



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2025 – 12:02 PM EDT

PDB ID : 4V9R
Title : Crystal structure of antibiotic DITYROMYCIN bound to 70S ribosome
Authors : Bulkley, D.P.; Brandi, L.; Polikanov, Y.S.; Fabbretti, A.; O'Connor, M.;
Gualerzi, C.O.; Steitz, T.A.
Deposited on : 2013-12-05
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

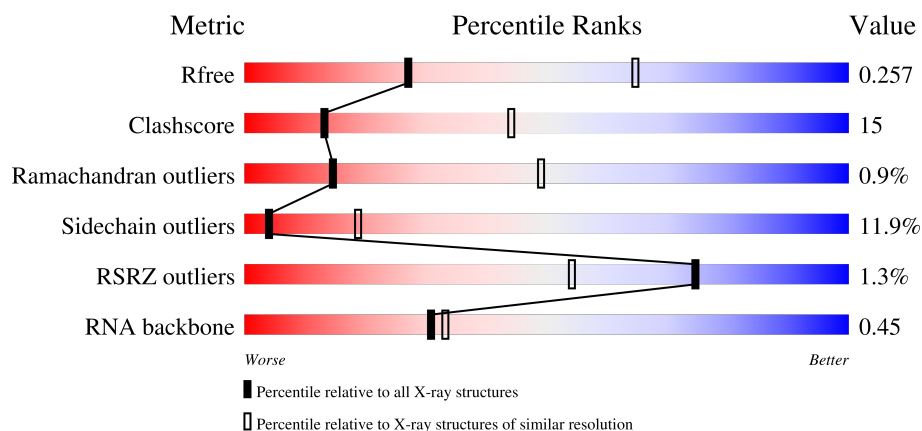
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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





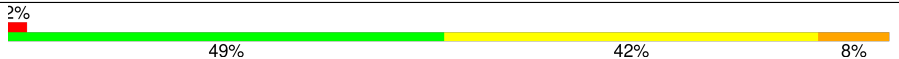



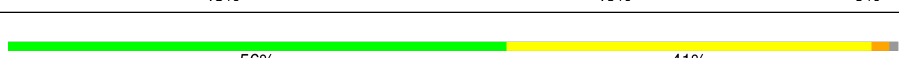
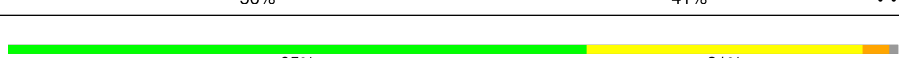
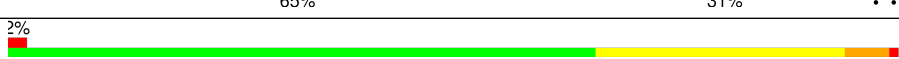

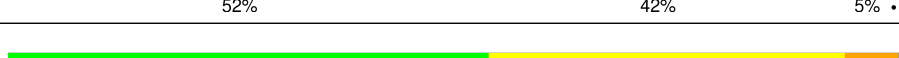





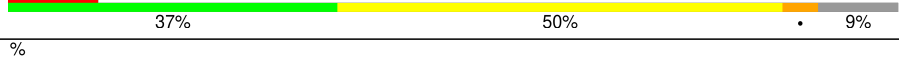

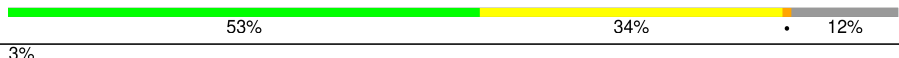
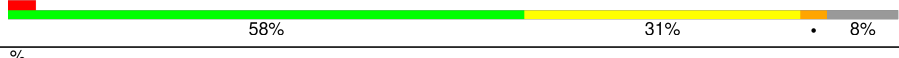

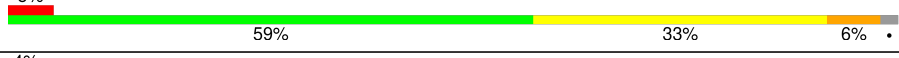



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)
RNA backbone	3690	1019 (3.20-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>2%</div> <div>29% 44% 20% 5%</div> </div>
1	CA	1522	<div> <div>%</div> <div>32% 43% 20%</div> </div>
2	AB	256	<div> <div>2%</div> <div>38% 41% 11% 10%</div> </div>
2	CB	256	<div> <div>3%</div> <div>36% 44% 10% 10%</div> </div>

