,27,27,27	0
60	MG	BA	3595	1/1	0.59	-	65,65,65,65	0
60	MG	AA	1758	1/1	0.49	-	98,98,98,98	0
60	MG	DA	3270	1/1	0.18	-	55,55,55,55	0
60	MG	AA	1656	1/1	0.30	-	98,98,98,98	1
60	MG	BA	3055	1/1	0.68	-	92,92,92,92	0
60	MG	BA	3039	1/1	0.73	-	81,81,81,81	0
60	MG	DA	3066	1/1	0.16	-	113,113,113,113	0
60	MG	BA	3537	1/1	0.28	-	28,28,28,28	0
60	MG	BA	3019	1/1	0.87	-	66,66,66,66	0
60	MG	AA	1707	1/1	0.32	-	97,97,97,97	0
60	MG	DA	3466	1/1	0.55	-	40,40,40,40	0
60	MG	DA	3280	1/1	0.20	-	58,58,58,58	0
60	MG	BA	3560	1/1	0.92	-	83,83,83,83	0
60	MG	DA	3088	1/1	0.11	-	65,65,65,65	0
60	MG	BA	3395	1/1	0.62	-	84,84,84,84	0
60	MG	DA	3706	1/1	0.72	-	66,66,66,66	0
60	MG	AA	1731	1/1	0.32	-	81,81,81,81	0
60	MG	BA	3582	1/1	0.43	-	63,63,63,63	0
60	MG	DA	3307	1/1	0.30	-	77,77,77,77	0
60	MG	BA	3358	1/1	0.13	-	100,100,100,100	0
60	MG	BA	3494	1/1	0.58	-	77,77,77,77	0
60	MG	DA	3677	1/1	0.31	-	45,45,45,45	0
60	MG	DA	3614	1/1	0.31	-	100,100,100,100	0
60	MG	DA	3729	1/1	0.24	-	96,96,96,96	0
60	MG	DB	211	1/1	0.37	-	80,80,80,80	0
60	MG	BA	3477	1/1	1.35	-	128,128,128,128	0
60	MG	DA	3749	1/1	0.23	-	80,80,80,80	1
60	MG	DA	3454	1/1	0.48	-	35,35,35,35	0
60	MG	BA	3277	1/1	0.46	-	44,44,44,44	0
60	MG	DA	3578	1/1	0.61	-	105,105,105,105	0
60	MG	AV	101	1/1	0.72	-	52,52,52,52	1
60	MG	D5	102	1/1	0.06	-	63,63,63,63	0
60	MG	DA	2948	1/1	0.35	-	75,75,75,75	0
60	MG	BA	3147	1/1	0.46	-	72,72,72,72	0
60	MG	BA	2975	1/1	0.57	-	57,57,57,57	0
60	MG	CA	1710	1/1	0.19	-	51,51,51,51	0
60	MG	DA	2968	1/1	0.17	-	1,1,1,1	1
60	MG	AA	1877	1/1	0.39	-	61,61,61,61	0
60	MG	DA	2957	1/1	0.43	-	47,47,47,47	0
60	MG	BA	3317	1/1	0.86	-	64,64,64,64	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1643	1/1	0.13	-	80,80,80,80	0
60	MG	DA	3091	1/1	0.37	-	119,119,119,119	0
60	MG	DA	3571	1/1	0.45	-	96,96,96,96	0
60	MG	DA	3456	1/1	0.72	-	56,56,56,56	0
60	MG	DA	3183	1/1	0.38	-	94,94,94,94	0
60	MG	AI	203	1/1	0.23	-	138,138,138,138	0
60	MG	DA	3420	1/1	0.49	-	100,100,100,100	0
60	MG	BA	2961	1/1	0.13	-	79,79,79,79	0
60	MG	DA	3022	1/1	0.48	-	71,71,71,71	0
60	MG	DA	3461	1/1	0.53	-	77,77,77,77	0
60	MG	DA	3316	1/1	0.44	-	59,59,59,59	1
60	MG	AA	1851	1/1	0.48	-	62,62,62,62	0
60	MG	AN	103	1/1	0.27	-	147,147,147,147	0
60	MG	DA	3406	1/1	1.55	-	38,38,38,38	1
60	MG	BA	3406	1/1	0.46	-	52,52,52,52	0
60	MG	DA	3208	1/1	0.35	-	91,91,91,91	0
60	MG	BA	3566	1/1	0.39	-	66,66,66,66	1
60	MG	CA	1645	1/1	0.14	-	50,50,50,50	0
60	MG	AA	1954	1/1	0.98	-	67,67,67,67	0
61	ZN	CD	301	1/1	0.25	-	151,151,151,151	0
60	MG	DB	209	1/1	0.23	-	95,95,95,95	0
60	MG	DA	3708	1/1	1.08	-	100,100,100,100	0
60	MG	DA	3438	1/1	0.25	-	76,76,76,76	0
60	MG	DA	3014	1/1	0.65	-	108,108,108,108	0
60	MG	BP	201	1/1	0.29	-	24,24,24,24	0
60	MG	CA	1771	1/1	0.79	-	96,96,96,96	0
60	MG	AA	1920	1/1	0.13	-	73,73,73,73	0
60	MG	DA	3337	1/1	0.24	-	90,90,90,90	0
60	MG	CA	1658	1/1	0.51	-	97,97,97,97	0
60	MG	DA	3408	1/1	0.28	-	41,41,41,41	0
60	MG	BA	3050	1/1	0.12	-	73,73,73,73	0
60	MG	AA	1706	1/1	0.06	-	44,44,44,44	1
60	MG	AA	1689	1/1	0.22	-	82,82,82,82	1
60	MG	BA	3176	1/1	0.21	-	50,50,50,50	0
60	MG	DA	3431	1/1	0.31	-	38,38,38,38	0
60	MG	DA	3312	1/1	0.30	-	48,48,48,48	0
60	MG	AA	1843	1/1	0.68	-	99,99,99,99	0
60	MG	DA	3641	1/1	0.71	-	68,68,68,68	0
60	MG	AC	301	1/1	0.10	-	173,173,173,173	0
60	MG	AA	1894	1/1	0.17	-	90,90,90,90	0
60	MG	BA	3072	1/1	0.29	-	101,101,101,101	0
60	MG	DA	3273	1/1	0.59	-	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3035	1/1	0.66	-	42,42,42,42	0
60	MG	BA	3146	1/1	1.07	-	113,113,113,113	0
60	MG	BA	3547	1/1	0.24	-	78,78,78,78	0
60	MG	BA	3318	1/1	0.47	-	63,63,63,63	0
60	MG	AA	1610	1/1	0.42	-	77,77,77,77	0
60	MG	DA	3415	1/1	0.52	-	41,41,41,41	0
60	MG	BA	3238	1/1	0.50	-	110,110,110,110	0
60	MG	BA	2910	1/1	0.22	-	83,83,83,83	1
60	MG	AA	1674	1/1	0.23	-	48,48,48,48	0
60	MG	AA	1849	1/1	0.19	-	80,80,80,80	0
60	MG	BE	304	1/1	0.42	-	46,46,46,46	1
60	MG	DA	3484	1/1	0.83	-	58,58,58,58	0
60	MG	BA	3254	1/1	0.21	-	93,93,93,93	0
60	MG	CA	1735	1/1	0.48	-	127,127,127,127	0
60	MG	BA	3005	1/1	1.20	-	105,105,105,105	0
60	MG	DA	3423	1/1	0.45	-	51,51,51,51	1
60	MG	AA	1931	1/1	0.22	-	87,87,87,87	0
60	MG	AD	302	1/1	0.08	-	96,96,96,96	0
60	MG	BB	204	1/1	0.16	-	109,109,109,109	0
60	MG	AA	1882	1/1	0.20	-	57,57,57,57	0
60	MG	DA	3613	1/1	0.12	-	56,56,56,56	1
60	MG	BA	3407	1/1	0.31	-	64,64,64,64	0
60	MG	AA	1755	1/1	0.29	-	34,34,34,34	1
60	MG	DA	3351	1/1	0.15	-	77,77,77,77	0
60	MG	CA	1686	1/1	0.29	-	74,74,74,74	0
60	MG	DA	3046	1/1	0.36	-	95,95,95,95	0
60	MG	DA	3489	1/1	0.52	-	59,59,59,59	1
60	MG	AA	1738	1/1	0.82	-	59,59,59,59	0
60	MG	BA	3466	1/1	0.28	-	38,38,38,38	0
60	MG	AA	1764	1/1	0.96	-	65,65,65,65	0
60	MG	BA	3455	1/1	0.75	-	65,65,65,65	0
60	MG	CA	1669	1/1	0.14	-	57,57,57,57	0
60	MG	BA	2974	1/1	0.53	-	38,38,38,38	0
60	MG	BA	3261	1/1	0.24	-	41,41,41,41	0
60	MG	BA	3363	1/1	0.47	-	92,92,92,92	0
60	MG	AA	1962	1/1	0.80	-	65,65,65,65	0
60	MG	BA	3394	1/1	0.32	-	85,85,85,85	0
60	MG	AA	1688	1/1	0.06	-	22,22,22,22	1
60	MG	DB	203	1/1	0.16	-	30,30,30,30	1
60	MG	AA	1658	1/1	0.14	-	106,106,106,106	0
60	MG	CA	1608	1/1	0.48	-	124,124,124,124	0
60	MG	DA	3538	1/1	0.56	-	118,118,118,118	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3306	1/1	0.25	-	57,57,57,57	0
60	MG	BA	3511	1/1	0.32	-	73,73,73,73	0
60	MG	BA	3288	1/1	0.47	-	38,38,38,38	0
60	MG	BA	3312	1/1	0.28	-	53,53,53,53	0
60	MG	DA	3643	1/1	0.39	-	113,113,113,113	0
60	MG	BA	3022	1/1	0.07	-	43,43,43,43	0
60	MG	AQ	201	1/1	0.09	-	97,97,97,97	1
60	MG	DA	3051	1/1	0.32	-	36,36,36,36	0
60	MG	AA	1860	1/1	0.39	-	61,61,61,61	0