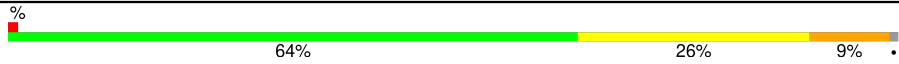

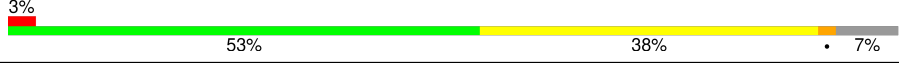

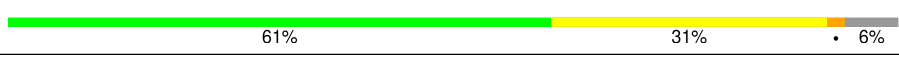
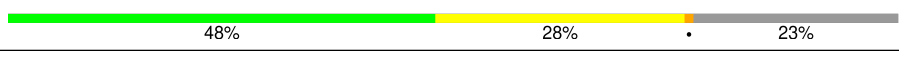
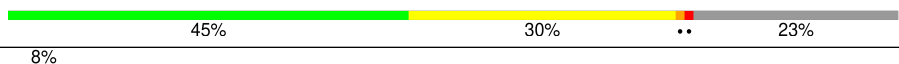
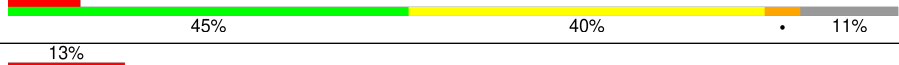
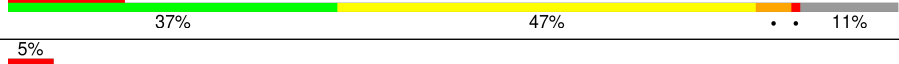


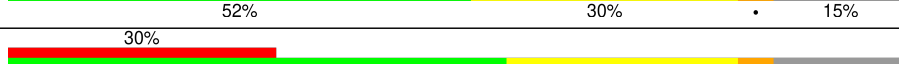


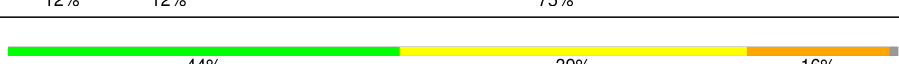
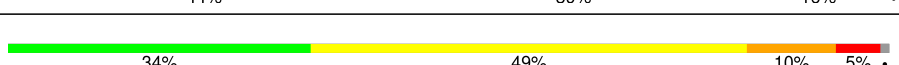


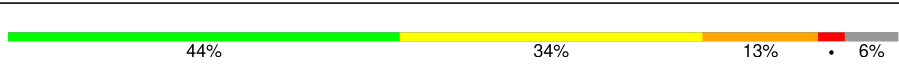


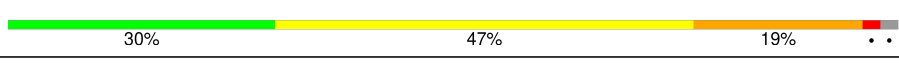
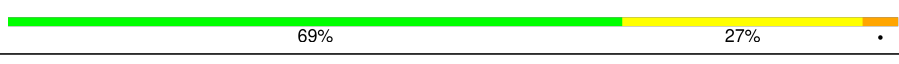


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	24	
22	CV	24	
23	AX	77	
23	CX	77	
24	AW	10	
24	CW	10	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	
27	BD	276	
27	DD	276	


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	118	
38	BS	112	
38	DS	112	
39	BT	146	
39	DT	146	
40	BU	118	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	
52	B6	54	
52	D6	54	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	D9	37	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	3030	-	-	-	X
56	MG	AA	3133	-	-	-	X
56	MG	CA	3030	-	-	-	X
56	MG	CA	3053	-	-	-	X
56	MG	DA	3113	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 286321 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1498	Total	C	N	O	P	0	0	0
			32196	14328	5966	10404	1498			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
2	CB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	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
			1231	766	243	216	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
8	CH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- 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
			983	623	193	167			
9	CI	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AJ	97	Total	C	N	O	0	0	0
			709	440	138	131			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O			
			714	445	138	131	0	0	0

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AK	114	Total	C	N	O	S		
			829	516	155	155	3	0	0
11	CK	114	Total	C	N	O	S		
			833	519	156	155	3	0	0

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S		
			930	585	185	159	1	0	0
12	CL	122	Total	C	N	O	S		
			930	585	185	159	1	0	0

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AM	123	Total	C	N	O	S		
			958	592	198	166	2	0	0
13	CM	122	Total	C	N	O	S		
			950	586	197	165	2	0	0

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

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

- 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		
			728	456	144	126	2	0	0
15	CO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
16	CP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	CR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
19	CS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
20	CT	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	7	Total	C	N	O	P	0	0	1
			114	49	22	37	6			
22	CV	6	Total	C	N	O	P	0	0	0
			113	49	22	36	6			

- Molecule 23 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	76	Total	C	N	O	P	0	0	0
			1623	723	294	530	76			
23	CX	76	Total	C	N	O	P	0	0	0
			1623	723	294	530	76			

- Molecule 24 is a protein called Dityromycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AW	10	Total	C	N	O	0	0	0
			93	67	10	16			
24	CW	10	Total	C	N	O	0	0	0
			93	67	10	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2731	Total	C	N	O	P	0	0	0
			58834	26185	11020	18899	2730			
25	DA	2714	Total	C	N	O	P	0	0	0
			58458	26018	10942	18786	2712			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	DB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 27 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
27	DD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 28 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
28	DE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 29 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
29	DF	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
30	DG	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- Molecule 31 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
31	DH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 32 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
32	DI	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	1			

- Molecule 33 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
33	DN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 34 is a protein called 50S Ribosomal Protein L14.

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

- Molecule 35 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
35	DP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 36 is a protein called 50S Ribosomal Protein L16.

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

- Molecule 37 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 38 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BS	110	Total	C	N	O		0	0	0
			877	553	175	149				
38	DS	110	Total	C	N	O		0	0	0
			870	549	173	148				

- Molecule 39 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
39	DT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 40 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
40	DU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 41 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
41	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 42 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 43 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
43	DX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 44 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
44	DY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 45 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BZ	171	Total	C	N	O	S	0	0	0
			1349	862	243	242	2			
45	DZ	174	Total	C	N	O	S	0	0	0
			1360	870	243	245	2			

- Molecule 46 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
46	D0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 47 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
47	D1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 48 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
48	D2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 49 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B3	59	Total	C	N	O	0	0	0
			469	298	90	81			
49	D3	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 50 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	69	Total	C	N	O	S	0	0	0
			551	348	99	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			531	338	97	91	5			

- Molecule 51 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
51	D5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 52 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
52	D6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 53 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
53	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 54 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			
54	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 55 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
55	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	222	Total	Mg	0	0
			222	222		
56	AD	1	Total	Mg	0	0
			1	1		
56	AF	1	Total	Mg	0	0
			1	1		
56	AK	1	Total	Mg	0	0
			1	1		
56	AL	1	Total	Mg	0	0
			1	1		
56	AM	2	Total	Mg	0	0
			2	2		
56	AN	1	Total	Mg	0	0
			1	1		
56	AS	1	Total	Mg	0	0
			1	1		
56	AV	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AX	9	Total 9	Mg 9	0	0
56	BA	739	Total 739	Mg 739	0	0
56	BB	18	Total 18	Mg 18	0	0
56	BD	12	Total 12	Mg 12	0	0
56	BE	9	Total 9	Mg 9	0	0
56	BF	6	Total 6	Mg 6	0	0
56	BG	4	Total 4	Mg 4	0	0
56	BN	6	Total 6	Mg 6	0	0
56	BO	1	Total 1	Mg 1	0	0
56	BP	4	Total 4	Mg 4	0	0
56	BQ	4	Total 4	Mg 4	0	0
56	BR	3	Total 3	Mg 3	0	0
56	BU	9	Total 9	Mg 9	0	0
56	BV	3	Total 3	Mg 3	0	0
56	BW	5	Total 5	Mg 5	0	0
56	BX	2	Total 2	Mg 2	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	B0	6	Total 6	Mg 6	0	0
56	B1	2	Total 2	Mg 2	0	0
56	B2	1	Total 1	Mg 1	0	0
56	B3	3	Total 3	Mg 3	0	0

Continued on next page...

Continued from previous page...

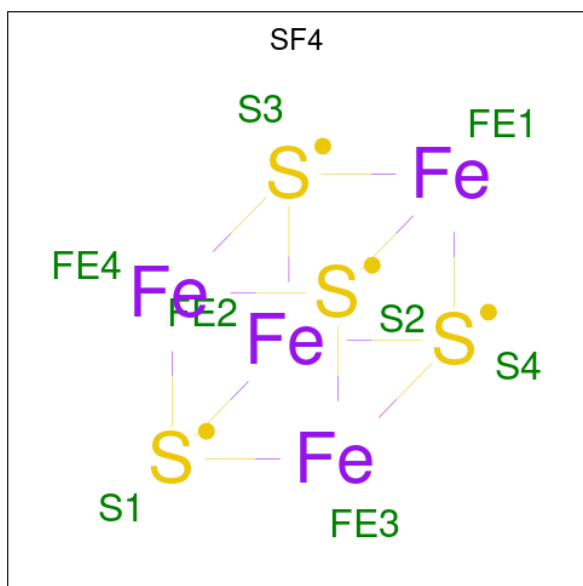
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B5	1	Total 1	Mg 1	0	0
56	B7	4	Total 4	Mg 4	0	0
56	B8	2	Total 2	Mg 2	0	0
56	B9	1	Total 1	Mg 1	0	0
56	CA	172	Total 172	Mg 172	0	0
56	CE	2	Total 2	Mg 2	0	0
56	CF	1	Total 1	Mg 1	0	0
56	CN	1	Total 1	Mg 1	0	0
56	CT	1	Total 1	Mg 1	0	0
56	CX	3	Total 3	Mg 3	0	0
56	DA	657	Total 657	Mg 657	0	0
56	DB	12	Total 12	Mg 12	0	0
56	DD	5	Total 5	Mg 5	0	0
56	DE	6	Total 6	Mg 6	0	0
56	DF	5	Total 5	Mg 5	0	0
56	DG	1	Total 1	Mg 1	0	0
56	DN	1	Total 1	Mg 1	0	0
56	DO	1	Total 1	Mg 1	0	0
56	DP	2	Total 2	Mg 2	0	0
56	DQ	4	Total 4	Mg 4	0	0
56	DR	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DU	2	Total	Mg	0	0
			2	2		
56	DV	3	Total	Mg	0	0
			3	3		
56	DW	2	Total	Mg	0	0
			2	2		
56	DY	1	Total	Mg	0	0
			1	1		
56	D3	1	Total	Mg	0	0
			1	1		
56	D5	2	Total	Mg	0	0
			2	2		
56	D8	1	Total	Mg	0	0
			1	1		