60	MG	BA	3601	1/1	0.39	-	79,79,79,79	0
60	MG	D3	101	1/1	1.93	-	1,1,1,1	1
60	MG	DA	3474	1/1	2.38	-	99,99,99,99	0
60	MG	D7	101	1/1	0.43	-	89,89,89,89	0
60	MG	DA	3111	1/1	0.33	-	83,83,83,83	0
60	MG	BA	3353	1/1	0.57	-	107,107,107,107	0
60	MG	DA	3092	1/1	0.67	-	106,106,106,106	0
60	MG	DA	3730	1/1	0.47	-	91,91,91,91	0
60	MG	DA	3632	1/1	0.49	-	56,56,56,56	0
60	MG	AA	1662	1/1	0.43	-	68,68,68,68	0
60	MG	BA	3381	1/1	0.32	-	42,42,42,42	0
60	MG	DA	3766	1/1	0.77	-	100,100,100,100	0
60	MG	BA	3528	1/1	0.53	-	73,73,73,73	0
60	MG	BA	2967	1/1	0.33	-	95,95,95,95	0
60	MG	DA	3360	1/1	0.21	-	99,99,99,99	0
60	MG	DA	3332	1/1	0.32	-	26,26,26,26	0
60	MG	CA	1757	1/1	0.15	-	83,83,83,83	0
60	MG	DA	3573	1/1	0.33	-	86,86,86,86	0
60	MG	DA	2937	1/1	0.38	-	63,63,63,63	1
60	MG	BA	3127	1/1	0.41	-	71,71,71,71	0
60	MG	AA	1665	1/1	0.67	-	60,60,60,60	0
60	MG	DA	3656	1/1	0.15	-	75,75,75,75	0
60	MG	BA	3328	1/1	0.68	-	76,76,76,76	0
60	MG	AA	1806	1/1	0.16	-	81,81,81,81	0
60	MG	CA	1773	1/1	0.42	-	106,106,106,106	0
60	MG	DA	3359	1/1	0.32	-	64,64,64,64	0
60	MG	BA	3117	1/1	0.68	-	98,98,98,98	0
60	MG	DA	3595	1/1	0.78	-	75,75,75,75	0
60	MG	BB	201	1/1	0.38	-	46,46,46,46	0
60	MG	CA	1709	1/1	0.15	-	85,85,85,85	1
60	MG	AA	1937	1/1	0.19	-	58,58,58,58	0
60	MG	DA	3157	1/1	0.22	-	52,52,52,52	0
60	MG	AA	1963	1/1	0.80	-	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3212	1/1	0.58	-	52,52,52,52	0
60	MG	CA	1781	1/1	0.18	-	74,74,74,74	0
60	MG	DA	3797	1/1	0.37	-	56,56,56,56	0
60	MG	DA	3477	1/1	0.63	-	76,76,76,76	0
60	MG	DA	3123	1/1	0.97	-	91,91,91,91	0
60	MG	DA	3063	1/1	0.23	-	50,50,50,50	0
60	MG	BA	3550	1/1	0.40	-	103,103,103,103	0
60	MG	AA	1949	1/1	0.47	-	42,42,42,42	1
60	MG	BU	202	1/1	0.33	-	39,39,39,39	0
60	MG	DA	3326	1/1	0.55	-	63,63,63,63	0
60	MG	DA	3114	1/1	0.50	-	55,55,55,55	0
60	MG	DA	3584	1/1	0.67	-	80,80,80,80	0
60	MG	DA	3299	1/1	0.46	-	75,75,75,75	0
60	MG	DA	3559	1/1	0.30	-	74,74,74,74	0
60	MG	AA	1602	1/1	0.17	-	71,71,71,71	0
60	MG	CA	1704	1/1	0.12	-	71,71,71,71	0
60	MG	DA	3790	1/1	1.04	-	29,29,29,29	1
60	MG	BR	204	1/1	0.17	-	26,26,26,26	0
60	MG	DA	2999	1/1	0.06	-	91,91,91,91	0
60	MG	BA	3461	1/1	0.48	-	41,41,41,41	0
60	MG	DA	3132	1/1	0.57	-	49,49,49,49	0
60	MG	BA	3579	1/1	0.70	-	71,71,71,71	0
60	MG	CA	1618	1/1	0.34	-	79,79,79,79	0
60	MG	DA	3442	1/1	0.48	-	71,71,71,71	0
60	MG	BA	3480	1/1	0.34	-	55,55,55,55	0
60	MG	DA	3422	1/1	0.69	-	63,63,63,63	0
60	MG	DA	3401	1/1	0.76	-	65,65,65,65	0
60	MG	AA	1867	1/1	0.35	-	65,65,65,65	0
60	MG	BA	2984	1/1	0.26	-	92,92,92,92	0
60	MG	AA	1829	1/1	0.57	-	91,91,91,91	0
60	MG	BA	3415	1/1	0.47	-	69,69,69,69	1
60	MG	BA	2951	1/1	1.41	-	142,142,142,142	0
60	MG	DA	3056	1/1	0.66	-	65,65,65,65	0
60	MG	CA	1656	1/1	0.47	-	73,73,73,73	0
60	MG	DA	3634	1/1	0.41	-	83,83,83,83	0
60	MG	AV	107	1/1	0.28	-	58,58,58,58	0
60	MG	DA	3197	1/1	0.18	-	67,67,67,67	0
60	MG	DA	3220	1/1	0.61	-	117,117,117,117	0
60	MG	AA	1722	1/1	0.70	-	116,116,116,116	0
60	MG	CV	107	1/1	0.31	-	115,115,115,115	0
60	MG	BA	3171	1/1	0.30	-	29,29,29,29	0
60	MG	BA	3080	1/1	0.58	-	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1613	1/1	0.33	-	73,73,73,73	0
60	MG	DA	3554	1/1	0.07	-	95,95,95,95	0
60	MG	BA	3087	1/1	0.47	-	87,87,87,87	0
60	MG	D1	102	1/1	0.26	-	80,80,80,80	0
60	MG	AO	101	1/1	0.40	-	111,111,111,111	0
60	MG	DA	2949	1/1	0.39	-	98,98,98,98	1
60	MG	BA	3562	1/1	0.50	-	71,71,71,71	0
60	MG	AA	1799	1/1	0.13	-	80,80,80,80	0
60	MG	BA	3428	1/1	1.05	-	72,72,72,72	0
60	MG	BA	3219	1/1	0.45	-	57,57,57,57	0
60	MG	DA	3564	1/1	0.32	-	42,42,42,42	0
60	MG	AA	1946	1/1	0.43	-	77,77,77,77	0
60	MG	BA	3564	1/1	0.76	-	113,113,113,113	0
60	MG	DA	3074	1/1	0.66	-	129,129,129,129	0
60	MG	BA	3432	1/1	0.44	-	59,59,59,59	0
60	MG	BA	3352	1/1	0.22	-	72,72,72,72	0
60	MG	DA	3274	1/1	0.08	-	73,73,73,73	0
60	MG	DA	3566	1/1	0.14	-	106,106,106,106	0
60	MG	D7	104	1/1	0.24	-	82,82,82,82	1
60	MG	DA	3547	1/1	0.72	-	89,89,89,89	0
60	MG	DA	2944	1/1	2.40	-	109,109,109,109	1
60	MG	AA	1942	1/1	0.20	-	98,98,98,98	0
60	MG	DA	3582	1/1	0.56	-	47,47,47,47	1
60	MG	BA	3532	1/1	1.34	-	88,88,88,88	0
60	MG	BA	2964	1/1	0.17	-	96,96,96,96	0
60	MG	DA	3756	1/1	0.44	-	106,106,106,106	0
60	MG	BA	3133	1/1	0.19	-	57,57,57,57	0
60	MG	AA	1619	1/1	0.49	-	111,111,111,111	0
60	MG	AA	1709	1/1	0.23	-	85,85,85,85	1
60	MG	BA	2976	1/1	0.14	-	97,97,97,97	0
60	MG	AA	1728	1/1	0.29	-	78,78,78,78	0
60	MG	AA	1830	1/1	0.33	-	86,86,86,86	0
60	MG	AA	1972	1/1	1.62	-	98,98,98,98	1
60	MG	DA	3663	1/1	0.57	-	55,55,55,55	0
60	MG	AA	1874	1/1	0.35	-	111,111,111,111	0
60	MG	AA	1634	1/1	0.44	-	70,70,70,70	1
60	MG	BA	3085	1/1	0.48	-	68,68,68,68	0
60	MG	DA	3642	1/1	0.53	-	88,88,88,88	0
60	MG	DA	3003	1/1	0.29	-	36,36,36,36	0
60	MG	BA	3068	1/1	0.65	-	59,59,59,59	0
60	MG	AA	1840	1/1	0.28	-	76,76,76,76	0
60	MG	BA	3496	1/1	0.32	-	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	2986	1/1	0.36	-	52,52,52,52	0
60	MG	DA	3516	1/1	0.85	-	97,97,97,97	0
60	MG	DA	3272	1/1	0.27	-	79,79,79,79	1
60	MG	DA	3736	1/1	0.21	-	77,77,77,77	1
60	MG	DA	3788	1/1	0.25	-	124,124,124,124	0
60	MG	DA	3473	1/1	0.55	-	38,38,38,38	0
60	MG	CA	1609	1/1	1.00	-	93,93,93,93	0
60	MG	DA	3026	1/1	0.34	-	60,60,60,60	0
60	MG	BA	3103	1/1	0.27	-	69,69,69,69	0
60	MG	AA	1792	1/1	0.17	-	102,102,102,102	0
60	MG	DA	3441	1/1	0.56	-	55,55,55,55	0
60	MG	BA	3474	1/1	0.53	-	53,53,53,53	0
60	MG	BA	3061	1/1	0.28	-	63,63,63,63	0
60	MG	AA	1951	1/1	0.27	-	82,82,82,82	0
60	MG	BA	3028	1/1	0.37	-	58,58,58,58	0
60	MG	BA	3440	1/1	0.36	-	72,72,72,72	0
60	MG	BA	3159	1/1	0.45	-	72,72,72,72	0