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

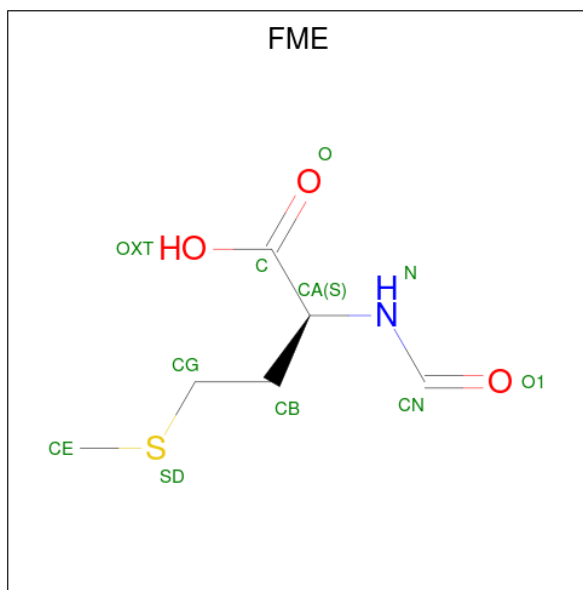


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AD	1	Total	Fe	S	0	0
			8	4	4		
57	CD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AN	1	Total Zn 1 1	0	0
58	BY	1	Total Zn 1 1	0	0
58	B4	1	Total Zn 1 1	0	0
58	B5	1	Total Zn 1 1	0	0
58	B6	1	Total Zn 1 1	0	0
58	B9	1	Total Zn 1 1	0	0
58	CN	1	Total Zn 1 1	0	0
58	DY	1	Total Zn 1 1	0	0
58	D4	1	Total Zn 1 1	0	0
58	D5	1	Total Zn 1 1	0	0
58	D6	1	Total Zn 1 1	0	0
58	D9	1	Total Zn 1 1	0	0

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	AX	1	Total	C	N	O	S	0	0
			10	6	1	2	1		
59	CX	1	Total	C	N	O	S	0	0
			10	6	1	2	1		

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	147	Total	O	0	0
			147	147		
61	AD	1	Total	O	0	0
			1	1		
61	AE	2	Total	O	0	0
			2	2		
61	AJ	1	Total	O	0	0
			1	1		
61	AL	2	Total	O	0	0
			2	2		
61	AO	2	Total	O	0	0
			2	2		
61	AU	1	Total	O	0	0
			1	1		
61	AV	2	Total	O	0	0
			2	2		
61	AX	1	Total	O	0	0
			1	1		
61	BA	1086	Total	O	0	0
			1086	1086		
61	BB	26	Total	O	0	0
			26	26		
61	BD	6	Total	O	0	0
			6	6		
61	BE	13	Total	O	0	0
			13	13		
61	BF	5	Total	O	0	0
			5	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BG	1	Total 1	O 1	0	0
61	BN	3	Total 3	O 3	0	0
61	BO	2	Total 2	O 2	0	0
61	BP	15	Total 15	O 15	0	0
61	BQ	3	Total 3	O 3	0	0
61	BR	1	Total 1	O 1	0	0
61	BT	2	Total 2	O 2	0	0
61	BU	5	Total 5	O 5	0	0
61	BV	2	Total 2	O 2	0	0
61	BW	4	Total 4	O 4	0	0
61	BX	4	Total 4	O 4	0	0
61	B0	4	Total 4	O 4	0	0
61	B1	2	Total 2	O 2	0	0
61	B5	2	Total 2	O 2	0	0
61	B7	1	Total 1	O 1	0	0
61	B8	7	Total 7	O 7	0	0
61	CA	186	Total 186	O 186	0	0
61	CE	2	Total 2	O 2	0	0
61	CN	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0
61	CX	2	Total 2	O 2	0	0

Continued on next page...