60	MG	DA	3055	1/1	0.47	-	51,51,51,51	0
60	MG	BA	3234	1/1	0.56	-	90,90,90,90	0
60	MG	AL	201	1/1	0.11	-	87,87,87,87	0
60	MG	AA	1871	1/1	0.22	-	144,144,144,144	0
60	MG	BA	3175	1/1	0.36	-	25,25,25,25	0
60	MG	AC	302	1/1	0.10	-	163,163,163,163	0
60	MG	AA	1886	1/1	0.67	-	84,84,84,84	0
60	MG	DA	3528	1/1	0.27	-	80,80,80,80	0
60	MG	CA	1651	1/1	0.16	-	84,84,84,84	0
60	MG	CA	1663	1/1	0.17	-	97,97,97,97	0
60	MG	AA	1928	1/1	0.33	-	42,42,42,42	0
60	MG	BA	3376	1/1	0.22	-	68,68,68,68	1
60	MG	DA	3348	1/1	0.55	-	43,43,43,43	0
60	MG	AA	1735	1/1	0.81	-	85,85,85,85	0
60	MG	DA	3412	1/1	0.52	-	42,42,42,42	0
60	MG	DA	3390	1/1	0.65	-	60,60,60,60	1
60	MG	DA	3043	1/1	0.41	-	80,80,80,80	0
60	MG	DA	2953	1/1	0.65	-	99,99,99,99	0
60	MG	BA	3265	1/1	0.32	-	66,66,66,66	0
60	MG	DA	3154	1/1	0.34	-	58,58,58,58	0
60	MG	AA	1940	1/1	0.24	-	86,86,86,86	0
60	MG	AA	1608	1/1	0.38	-	58,58,58,58	0
60	MG	AL	202	1/1	0.12	-	73,73,73,73	0
60	MG	DA	3110	1/1	0.69	-	200,200,200,200	0
60	MG	AV	102	1/1	0.72	-	106,106,106,106	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3049	1/1	0.19	-	66,66,66,66	0
60	MG	DA	3037	1/1	0.53	-	58,58,58,58	0
60	MG	DA	3615	1/1	0.82	-	86,86,86,86	0
60	MG	DA	3504	1/1	0.29	-	60,60,60,60	0
60	MG	BA	3143	1/1	0.39	-	149,149,149,149	0
60	MG	DA	3190	1/1	0.27	-	97,97,97,97	0
60	MG	DA	3258	1/1	0.21	-	48,48,48,48	0
60	MG	D1	101	1/1	0.19	-	75,75,75,75	0
60	MG	BA	3515	1/1	0.15	-	47,47,47,47	1
60	MG	BA	3385	1/1	0.35	-	63,63,63,63	1
60	MG	BA	3505	1/1	0.43	-	95,95,95,95	0
60	MG	BA	2987	1/1	0.26	-	104,104,104,104	0
60	MG	BA	3141	1/1	0.64	-	104,104,104,104	0
60	MG	DA	3262	1/1	0.30	-	59,59,59,59	1
60	MG	BA	3454	1/1	0.56	-	64,64,64,64	0
60	MG	BA	3447	1/1	0.12	-	90,90,90,90	0
60	MG	BA	3297	1/1	0.21	-	34,34,34,34	0
60	MG	CA	1752	1/1	0.66	-	113,113,113,113	0
60	MG	DA	3096	1/1	0.40	-	80,80,80,80	0
60	MG	CA	1717	1/1	0.14	-	78,78,78,78	0
60	MG	DA	3317	1/1	0.51	-	62,62,62,62	0
60	MG	AA	1836	1/1	0.27	-	114,114,114,114	0
60	MG	DA	2987	1/1	0.27	-	68,68,68,68	0
60	MG	CA	1766	1/1	0.31	-	118,118,118,118	0
60	MG	BA	3082	1/1	0.29	-	90,90,90,90	0
60	MG	DA	3666	1/1	0.97	-	66,66,66,66	0
60	MG	BA	3168	1/1	0.31	-	24,24,24,24	0
60	MG	BA	2921	1/1	0.12	-	51,51,51,51	0
60	MG	BA	3043	1/1	0.35	-	80,80,80,80	0
60	MG	DA	3397	1/1	0.44	-	72,72,72,72	0
60	MG	DA	3395	1/1	0.34	-	83,83,83,83	0
60	MG	BA	3038	1/1	0.19	-	17,17,17,17	0
60	MG	BA	2919	1/1	0.40	-	44,44,44,44	1
60	MG	DA	3175	1/1	0.19	-	28,28,28,28	0
60	MG	DA	3601	1/1	0.19	-	39,39,39,39	0
60	MG	BA	3396	1/1	0.58	-	86,86,86,86	0
60	MG	DA	3775	1/1	0.62	-	86,86,86,86	0
60	MG	BA	3433	1/1	0.20	-	61,61,61,61	0
60	MG	BA	3573	1/1	0.62	-	75,75,75,75	0
60	MG	DA	3631	1/1	0.40	-	41,41,41,41	0
60	MG	DB	202	1/1	0.48	-	55,55,55,55	0
60	MG	BA	3105	1/1	1.07	-	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	2924	1/1	0.31	-	65,65,65,65	0
60	MG	AA	1637	1/1	0.15	-	78,78,78,78	1
60	MG	DA	3083	1/1	0.45	-	104,104,104,104	0
60	MG	DA	3402	1/1	0.28	-	16,16,16,16	0
60	MG	DA	3002	1/1	0.08	-	78,78,78,78	0
60	MG	DA	3580	1/1	0.22	-	34,34,34,34	0
60	MG	BA	3345	1/1	0.57	-	37,37,37,37	0
60	MG	DA	3343	1/1	0.45	-	69,69,69,69	0
60	MG	AA	1784	1/1	0.26	-	92,92,92,92	0
60	MG	BA	3179	1/1	0.27	-	66,66,66,66	0
60	MG	BA	2963	1/1	1.28	-	113,113,113,113	0
60	MG	BR	202	1/1	0.17	-	24,24,24,24	0
60	MG	BA	3031	1/1	0.37	-	58,58,58,58	0
60	MG	AA	1924	1/1	0.95	-	84,84,84,84	0
60	MG	DA	3476	1/1	0.38	-	120,120,120,120	0
60	MG	BA	3516	1/1	0.78	-	64,64,64,64	0
60	MG	BA	3023	1/1	0.24	-	64,64,64,64	0
60	MG	AA	1779	1/1	0.19	-	114,114,114,114	0
60	MG	DA	3296	1/1	0.29	-	46,46,46,46	1
60	MG	AA	1639	1/1	1.24	-	79,79,79,79	0
60	MG	DA	3323	1/1	0.77	-	58,58,58,58	0
60	MG	CA	1760	1/1	0.25	-	52,52,52,52	1
60	MG	BA	3106	1/1	0.11	-	35,35,35,35	0
60	MG	AA	1659	1/1	0.20	-	107,107,107,107	0
60	MG	AA	1618	1/1	0.52	-	78,78,78,78	0
60	MG	AA	1657	1/1	0.12	-	77,77,77,77	0
60	MG	BA	3419	1/1	0.21	-	49,49,49,49	0
60	MG	BA	3540	1/1	0.90	-	66,66,66,66	1
60	MG	DA	3781	1/1	0.77	-	143,143,143,143	0
60	MG	DA	3315	1/1	0.34	-	77,77,77,77	0
60	MG	CA	1721	1/1	0.78	-	111,111,111,111	0
60	MG	BA	3565	1/1	0.37	-	79,79,79,79	0
60	MG	AX	103	1/1	0.58	-	112,112,112,112	0
60	MG	BA	2923	1/1	1.05	-	96,96,96,96	0
60	MG	CA	1696	1/1	1.03	-	79,79,79,79	0
60	MG	DA	3407	1/1	0.45	-	77,77,77,77	1
60	MG	DA	3253	1/1	0.44	-	52,52,52,52	0
60	MG	BA	3256	1/1	0.33	-	122,122,122,122	0
60	MG	AA	1887	1/1	0.23	-	72,72,72,72	0
60	MG	DA	3336	1/1	0.54	-	31,31,31,31	0
60	MG	BA	2914	1/1	1.69	-	106,106,106,106	0
60	MG	BA	3481	1/1	0.40	-	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3220	1/1	0.62	-	54,54,54,54	0
60	MG	CA	1783	1/1	0.11	-	83,83,83,83	0
60	MG	DA	3618	1/1	0.64	-	72,72,72,72	0
60	MG	CA	1774	1/1	1.35	-	111,111,111,111	1
60	MG	DA	3703	1/1	0.18	-	41,41,41,41	0
60	MG	BA	3568	1/1	0.42	-	58,58,58,58	0
60	MG	AA	1682	1/1	0.96	-	104,104,104,104	0
60	MG	BA	3108	1/1	0.65	-	56,56,56,56	0
60	MG	AA	1748	1/1	0.40	-	23,23,23,23	1
60	MG	CA	1739	1/1	0.59	-	104,104,104,104	0
60	MG	DA	2938	1/1	0.18	-	17,17,17,17	1
60	MG	DA	3193	1/1	0.18	-	68,68,68,68	0
60	MG	AA	1908	1/1	0.28	-	65,65,65,65	0
60	MG	BA	3153	1/1	0.09	-	93,93,93,93	0
60	MG	AA	1660	1/1	0.20	-	82,82,82,82	0
60	MG	BA	3223	1/1	0.20	-	80,80,80,80	0
60	MG	BA	3099	1/1	0.40	-	30,30,30,30	0
60	MG	AA	1903	1/1	0.38	-	79,79,79,79	0
60	MG	AA	1872	1/1	0.67	-	77,77,77,77	0
60	MG	D0	101	1/1	0.16	-	16,16,16,16	1
60	MG	DA	2904	1/1	0.98	-	66,66,66,66	0
60	MG	BA	3594	1/1	0.22	-	83,83,83,83	0
60	MG	AA	1690	1/1	0.23	-	81,81,81,81	1
60	MG	CV	102	1/1	0.08	-	92,92,92,92	0
60	MG	BA	3192	1/1	0.78	-	90,90,90,90	0