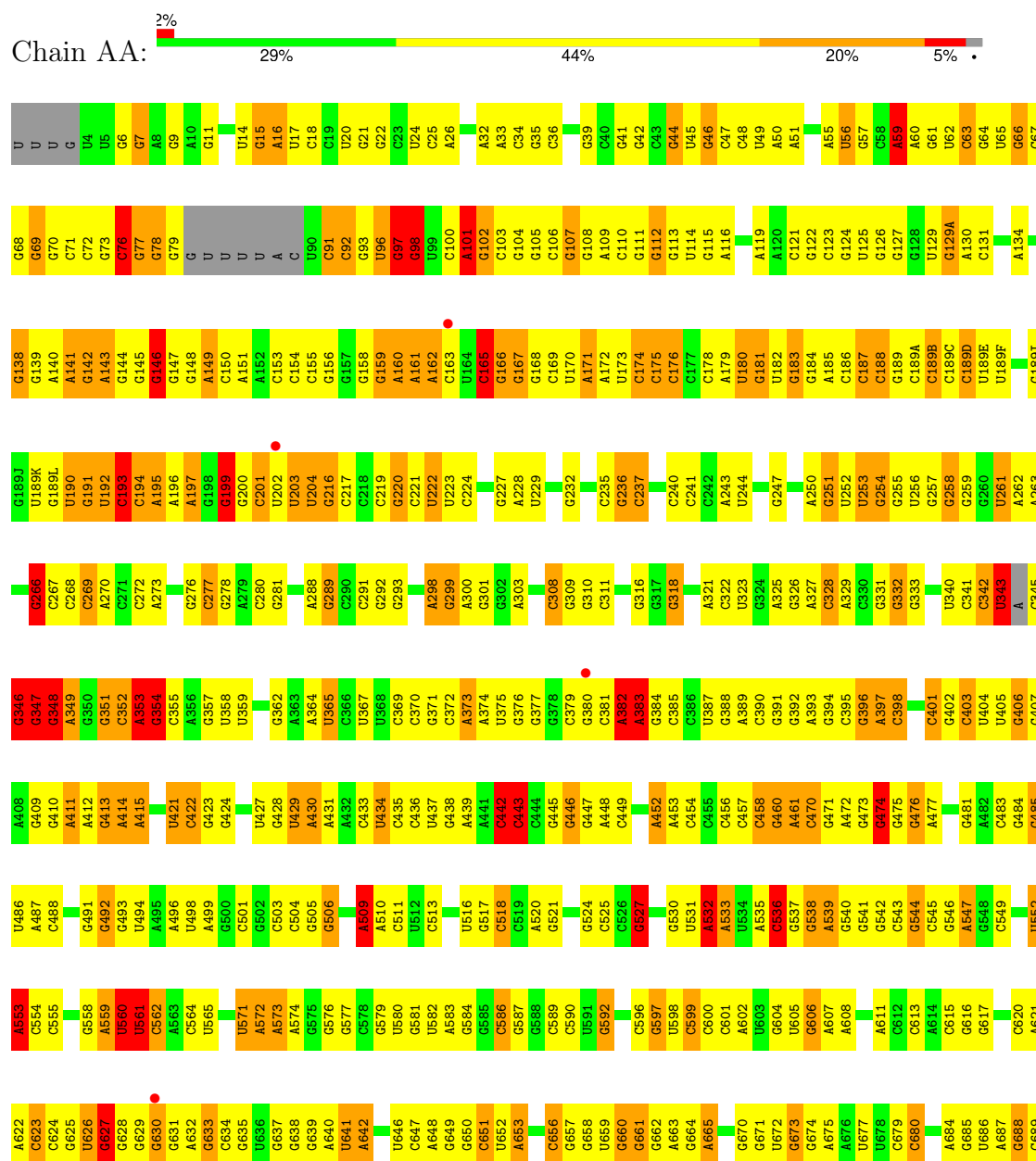
Continued from previous page...