60	MG	BA	3134	1/1	0.08	-	65,65,65,65	0
60	MG	BA	3522	1/1	0.24	-	74,74,74,74	0
60	MG	AA	1705	1/1	0.73	-	105,105,105,105	0
60	MG	B7	101	1/1	0.85	-	93,93,93,93	0
60	MG	CA	1734	1/1	0.17	-	56,56,56,56	0
60	MG	DA	3540	1/1	0.17	-	152,152,152,152	0
60	MG	DA	3093	1/1	0.37	-	67,67,67,67	0
60	MG	DA	3115	1/1	0.49	-	39,39,39,39	0
60	MG	BA	3243	1/1	0.45	-	25,25,25,25	0
60	MG	DA	3687	1/1	0.18	-	43,43,43,43	0
60	MG	DA	3030	1/1	0.66	-	59,59,59,59	0
60	MG	AA	1965	1/1	1.12	-	97,97,97,97	0
60	MG	BA	3578	1/1	0.18	-	76,76,76,76	0
60	MG	AA	1835	1/1	1.89	-	102,102,102,102	0
60	MG	DA	3086	1/1	0.24	-	60,60,60,60	0
60	MG	CA	1694	1/1	0.18	-	93,93,93,93	0
60	MG	BA	3476	1/1	0.24	-	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3457	1/1	0.66	-	68,68,68,68	0
60	MG	DA	3075	1/1	0.14	-	98,98,98,98	0
60	MG	BA	3421	1/1	0.32	-	68,68,68,68	0
60	MG	DA	3080	1/1	0.22	-	56,56,56,56	0
60	MG	DA	3185	1/1	0.23	-	79,79,79,79	0
60	MG	DA	3409	1/1	0.18	-	53,53,53,53	1
60	MG	DA	3451	1/1	0.14	-	80,80,80,80	1
60	MG	DA	2967	1/1	0.28	-	35,35,35,35	1
60	MG	DA	3200	1/1	0.55	-	62,62,62,62	0
60	MG	BA	3247	1/1	0.17	-	62,62,62,62	1
60	MG	BA	2952	1/1	0.41	-	96,96,96,96	0
60	MG	BA	3135	1/1	0.24	-	86,86,86,86	0
60	MG	BA	3000	1/1	0.11	-	80,80,80,80	0
60	MG	BA	3370	1/1	0.55	-	105,105,105,105	0
60	MG	DA	3722	1/1	0.49	-	86,86,86,86	0
60	MG	CA	1655	1/1	0.26	-	84,84,84,84	0
60	MG	DA	3607	1/1	0.26	-	104,104,104,104	0
60	MG	DA	3388	1/1	0.65	-	78,78,78,78	0
60	MG	AA	1898	1/1	0.29	-	65,65,65,65	0
60	MG	DA	3031	1/1	0.38	-	51,51,51,51	0
60	MG	AA	1933	1/1	0.24	-	67,67,67,67	0
60	MG	DE	301	1/1	0.42	-	67,67,67,67	0
60	MG	DR	202	1/1	0.37	-	65,65,65,65	1
60	MG	DA	3541	1/1	0.22	-	96,96,96,96	0
60	MG	AA	1640	1/1	1.58	-	127,127,127,127	0
60	MG	DA	3375	1/1	0.41	-	57,57,57,57	0
60	MG	CA	1679	1/1	0.17	-	65,65,65,65	1
60	MG	AA	1805	1/1	0.16	-	102,102,102,102	0
60	MG	BA	3191	1/1	0.72	-	78,78,78,78	0
60	MG	AA	1654	1/1	0.11	-	58,58,58,58	1
60	MG	AA	1873	1/1	0.34	-	117,117,117,117	0
60	MG	BA	3253	1/1	0.33	-	52,52,52,52	1
60	MG	DA	3137	1/1	0.27	-	70,70,70,70	0
60	MG	AY	102	1/1	0.75	-	104,104,104,104	1
60	MG	BA	3592	1/1	0.24	-	100,100,100,100	0
60	MG	AA	1808	1/1	0.48	-	57,57,57,57	0
60	MG	BA	3520	1/1	0.20	-	80,80,80,80	0
60	MG	DA	2925	1/1	1.00	-	108,108,108,108	0
60	MG	CA	1615	1/1	1.43	-	104,104,104,104	0
60	MG	AA	1821	1/1	0.40	-	65,65,65,65	0
60	MG	DA	3310	1/1	0.41	-	90,90,90,90	1
60	MG	DA	3437	1/1	0.17	-	12,12,12,12	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1632	1/1	0.26	-	97,97,97,97	0
60	MG	DA	2988	1/1	0.59	-	40,40,40,40	1
60	MG	DA	3733	1/1	0.14	-	43,43,43,43	0
60	MG	DA	3664	1/1	0.19	-	85,85,85,85	0
60	MG	DB	205	1/1	0.51	-	82,82,82,82	0
60	MG	CA	1642	1/1	0.22	-	85,85,85,85	0
60	MG	BA	2905	1/1	0.36	-	52,52,52,52	0
60	MG	BA	3402	1/1	0.44	-	37,37,37,37	0
60	MG	DA	3508	1/1	0.29	-	88,88,88,88	0
60	MG	AA	1736	1/1	1.31	-	101,101,101,101	0
60	MG	DA	3000	1/1	0.07	-	105,105,105,105	0
60	MG	DA	3124	1/1	0.52	-	81,81,81,81	0
60	MG	DA	3519	1/1	0.35	-	77,77,77,77	0
60	MG	D2	101	1/1	0.36	-	62,62,62,62	0
60	MG	BA	2962	1/1	0.57	-	70,70,70,70	0
60	MG	DA	2945	1/1	0.67	-	102,102,102,102	0
60	MG	AA	1901	1/1	0.70	-	65,65,65,65	0
60	MG	DA	3149	1/1	0.30	-	26,26,26,26	0
60	MG	BA	2947	1/1	0.31	-	45,45,45,45	0
60	MG	BA	3120	1/1	0.14	-	101,101,101,101	0
60	MG	BA	2971	1/1	1.01	-	92,92,92,92	0
60	MG	DA	3370	1/1	0.54	-	68,68,68,68	0
60	MG	DA	2947	1/1	0.12	-	86,86,86,86	0
60	MG	BA	3301	1/1	0.59	-	67,67,67,67	0
60	MG	DA	3561	1/1	0.45	-	81,81,81,81	1
60	MG	DA	3333	1/1	0.35	-	55,55,55,55	0
60	MG	DA	2905	1/1	0.10	-	80,80,80,80	0
60	MG	BA	2941	1/1	0.30	-	62,62,62,62	0
60	MG	AA	1957	1/1	0.77	-	75,75,75,75	0
60	MG	DA	3305	1/1	0.55	-	52,52,52,52	0
60	MG	BA	2916	1/1	0.34	-	78,78,78,78	0
60	MG	BA	3323	1/1	0.51	-	36,36,36,36	0
60	MG	BA	3344	1/1	0.51	-	45,45,45,45	0
60	MG	BA	3438	1/1	0.24	-	29,29,29,29	0
60	MG	BA	3237	1/1	0.23	-	58,58,58,58	0
60	MG	DA	3264	1/1	0.29	-	47,47,47,47	1
60	MG	DA	2917	1/1	0.91	-	89,89,89,89	0
60	MG	DA	3453	1/1	0.26	-	84,84,84,84	0
60	MG	DP	202	1/1	0.63	-	49,49,49,49	1
60	MG	AA	1793	1/1	0.19	-	75,75,75,75	0
60	MG	BA	3596	1/1	1.12	-	107,107,107,107	0
60	MG	DA	3490	1/1	0.12	-	29,29,29,29	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3129	1/1	0.38	-	72,72,72,72	0
60	MG	DA	3612	1/1	0.53	-	77,77,77,77	0
60	MG	DA	3488	1/1	0.32	-	28,28,28,28	0
60	MG	AA	1765	1/1	0.09	-	107,107,107,107	1
60	MG	AA	1922	1/1	0.40	-	82,82,82,82	0
60	MG	DU	202	1/1	0.26	-	8,8,8,8	1
60	MG	BA	3188	1/1	0.09	-	58,58,58,58	0
60	MG	DA	3071	1/1	0.30	-	71,71,71,71	0
60	MG	BA	2998	1/1	0.22	-	54,54,54,54	0
60	MG	DA	3102	1/1	0.32	-	86,86,86,86	0
60	MG	BA	3351	1/1	0.31	-	26,26,26,26	0
60	MG	CA	1678	1/1	0.12	-	45,45,45,45	1
60	MG	DA	3352	1/1	0.27	-	58,58,58,58	0
60	MG	BA	3215	1/1	0.57	-	4,4,4,4	1
60	MG	DA	3038	1/1	0.35	-	32,32,32,32	0
60	MG	BA	3172	1/1	0.42	-	80,80,80,80	0
60	MG	BA	3489	1/1	0.10	-	22,22,22,22	0
60	MG	DA	3468	1/1	0.38	-	76,76,76,76	0
60	MG	AA	1907	1/1	0.43	-	96,96,96,96	0
60	MG	DA	3174	1/1	0.43	-	93,93,93,93	0
60	MG	BY	201	1/1	0.26	-	50,50,50,50	0
60	MG	DA	3355	1/1	0.13	-	80,80,80,80	0
60	MG	DA	2963	1/1	0.34	-	39,39,39,39	1
60	MG	BA	3185	1/1	0.36	-	75,75,75,75	0
60	MG	BA	3292	1/1	0.23	-	29,29,29,29	0
60	MG	DA	3087	1/1	0.32	-	33,33,33,33	0
60	MG	DA	3225	1/1	0.44	-	32,32,32,32	0
60	MG	BA	3060	1/1	1.07	-	98,98,98,98	0
60	MG	CA	1743	1/1	1.95	-	81,81,81,81	0
60	MG	BA	3314	1/1	0.49	-	29,29,29,29	0
60	MG	DA	3452	1/1	0.41	-	30,30,30,30	0
60	MG	DA	3133	1/1	0.88	-	120,120,120,120	0
60	MG	BA	3457	1/1	0.52	-	72,72,72,72	0
60	MG	BA	3426	1/1	0.77	-	77,77,77,77	0
60	MG	DA	3686	1/1	0.34	-	107,107,107,107	0
60	MG	DA	3713	1/1	0.17	-	67,67,67,67	0
60	MG	CA	1688	1/1	0.12	-	79,79,79,79	0
60	MG	AA	1880	1/1	0.52	-	102,102,102,102	0
60	MG	BA	3311	1/1	0.35	-	80,80,80,80	0
60	MG	DA	2935	1/1	1.27	-	12,12,12,12	1
60	MG	DA	3458	1/1	0.49	-	59,59,59,59	0
60	MG	DA	3572	1/1	0.39	-	56,56,56,56	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3231	1/1	0.43	-	98,98,98,98	0
60	MG	DA	3543	1/1	0.33	-	71,71,71,71	0
60	MG	BA	3213	1/1	0.57	-	135,135,135,135	0
60	MG	CA	1725	1/1	0.41	-	76,76,76,76	1
60	MG	BA	3248	1/1	0.35	-	101,101,101,101	0
60	MG	BA	3319	1/1	0.51	-	33,33,33,33	0
60	MG	DA	3346	1/1	0.37	-	59,59,59,59	0
60	MG	BA	3525	1/1	0.26	-	44,44,44,44	0
60	MG	BA	3425	1/1	0.44	-	48,48,48,48	0
60	MG	CA	1674	1/1	0.18	-	90,90,90,90	0
60	MG	CA	1607	1/1	0.13	-	94,94,94,94	0
60	MG	BA	3410	1/1	0.49	-	42,42,42,42	0
60	MG	BA	3204	1/1	0.87	-	71,71,71,71	0
60	MG	DA	3555	1/1	1.04	-	105,105,105,105	0
60	MG	AA	1760	1/1	0.39	-	45,45,45,45	0
60	MG	CA	1653	1/1	0.35	-	39,39,39,39	0
60	MG	CA	1768	1/1	0.17	-	71,71,71,71	0
60	MG	DA	3069	1/1	0.18	-	50,50,50,50	0
60	MG	AA	1617	1/1	0.16	-	109,109,109,109	0
60	MG	CA	1692	1/1	0.20	-	140,140,140,140	0
60	MG	DB	208	1/1	0.16	-	86,86,86,86	0
60	MG	DA	2929	1/1	0.24	-	10,10,10,10	1
60	MG	DA	3688	1/1	0.32	-	107,107,107,107	1
60	MG	DA	3398	1/1	0.44	-	31,31,31,31	1
60	MG	DA	3381	1/1	0.67	-	43,43,43,43	0
60	MG	DA	3179	1/1	0.51	-	66,66,66,66	0
60	MG	BA	3278	1/1	0.36	-	71,71,71,71	0
60	MG	DA	3373	1/1	0.66	-	75,75,75,75	0
60	MG	DA	3163	1/1	0.32	-	49,49,49,49	0
60	MG	CA	1617	1/1	0.07	-	66,66,66,66	0
60	MG	CA	1714	1/1	0.56	-	83,83,83,83	0
60	MG	CA	1689	1/1	0.13	-	96,96,96,96	1
60	MG	DA	3425	1/1	0.23	-	56,56,56,56	0
60	MG	AA	1732	1/1	0.11	-	52,52,52,52	0
60	MG	BA	3372	1/1	0.37	-	70,70,70,70	0
60	MG	DA	2926	1/1	0.41	-	45,45,45,45	1
60	MG	AA	1676	1/1	0.27	-	68,68,68,68	0
60	MG	DA	3728	1/1	0.45	-	46,46,46,46	1
60	MG	BA	3181	1/1	0.52	-	42,42,42,42	0
60	MG	AA	1815	1/1	0.29	-	76,76,76,76	0
60	MG	DA	3482	1/1	0.27	-	37,37,37,37	1
60	MG	DA	3647	1/1	0.47	-	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1661	1/1	0.41	-	34,34,34,34	1
60	MG	BA	3250	1/1	0.27	-	51,51,51,51	0
60	MG	DA	3416	1/1	0.33	-	35,35,35,35	0
60	MG	CA	1687	1/1	0.08	-	63,63,63,63	0
60	MG	AA	1855	1/1	0.29	-	69,69,69,69	0
60	MG	DA	2952	1/1	0.48	-	44,44,44,44	0
60	MG	BA	3044	1/1	0.57	-	64,64,64,64	0
60	MG	BA	3609	1/1	0.24	-	56,56,56,56	0
60	MG	DA	3177	1/1	0.21	-	71,71,71,71	0
60	MG	BA	3209	1/1	0.29	-	61,61,61,61	0
60	MG	DA	3134	1/1	0.31	-	74,74,74,74	0
60	MG	DA	3486	1/1	0.60	-	38,38,38,38	0
60	MG	AA	1857	1/1	0.17	-	57,57,57,57	0
60	MG	DF	302	1/1	1.39	-	98,98,98,98	0
60	MG	DA	3570	1/1	0.37	-	62,62,62,62	0
60	MG	DA	3324	1/1	0.30	-	66,66,66,66	1
60	MG	DA	3787	1/1	0.52	-	95,95,95,95	0
60	MG	DA	3041	1/1	0.20	-	78,78,78,78	0
60	MG	DA	3740	1/1	0.25	-	50,50,50,50	0
60	MG	DA	2991	1/1	0.29	-	44,44,44,44	1
60	MG	BA	3423	1/1	0.32	-	67,67,67,67	1
60	MG	DA	3261	1/1	0.73	-	34,34,34,34	1
60	MG	BA	3517	1/1	0.26	-	98,98,98,98	0
60	MG	AA	1648	1/1	0.89	-	108,108,108,108	0
60	MG	AA	1673	1/1	0.89	-	90,90,90,90	0
60	MG	DA	3367	1/1	0.59	-	28,28,28,28	1
60	MG	BA	3362	1/1	0.50	-	43,43,43,43	0
60	MG	BA	3557	1/1	0.89	-	37,37,37,37	1
60	MG	BA	3552	1/1	0.14	-	54,54,54,54	1
60	MG	DA	3085	1/1	0.14	-	68,68,68,68	0
60	MG	CA	1744	1/1	0.24	-	57,57,57,57	0
60	MG	DA	3685	1/1	0.15	-	69,69,69,69	0
60	MG	DA	2966	1/1	0.94	-	51,51,51,51	1
60	MG	AA	1615	1/1	1.12	-	67,67,67,67	0
60	MG	BA	3017	1/1	0.98	-	93,93,93,93	0
60	MG	BA	3339	1/1	0.81	-	63,63,63,63	1
60	MG	DA	3233	1/1	0.18	-	152,152,152,152	0
60	MG	DA	3159	1/1	0.39	-	85,85,85,85	0
60	MG	DA	3150	1/1	0.16	-	98,98,98,98	0
60	MG	CA	1631	1/1	0.32	-	59,59,59,59	0
60	MG	BA	2972	1/1	0.43	-	63,63,63,63	1
60	MG	DB	207	1/1	0.40	-	53,53,53,53	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1902	1/1	0.10	-	90,90,90,90	0
60	MG	BA	3165	1/1	0.62	-	77,77,77,77	0
60	MG	DA	3252	1/1	0.18	-	87,87,87,87	0
60	MG	BA	3221	1/1	0.58	-	42,42,42,42	0
60	MG	AA	1781	1/1	0.33	-	111,111,111,111	0
60	MG	AP	101	1/1	0.14	-	93,93,93,93	0
60	MG	BA	3506	1/1	0.17	-	42,42,42,42	0
60	MG	DA	3626	1/1	0.27	-	34,34,34,34	0
60	MG	BA	2978	1/1	0.42	-	75,75,75,75	0
60	MG	CA	1720	1/1	0.26	-	106,106,106,106	0
60	MG	BA	3101	1/1	0.40	-	79,79,79,79	0
60	MG	AA	1729	1/1	0.24	-	50,50,50,50	0
60	MG	BN	201	1/1	0.45	-	64,64,64,64	0
60	MG	AA	1612	1/1	0.08	-	55,55,55,55	0
60	MG	CA	1756	1/1	0.66	-	87,87,87,87	0
60	MG	CA	1758	1/1	0.44	-	126,126,126,126	0
60	MG	BA	3337	1/1	0.73	-	37,37,37,37	0
60	MG	DA	3275	1/1	0.24	-	63,63,63,63	0
60	MG	DA	2932	1/1	0.22	-	1,1,1,1	1
60	MG	AA	1719	1/1	0.82	-	76,76,76,76	1
60	MG	AA	1701	1/1	0.32	-	77,77,77,77	0
60	MG	AA	1929	1/1	0.26	-	69,69,69,69	0
60	MG	DA	3224	1/1	0.34	-	85,85,85,85	0
60	MG	BA	3478	1/1	0.42	-	28,28,28,28	0
60	MG	DA	3247	1/1	0.56	-	41,41,41,41	0
60	MG	CA	1765	1/1	0.97	-	94,94,94,94	0
60	MG	BA	3388	1/1	0.56	-	100,100,100,100	0
60	MG	BA	3274	1/1	0.44	-	83,83,83,83	0
60	MG	DA	3497	1/1	0.32	-	103,103,103,103	0
60	MG	BA	3246	1/1	0.24	-	68,68,68,68	0
60	MG	BA	3598	1/1	0.48	-	110,110,110,110	0
60	MG	AA	1969	1/1	0.68	-	83,83,83,83	0
60	MG	AA	1913	1/1	0.11	-	72,72,72,72	0
60	MG	DA	3605	1/1	0.31	-	63,63,63,63	0
60	MG	DA	2911	1/1	0.58	-	91,91,91,91	0
60	MG	BQ	201	1/1	0.29	-	72,72,72,72	0
60	MG	BA	3325	1/1	0.38	-	84,84,84,84	0
60	MG	BA	2945	1/1	0.46	-	113,113,113,113	0
60	MG	BA	3408	1/1	0.38	-	73,73,73,73	0
60	MG	BA	3356	1/1	0.28	-	45,45,45,45	0
60	MG	DA	3739	1/1	0.27	-	95,95,95,95	0