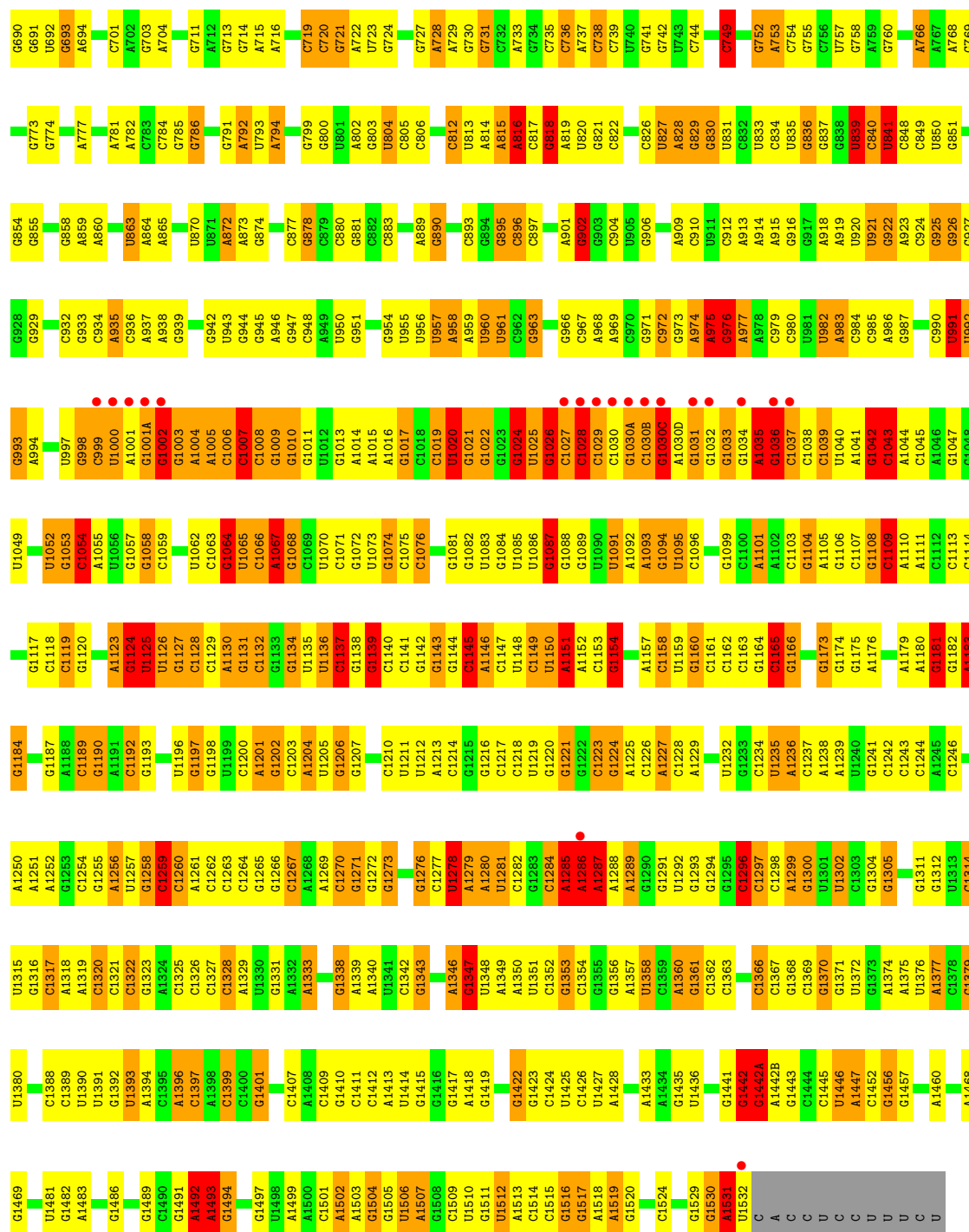
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DA	906	Total 906	O 906	0	0
61	DB	7	Total 7	O 7	0	0
61	DD	10	Total 10	O 10	0	0
61	DE	11	Total 11	O 11	0	0
61	DF	4	Total 4	O 4	0	0
61	DO	1	Total 1	O 1	0	0
61	DP	14	Total 14	O 14	0	0
61	DQ	3	Total 3	O 3	0	0
61	DR	1	Total 1	O 1	0	0
61	DU	4	Total 4	O 4	0	0
61	DV	1	Total 1	O 1	0	0
61	DX	2	Total 2	O 2	0	0
61	DY	1	Total 1	O 1	0	0
61	D0	3	Total 3	O 3	0	0
61	D1	1	Total 1	O 1	0	0
61	D3	1	Total 1	O 1	0	0
61	D7	1	Total 1	O 1	0	0
61	D8	4	Total 4	O 4	0	0

3 Residue-property plots

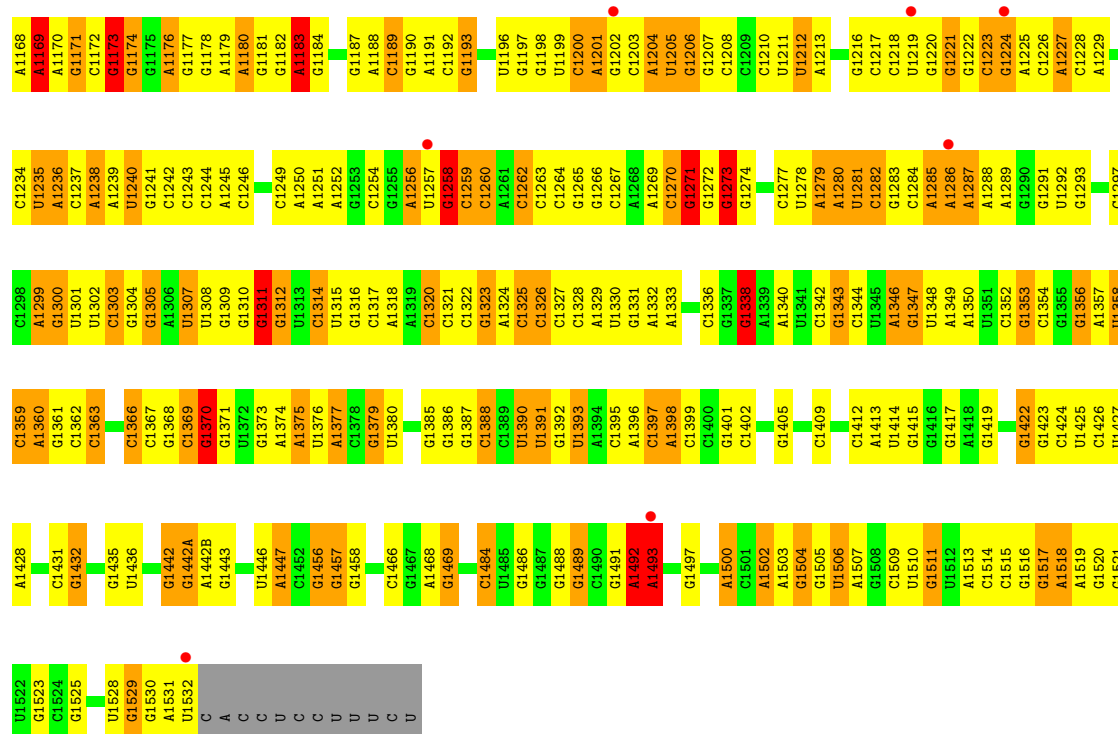
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S Ribosomal RNA