60	MG	DA	3446	1/1	0.36	-	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3202	1/1	0.27	-	24,24,24,24	0
60	MG	BA	2973	1/1	0.88	-	85,85,85,85	0
60	MG	AA	1745	1/1	0.57	-	50,50,50,50	1
60	MG	DB	206	1/1	0.09	-	65,65,65,65	1
60	MG	AA	1878	1/1	0.16	-	76,76,76,76	0
60	MG	DA	3384	1/1	0.76	-	120,120,120,120	0
60	MG	CA	1733	1/1	0.17	-	76,76,76,76	0
60	MG	BA	3069	1/1	0.58	-	100,100,100,100	0
60	MG	DA	3164	1/1	0.26	-	55,55,55,55	0
60	MG	DA	3394	1/1	0.30	-	63,63,63,63	0
60	MG	DA	3329	1/1	0.44	-	110,110,110,110	0
60	MG	DA	3166	1/1	0.26	-	30,30,30,30	0
60	MG	BA	3094	1/1	0.40	-	32,32,32,32	0
60	MG	BA	3399	1/1	0.69	-	146,146,146,146	0
60	MG	DA	3301	1/1	0.17	-	32,32,32,32	0
60	MG	DA	3035	1/1	0.30	-	84,84,84,84	0
60	MG	DA	3611	1/1	0.45	-	31,31,31,31	0
60	MG	BA	3257	1/1	0.72	-	42,42,42,42	0
60	MG	BA	3040	1/1	0.62	-	79,79,79,79	0
60	MG	DA	3548	1/1	0.44	-	50,50,50,50	1
60	MG	DA	3072	1/1	0.41	-	81,81,81,81	0
60	MG	DA	3121	1/1	0.35	-	69,69,69,69	0
60	MG	DA	3417	1/1	0.56	-	48,48,48,48	1
60	MG	BA	3214	1/1	0.60	-	85,85,85,85	0
60	MG	AA	1844	1/1	0.22	-	107,107,107,107	0
60	MG	AA	1653	1/1	0.06	-	68,68,68,68	1
60	MG	BA	3365	1/1	1.13	-	112,112,112,112	0
60	MG	AA	1718	1/1	0.23	-	98,98,98,98	0
60	MG	DA	3249	1/1	0.34	-	68,68,68,68	0
60	MG	BA	3604	1/1	0.67	-	82,82,82,82	0
60	MG	AA	1669	1/1	0.28	-	50,50,50,50	0
60	MG	DA	3700	1/1	0.32	-	59,59,59,59	0
60	MG	BA	3450	1/1	0.60	-	60,60,60,60	0
60	MG	BA	2954	1/1	0.27	-	59,59,59,59	0
60	MG	DA	3709	1/1	0.25	-	61,61,61,61	0
60	MG	DA	3692	1/1	0.87	-	61,61,61,61	0
60	MG	AA	1868	1/1	0.29	-	100,100,100,100	0
60	MG	DT	201	1/1	0.66	-	5,5,5,5	1
60	MG	DA	3785	1/1	1.00	-	35,35,35,35	1
60	MG	DP	203	1/1	0.33	-	53,53,53,53	0
60	MG	DE	304	1/1	0.35	-	22,22,22,22	0
60	MG	BA	3081	1/1	0.59	-	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3623	1/1	0.15	-	28,28,28,28	0
60	MG	DA	3741	1/1	0.27	-	43,43,43,43	0
60	MG	AA	1854	1/1	0.20	-	71,71,71,71	0
60	MG	CA	1698	1/1	0.66	-	73,73,73,73	1
60	MG	DA	3139	1/1	0.28	-	89,89,89,89	0
60	MG	BA	3543	1/1	0.61	-	71,71,71,71	0
60	MG	BP	204	1/1	0.25	-	24,24,24,24	1
60	MG	AA	1703	1/1	0.17	-	44,44,44,44	1
60	MG	BA	3404	1/1	0.29	-	34,34,34,34	0
60	MG	AA	1699	1/1	0.18	-	71,71,71,71	0
60	MG	DA	3278	1/1	0.29	-	57,57,57,57	0
60	MG	AA	1607	1/1	0.28	-	73,73,73,73	0
60	MG	CA	1639	1/1	0.22	-	95,95,95,95	0
60	MG	AA	1858	1/1	0.27	-	60,60,60,60	0
60	MG	DA	2909	1/1	0.51	-	83,83,83,83	0
60	MG	BA	3383	1/1	0.12	-	126,126,126,126	0
60	MG	DA	3429	1/1	0.62	-	23,23,23,23	1
60	MG	AA	1970	1/1	0.33	-	107,107,107,107	0
60	MG	BA	3384	1/1	0.74	-	95,95,95,95	0
60	MG	AA	1768	1/1	0.89	-	107,107,107,107	0
60	MG	BA	3412	1/1	0.35	-	95,95,95,95	0
60	MG	DR	201	1/1	0.24	-	108,108,108,108	0
60	MG	AQ	202	1/1	0.47	-	97,97,97,97	0
60	MG	DA	3257	1/1	0.68	-	29,29,29,29	0
60	MG	AL	206	1/1	0.19	-	53,53,53,53	1
60	MG	CA	1633	1/1	0.10	-	70,70,70,70	0
60	MG	AA	1685	1/1	0.38	-	30,30,30,30	1
60	MG	AA	1967	1/1	0.26	-	67,67,67,67	0
60	MG	DA	3376	1/1	0.81	-	93,93,93,93	0
60	MG	BA	2994	1/1	0.48	-	80,80,80,80	0
60	MG	BD	304	1/1	0.32	-	49,49,49,49	0
60	MG	AA	1817	1/1	0.16	-	71,71,71,71	0
60	MG	DA	3602	1/1	0.32	-	76,76,76,76	0
60	MG	BA	3033	1/1	0.33	-	69,69,69,69	0
60	MG	BA	3150	1/1	0.41	-	145,145,145,145	0
60	MG	DA	3207	1/1	0.19	-	84,84,84,84	0
60	MG	DA	3358	1/1	0.31	-	93,93,93,93	0
60	MG	BA	3443	1/1	0.19	-	76,76,76,76	0
60	MG	DA	3609	1/1	0.53	-	63,63,63,63	0
60	MG	AA	1628	1/1	0.10	-	84,84,84,84	0
60	MG	DA	3712	1/1	0.85	-	108,108,108,108	0
60	MG	CA	1750	1/1	1.07	-	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1622	1/1	0.72	-	99,99,99,99	0
60	MG	DA	3167	1/1	0.29	-	40,40,40,40	0
60	MG	AA	1838	1/1	0.81	-	80,80,80,80	0
60	MG	BA	3290	1/1	0.33	-	86,86,86,86	0
60	MG	DA	3495	1/1	0.64	-	75,75,75,75	0
60	MG	AA	1715	1/1	0.98	-	126,126,126,126	0
60	MG	DA	3424	1/1	0.99	-	84,84,84,84	0
60	MG	DA	3392	1/1	0.38	-	81,81,81,81	0
60	MG	BD	303	1/1	0.20	-	35,35,35,35	0
60	MG	BA	3098	1/1	0.43	-	62,62,62,62	0
60	MG	AA	1896	1/1	0.20	-	78,78,78,78	0
60	MG	DA	3065	1/1	0.69	-	128,128,128,128	0
60	MG	CA	1779	1/1	0.53	-	102,102,102,102	0
60	MG	DA	3012	1/1	0.59	-	30,30,30,30	0
60	MG	DA	3418	1/1	0.17	-	88,88,88,88	0
60	MG	BA	3167	1/1	0.28	-	36,36,36,36	0
60	MG	BA	2938	1/1	0.18	-	64,64,64,64	1
60	MG	DA	3793	1/1	0.31	-	130,130,130,130	0
60	MG	CV	105	1/1	0.18	-	82,82,82,82	0
60	MG	DA	3289	1/1	0.58	-	78,78,78,78	0
60	MG	AA	1756	1/1	0.22	-	91,91,91,91	0
60	MG	BA	3251	1/1	0.43	-	100,100,100,100	0
60	MG	AD	304	1/1	0.12	-	135,135,135,135	0
60	MG	CC	303	1/1	0.18	-	113,113,113,113	0
60	MG	DA	3313	1/1	0.22	-	101,101,101,101	0
60	MG	CA	1770	1/1	0.61	-	54,54,54,54	1
60	MG	BA	3056	1/1	0.22	-	156,156,156,156	0
60	MG	AA	1786	1/1	0.14	-	123,123,123,123	0
60	MG	AA	1744	1/1	0.14	-	80,80,80,80	0
60	MG	BA	3342	1/1	0.59	-	127,127,127,127	0
60	MG	DA	3396	1/1	0.29	-	62,62,62,62	0
60	MG	AA	1939	1/1	0.28	-	74,74,74,74	1
60	MG	BA	3427	1/1	0.57	-	63,63,63,63	0
60	MG	CA	1649	1/1	0.90	-	92,92,92,92	0
60	MG	BA	3507	1/1	0.41	-	55,55,55,55	0
60	MG	AA	1664	1/1	0.09	-	17,17,17,17	1
60	MG	AA	1623	1/1	0.93	-	66,66,66,66	0
60	MG	BA	3541	1/1	0.92	-	82,82,82,82	0
60	MG	DA	3583	1/1	0.44	-	64,64,64,64	0
60	MG	BA	3178	1/1	0.92	-	79,79,79,79	0
60	MG	BA	3482	1/1	0.43	-	144,144,144,144	0
60	MG	BA	3184	1/1	0.34	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3621	1/1	0.33	-	76,76,76,76	1
60	MG	DA	3448	1/1	0.21	-	55,55,55,55	0
60	MG	DA	3186	1/1	0.16	-	42,42,42,42	0
60	MG	AA	1934	1/1	0.22	-	68,68,68,68	0
60	MG	BA	3132	1/1	0.42	-	81,81,81,81	0
60	MG	DA	3196	1/1	0.26	-	100,100,100,100	0
60	MG	BA	3186	1/1	0.11	-	81,81,81,81	0
60	MG	DA	3180	1/1	0.33	-	115,115,115,115	0
60	MG	BA	3239	1/1	0.29	-	77,77,77,77	0
60	MG	DA	2990	1/1	0.47	-	43,43,43,43	1
60	MG	BA	3307	1/1	0.41	-	75,75,75,75	0
60	MG	AA	1651	1/1	0.19	-	76,76,76,76	0
60	MG	AA	1720	1/1	0.41	-	37,37,37,37	1
60	MG	DA	2978	1/1	0.32	-	33,33,33,33	0
60	MG	DA	2907	1/1	0.41	-	83,83,83,83	0
60	MG	CA	1619	1/1	0.20	-	116,116,116,116	0
60	MG	DA	3156	1/1	0.59	-	73,73,73,73	0
60	MG	DA	3472	1/1	0.36	-	79,79,79,79	1
60	MG	BH	201	1/1	0.30	-	71,71,71,71	1
60	MG	DA	3645	1/1	0.29	-	78,78,78,78	0
60	MG	BA	3230	1/1	0.43	-	85,85,85,85	0
60	MG	BA	3491	1/1	0.15	-	70,70,70,70	0
60	MG	BA	3298	1/1	0.24	-	67,67,67,67	0
60	MG	BA	3380	1/1	0.92	-	133,133,133,133	0
60	MG	CA	1723	1/1	0.43	-	82,82,82,82	0
60	MG	AA	1841	1/1	0.42	-	42,42,42,42	0
60	MG	DA	3608	1/1	0.35	-	61,61,61,61	0
60	MG	DA	3432	1/1	0.48	-	86,86,86,86	1
60	MG	DA	3287	1/1	0.14	-	66,66,66,66	0
60	MG	BA	3553	1/1	0.30	-	106,106,106,106	0
60	MG	BA	3513	1/1	0.35	-	77,77,77,77	0
60	MG	DA	2920	1/1	0.21	-	15,15,15,15	1
60	MG	BA	3569	1/1	1.01	-	113,113,113,113	0
60	MG	DA	3598	1/1	0.72	-	83,83,83,83	0
60	MG	DA	3765	1/1	0.55	-	69,69,69,69	0
60	MG	BA	3498	1/1	0.97	-	85,85,85,85	1
60	MG	AA	1609	1/1	0.49	-	59,59,59,59	0
60	MG	BA	3096	1/1	0.90	-	102,102,102,102	0
60	MG	DA	3680	1/1	0.73	-	98,98,98,98	0
60	MG	BA	3448	1/1	0.40	-	40,40,40,40	0
60	MG	AA	1826	1/1	0.14	-	83,83,83,83	0
60	MG	AA	1900	1/1	0.17	-	128,128,128,128	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3435	1/1	0.26	-	47,47,47,47	0
60	MG	BA	3260	1/1	0.34	-	77,77,77,77	0
60	MG	DA	3199	1/1	0.38	-	30,30,30,30	0
60	MG	CA	1672	1/1	0.19	-	92,92,92,92	0
60	MG	AA	1802	1/1	0.28	-	119,119,119,119	0
60	MG	AA	1812	1/1	1.02	-	70,70,70,70	0
60	MG	DA	3241	1/1	0.46	-	34,34,34,34	1
60	MG	DA	3015	1/1	0.44	-	81,81,81,81	0
60	MG	DA	3173	1/1	0.44	-	48,48,48,48	0
60	MG	AA	1751	1/1	0.07	-	104,104,104,104	0
60	MG	BA	3264	1/1	0.36	-	42,42,42,42	0
60	MG	DA	3117	1/1	0.41	-	88,88,88,88	0
60	MG	DA	3427	1/1	0.39	-	78,78,78,78	0
60	MG	CA	1727	1/1	0.13	-	74,74,74,74	0
60	MG	DA	3095	1/1	0.55	-	42,42,42,42	0
60	MG	AA	1686	1/1	0.17	-	81,81,81,81	0
60	MG	DA	2942	1/1	0.74	-	27,27,27,27	1
60	MG	BA	3452	1/1	0.45	-	45,45,45,45	0
60	MG	DA	2996	1/1	0.49	-	71,71,71,71	1
60	MG	DA	3637	1/1	1.04	-	88,88,88,88	0
60	MG	DA	3079	1/1	0.63	-	127,127,127,127	0
60	MG	DA	3387	1/1	0.39	-	77,77,77,77	0
60	MG	DA	3068	1/1	0.32	-	51,51,51,51	0
60	MG	DA	2979	1/1	0.33	-	42,42,42,42	0
60	MG	DA	3090	1/1	0.22	-	35,35,35,35	0
60	MG	DA	3366	1/1	0.62	-	9,9,9,9	1
60	MG	DA	2984	1/1	0.41	-	66,66,66,66	1
60	MG	BA	3316	1/1	0.61	-	98,98,98,98	0
60	MG	CH	201	1/1	0.55	-	37,37,37,37	1
60	MG	DA	3771	1/1	0.65	-	71,71,71,71	0
60	MG	DA	3118	1/1	0.15	-	63,63,63,63	0
60	MG	AA	1870	1/1	0.36	-	73,73,73,73	0
60	MG	AA	1778	1/1	0.10	-	84,84,84,84	0
60	MG	BA	3222	1/1	1.02	-	108,108,108,108	0
60	MG	CA	1682	1/1	0.34	-	53,53,53,53	0
60	MG	DA	3138	1/1	0.97	-	139,139,139,139	0
60	MG	BA	3581	1/1	1.40	-	95,95,95,95	0
60	MG	BA	3544	1/1	0.28	-	62,62,62,62	0
60	MG	BA	3326	1/1	0.55	-	77,77,77,77	0
60	MG	DA	3128	1/1	0.30	-	86,86,86,86	0
60	MG	DA	3670	1/1	0.50	-	88,88,88,88	0
60	MG	BA	3465	1/1	0.54	-	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3039	1/1	0.36	-	88,88,88,88	0
60	MG	DA	3532	1/1	0.27	-	79,79,79,79	0
60	MG	BA	3119	1/1	0.33	-	30,30,30,30	0
60	MG	DA	3672	1/1	0.23	-	74,74,74,74	0
60	MG	BA	2955	1/1	0.67	-	84,84,84,84	0
60	MG	AH	201	1/1	0.85	-	102,102,102,102	0
60	MG	BA	3276	1/1	0.87	-	125,125,125,125	0
60	MG	DA	3187	1/1	0.55	-	44,44,44,44	0
60	MG	DA	3151	1/1	0.82	-	73,73,73,73	0
60	MG	CA	1761	1/1	0.26	-	87,87,87,87	0
60	MG	DA	3619	1/1	0.28	-	69,69,69,69	0
60	MG	DA	3259	1/1	0.48	-	32,32,32,32	0
60	MG	DA	3411	1/1	0.17	-	67,67,67,67	1
60	MG	BA	3227	1/1	0.23	-	78,78,78,78	0
60	MG	CA	1706	1/1	0.09	-	47,47,47,47	0
60	MG	DA	3470	1/1	0.57	-	75,75,75,75	0
60	MG	BA	3210	1/1	0.51	-	106,106,106,106	0
60	MG	BA	3122	1/1	0.73	-	106,106,106,106	0
60	MG	DA	3320	1/1	0.14	-	78,78,78,78	0
60	MG	DA	2916	1/1	0.15	-	57,57,57,57	0
60	MG	DA	3082	1/1	0.17	-	82,82,82,82	0
60	MG	AA	1968	1/1	0.49	-	95,95,95,95	0
60	MG	AA	1645	1/1	0.95	-	56,56,56,56	1
60	MG	BA	2911	1/1	0.30	-	94,94,94,94	0
60	MG	AA	1891	1/1	0.35	-	54,54,54,54	1
60	MG	CA	1702	1/1	0.16	-	104,104,104,104	0
60	MG	BA	3403	1/1	0.15	-	69,69,69,69	0
60	MG	DA	3534	1/1	0.60	-	73,73,73,73	1
60	MG	BA	3464	1/1	0.50	-	43,43,43,43	0
60	MG	DA	2986	1/1	0.18	-	142,142,142,142	0
60	MG	DA	3768	1/1	0.07	-	58,58,58,58	1
60	MG	DA	3773	1/1	0.26	-	90,90,90,90	0
60	MG	BA	3266	1/1	0.19	-	65,65,65,65	0
60	MG	DA	2922	1/1	0.31	-	65,65,65,65	0
60	MG	CA	1646	1/1	0.78	-	102,102,102,102	0
60	MG	DA	3153	1/1	0.50	-	68,68,68,68	0
60	MG	CA	1732	1/1	0.20	-	70,70,70,70	0
60	MG	AA	1846	1/1	0.43	-	45,45,45,45	0
60	MG	CA	1638	1/1	0.29	-	61,61,61,61	0
60	MG	DA	3667	1/1	0.45	-	46,46,46,46	1
60	MG	CA	1772	1/1	0.12	-	79,79,79,79	0
60	MG	CA	1777	1/1	0.18	-	125,125,125,125	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1714	1/1	0.23	-	66,66,66,66	0
60	MG	BA	2917	1/1	0.25	-	84,84,84,84	0
60	MG	B5	102	1/1	0.21	-	32,32,32,32	1
60	MG	DB	201	1/1	0.17	-	59,59,59,59	0
60	MG	BA	3271	1/1	0.46	-	29,29,29,29	0
60	MG	CA	1612	1/1	0.27	-	58,58,58,58	0
60	MG	DA	3120	1/1	0.18	-	106,106,106,106	0
60	MG	CJ	201	1/1	0.42	-	115,115,115,115	0
60	MG	AA	1864	1/1	0.21	-	67,67,67,67	0
60	MG	BA	3052	1/1	0.41	-	64,64,64,64	0
60	MG	DA	3284	1/1	0.39	-	25,25,25,25	0
60	MG	BA	3244	1/1	0.47	-	88,88,88,88	0
60	MG	AA	1708	1/1	0.37	-	65,65,65,65	1