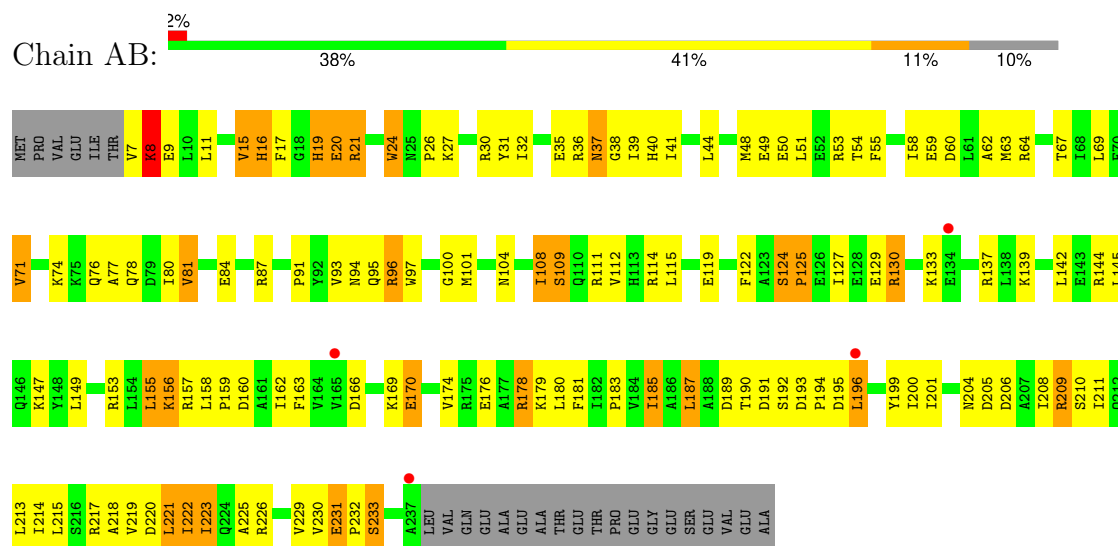




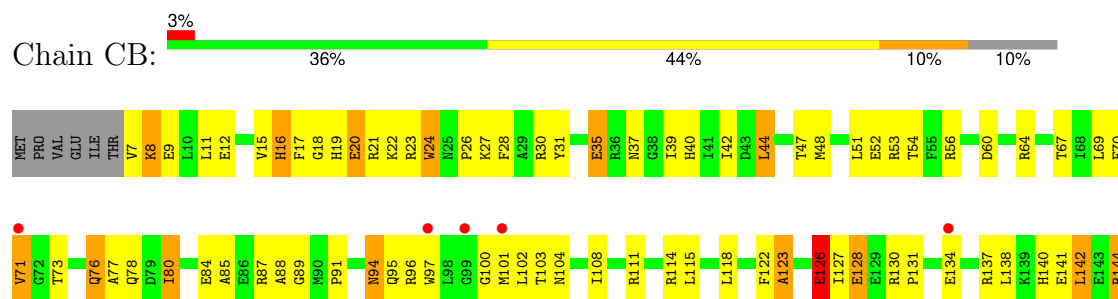
C1107	G1108	C1109	A1110	A1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139	C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	C1148	C1149	A1151	A1152	C1153	C1154	C1155	C1156	A1157	C1158	C1159	C1160	C1161	C1162	C1163	C1164	C1165	C1166																																																																																																	
C1043	A1044	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061	U1062	C1063	C1064	C1065	C1066	A1067	C1068	C1069	C1070	C1071	C1072	C1073	C1074	C1075	C1076	C1077	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	A1101	C1103	C1103	C1103	C1104	A1105	C1106																																																																																																
A986	C990	U991	U992	U993	A994	C995	A996	U997	G998	C999	U1000	A1001	G1001A	G1002	G1003	A1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	A1014	A1015	A1016	C1017	C1018	C1019	U1020	C1021	G1022	C1023	U1024	C1025	A964	A965	C966	C967	C968	C1029	C1030	G1030A	C1030B	C1030C	A1030D	C1031	U1095	G1032	C1033	C1034	A977	A978	C979	C980	U981	C1038	C1039	U1040	A983	A1041	C1042																																																																																											
U920	U921	G922	A923	C924	C925	G926	G927	C931	C932	C933	C934	A935	C936	A937	A938	G939	C940	G941	G942	U943	C944	G945	G946	C947	C948	U952	G953	C954	U955	U956	U957	A958	U959	U960	U961	A964	A965	G966	G967	A968	A969	C970	C971	C972	C973	A974	U975	C976	C977	A978	A979	C980	U981	U982	A983	C984	C985																																																																																																		
C840	U841	C848	C849	U850	C851	G852	G853	G854	G855	C856	C857	G858	A859	A860	G861	A865	C866	G867	C868	G869	U870	U871	A872	A873	G874	C875	C876	C877	G878	C879	C880	C881	G885	G886	G889	C893	G894	C897	C898	A900	A901	G902	G903	A904	A905	A906	A907	A908	A909	C910	A913	A914	A915	G916	G917	G918	A919																																																																																																		
U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883																																																																																												
C689	C690	G691	G692	G693	G694	G700	G701	A704	G708	G709	G710	G711	A712	G713	G714	A715	C719	C720	G721	G722	U723	G724	G727	G728	A729	G730	G731	C732	A733	G734	C735	C736	A737	C738	C739	U740	G741	G742	C745	C749	G752	A753	C754	G755	C756	G757	G758	A759	G760	A766																																																																																																									