60	MG	BA	3310	1/1	0.58	-	68,68,68,68	0
60	MG	BA	2942	1/1	0.65	-	110,110,110,110	0
60	MG	BA	3014	1/1	0.39	-	79,79,79,79	0
60	MG	CY	101	1/1	0.33	-	143,143,143,143	0
60	MG	BA	3398	1/1	0.64	-	53,53,53,53	0
60	MG	AA	1861	1/1	0.55	-	77,77,77,77	0
60	MG	BA	3546	1/1	0.68	-	83,83,83,83	0
60	MG	AA	1852	1/1	0.37	-	56,56,56,56	0
60	MG	AA	1910	1/1	0.16	-	120,120,120,120	0
60	MG	BA	3233	1/1	0.15	-	73,73,73,73	0
60	MG	DA	3502	1/1	0.31	-	74,74,74,74	0
60	MG	DA	3737	1/1	0.77	-	74,74,74,74	0
60	MG	DA	3487	1/1	0.67	-	42,42,42,42	1
60	MG	DA	3116	1/1	0.16	-	78,78,78,78	0
60	MG	BA	3377	1/1	0.24	-	59,59,59,59	0
60	MG	DA	3743	1/1	0.26	-	50,50,50,50	1
60	MG	CA	1718	1/1	0.27	-	87,87,87,87	0
60	MG	DA	3657	1/1	0.29	-	59,59,59,59	0
60	MG	AA	1620	1/1	0.57	-	71,71,71,71	0
60	MG	DA	3024	1/1	0.24	-	92,92,92,92	0
60	MG	DA	2906	1/1	0.29	-	93,93,93,93	1
60	MG	BA	3027	1/1	0.33	-	74,74,74,74	0
60	MG	BA	3021	1/1	0.53	-	78,78,78,78	0
60	MG	AA	1956	1/1	0.57	-	58,58,58,58	0
60	MG	BA	3232	1/1	0.32	-	64,64,64,64	0
60	MG	DA	3469	1/1	0.34	-	65,65,65,65	0
60	MG	BA	3554	1/1	0.24	-	109,109,109,109	0
60	MG	BA	2922	1/1	1.10	-	95,95,95,95	0
60	MG	DA	3279	1/1	0.59	-	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1890	1/1	0.50	-	78,78,78,78	0
60	MG	DA	3236	1/1	0.37	-	63,63,63,63	0
60	MG	BA	3305	1/1	0.39	-	28,28,28,28	0
60	MG	DA	3106	1/1	0.23	-	77,77,77,77	0
60	MG	DA	3724	1/1	0.30	-	73,73,73,73	0
60	MG	BA	3529	1/1	0.69	-	70,70,70,70	0
60	MG	DA	3005	1/1	0.12	-	69,69,69,69	0
60	MG	BA	3441	1/1	0.16	-	40,40,40,40	0
60	MG	BA	3591	1/1	0.85	-	93,93,93,93	0
60	MG	DA	2915	1/1	0.35	-	48,48,48,48	0
60	MG	DP	206	1/1	0.95	-	82,82,82,82	0
60	MG	BA	3008	1/1	0.32	-	123,123,123,123	0
60	MG	DA	3704	1/1	0.22	-	74,74,74,74	0
60	MG	AA	1753	1/1	0.05	-	110,110,110,110	0
60	MG	DA	2914	1/1	0.61	-	83,83,83,83	0
60	MG	BA	3242	1/1	0.38	-	60,60,60,60	0
60	MG	DA	3184	1/1	0.24	-	63,63,63,63	0
60	MG	DA	3101	1/1	1.22	-	97,97,97,97	0
60	MG	DA	3545	1/1	0.10	-	58,58,58,58	0
60	MG	AA	1893	1/1	0.26	-	56,56,56,56	0
60	MG	DA	3699	1/1	0.16	-	62,62,62,62	0
60	MG	CA	1767	1/1	0.42	-	73,73,73,73	0
60	MG	DA	3498	1/1	0.42	-	82,82,82,82	0
60	MG	CA	1690	1/1	0.42	-	60,60,60,60	0
60	MG	DU	201	1/1	0.23	-	68,68,68,68	0
60	MG	BA	3510	1/1	0.67	-	41,41,41,41	0
60	MG	DN	202	1/1	0.58	-	78,78,78,78	0
60	MG	BA	3125	1/1	0.21	-	70,70,70,70	0
60	MG	AA	1613	1/1	0.90	-	74,74,74,74	0
60	MG	DA	3321	1/1	0.34	-	88,88,88,88	0
60	MG	BA	3211	1/1	0.19	-	67,67,67,67	0
60	MG	BA	3414	1/1	0.34	-	67,67,67,67	0
60	MG	AA	1853	1/1	0.27	-	74,74,74,74	0
60	MG	BA	2956	1/1	0.20	-	37,37,37,37	1
60	MG	CA	1635	1/1	0.20	-	93,93,93,93	0
60	MG	DA	3492	1/1	0.88	-	62,62,62,62	0
60	MG	AA	1927	1/1	0.12	-	113,113,113,113	0
60	MG	BA	2929	1/1	0.26	-	90,90,90,90	0
60	MG	DE	303	1/1	0.22	-	42,42,42,42	0
60	MG	DA	3512	1/1	0.45	-	104,104,104,104	0
60	MG	D5	103	1/1	0.12	-	88,88,88,88	0
60	MG	DA	3644	1/1	0.62	-	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1605	1/1	0.81	-	49,49,49,49	1
60	MG	BA	3066	1/1	0.67	-	57,57,57,57	0
60	MG	BA	3424	1/1	0.34	-	64,64,64,64	0
60	MG	BD	301	1/1	0.37	-	25,25,25,25	0
60	MG	CA	1719	1/1	0.26	-	95,95,95,95	0
60	MG	BA	3462	1/1	0.45	-	28,28,28,28	0
60	MG	BA	3224	1/1	0.29	-	79,79,79,79	0
60	MG	BA	3164	1/1	0.80	-	44,44,44,44	0
60	MG	BA	3020	1/1	0.44	-	103,103,103,103	0
60	MG	DA	3625	1/1	0.43	-	29,29,29,29	0
60	MG	DA	3610	1/1	0.20	-	112,112,112,112	0
60	MG	DA	3182	1/1	0.17	-	73,73,73,73	0
60	MG	AA	1621	1/1	1.39	-	98,98,98,98	0
60	MG	DP	204	1/1	0.25	-	15,15,15,15	0
60	MG	BA	3118	1/1	0.07	-	59,59,59,59	0
60	MG	CA	1616	1/1	0.15	-	62,62,62,62	0
60	MG	AA	1627	1/1	1.03	-	142,142,142,142	0
60	MG	DA	3223	1/1	0.35	-	37,37,37,37	0
60	MG	BA	3313	1/1	0.17	-	70,70,70,70	0
60	MG	DA	3505	1/1	0.91	-	125,125,125,125	0
60	MG	BA	3095	1/1	0.40	-	95,95,95,95	0
60	MG	AA	1912	1/1	0.33	-	57,57,57,57	1
60	MG	DA	3170	1/1	0.42	-	98,98,98,98	0
60	MG	CA	1676	1/1	0.25	-	88,88,88,88	0
60	MG	AA	1909	1/1	0.13	-	87,87,87,87	1
60	MG	BA	3473	1/1	0.87	-	87,87,87,87	0
60	MG	BA	3446	1/1	0.34	-	99,99,99,99	0
60	MG	DA	3795	1/1	0.43	-	25,25,25,25	0
60	MG	BA	3079	1/1	0.15	-	37,37,37,37	0
60	MG	DA	3517	1/1	0.34	-	107,107,107,107	0
60	MG	AA	1944	1/1	0.28	-	76,76,76,76	0
60	MG	DA	3308	1/1	0.25	-	103,103,103,103	0
60	MG	DA	3240	1/1	0.09	-	128,128,128,128	0
60	MG	BA	3371	1/1	0.15	-	63,63,63,63	0
60	MG	DA	3589	1/1	0.67	-	47,47,47,47	0
60	MG	BA	3255	1/1	0.26	-	55,55,55,55	0
60	MG	BA	2904	1/1	1.74	-	104,104,104,104	0
60	MG	DA	3212	1/1	0.43	-	105,105,105,105	0
60	MG	DA	3658	1/1	0.24	-	53,53,53,53	0
60	MG	DA	2918	1/1	0.37	-	91,91,91,91	0
60	MG	AX	102	1/1	0.14	-	87,87,87,87	0
60	MG	BA	3379	1/1	1.49	-	114,114,114,114	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3009	1/1	0.46	-	80,80,80,80	0
60	MG	BA	3556	1/1	0.86	-	116,116,116,116	0
60	MG	BA	3293	1/1	0.20	-	82,82,82,82	0
60	MG	AA	1785	1/1	0.03	-	108,108,108,108	0
60	MG	BA	3225	1/1	0.18	-	62,62,62,62	0
60	MG	BA	3047	1/1	0.61	-	89,89,89,89	0
60	MG	DA	3198	1/1	0.52	-	31,31,31,31	0
60	MG	AA	1803	1/1	0.52	-	98,98,98,98	0
60	MG	AA	1739	1/1	0.85	-	73,73,73,73	1
60	MG	AA	1791	1/1	0.26	-	93,93,93,93	0
60	MG	DA	3076	1/1	0.25	-	75,75,75,75	0
60	MG	DA	3597	1/1	0.29	-	66,66,66,66	0
60	MG	DA	3526	1/1	0.11	-	11,11,11,11	1
60	MG	BA	3123	1/1	0.42	-	105,105,105,105	0
60	MG	AL	203	1/1	0.26	-	81,81,81,81	0
60	MG	BA	2925	1/1	0.45	-	33,33,33,33	0
60	MG	DA	3265	1/1	0.75	-	82,82,82,82	0
60	MG	BA	3092	1/1	0.21	-	101,101,101,101	0
60	MG	AA	1635	1/1	0.69	-	108,108,108,108	0

6.5 Other polymers ⓘ

There are no such residues in this entry.