G546	A547	U552	A553	C554	C555	C556	C557	C558	C559	C560	C561	C562	C563	C564	C565	C566	C567	C568	C569	C570	C571	C572	C573	C574	C575	C576	C577	C578	C579	C580	C581	C582	C583	C584	C585	C586	C587	C588	C589	C590	C591	C592	C593	C594	C595	C596	C597	C598	C599	C600	C601	A602	U605	G606	A607	A608	A609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620																																																																																							
C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500	C501	C502	C503	C504	C505	C506	C507	C508	C509	C510	C511	C512	C513	C514	C515	C516	C517	C518	C519	C520	C521	C522	C523	C524	C525	C526	C527	C528	C529	C530	C531	C532	C533	C534	C535	C536	C537	C538	C539	C540	C541	C542	C543	C544	C545																																																																																			
C401	C402	C403	U404	U405	C406	C407	G410	A411	A412	C413	A414	A415	C418	C419	U420	U421	C422	C423	C424	C425	C426	U427	C428	U429	A430	C431	A432	C433	U434	C435	U436	C437	C438	A439	A441	C442	C443	C444	C445	C446	C447	A448	C449	A451	A452	A453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500	C501	C502	C503	C504	C505	C506	C507	C508	C509	C510	C511	C512	C513	C514	C515	C516	C517	C518	C519	C520	C521	C522	C523	C524	C525	C526	C527	C528	C529	C530	C531	C532	C533	C534	C535	C536	C537	C538	C539	C540	C541	C542	C543	C544	C545																	
A329	C330	G331	G332	G333	C337	A338	C339	U340	C341	C342	C343	C344	C345	C346	C347	C348	C349	C350	C351	C352	C353	C354	C355	U358	U359	A364	C365	C366	C367	C368	C369	C370	C371	C372	C373	C374	C375	C376	C377	C378	C379	C380	C381	C382	C383	C384	C385	C386	C387	C388	C389	C390	C391	C392	C393	C394	C395	C396	C397	C398	C399	C400																																																																																													
U164	C165	G166	U169	U170	U171	U172	U173	C174	C175	C178	U179	U180	G181	U182	C187	C188	C189	C189A	C189B	C189C	C189D	C189E	U189F	U189G	U189H	C189J	C189K	C189L	U190	C191	C192	C193	C194	C195	C196	C197	C198	C199	C200	C201	C202	C203	C204	C205	C206	C207	C208	C209	C210	C211	C212	C213	C214	C215	C216	C217	C218	C219	C220	C221	C222	C223	C224	C225	C226	C227	C228	C229	C230	C231	C232	C233	C234	C235	C236	C237	C238	C239	C240	C241	C242																																																																										
A243	C244	C245	A246	C247	A250	C251	U252	C253	C254	C255	C256	C257	C258	C259	C260	C261	C262	C263	C264	C265	C266	C267	C268	C269	C270	C271	C272	C273	C274	C275	C276	C277	C278	C279	C280	C281	C282	C283	C284	C285	C286	C287	C288	C289	C290	C291	C292	C293	C294	C295	C296	C297	C298	C299	C300	C301	C302	C303	C304	C305	C306	C307	C308	C309	C310	C311	C312	C313	C314	C315	C316	C317	C318	C319	C320	C321	C322	C323	C324	C325	C326	C327	C328	C329	C330	C331	C332	C333	C334	C335	C336	C337	C338	C339	C340	C341	C342	C343	C344	C345	C346	C347	C348	C349	C350	C351	C352	C353	C354	C355	C356	C357	C358	C359	C360	C361	C362	C363	C364	C365	C366	C367	C368	C369	C370	C371	C372	C373	C374	C375	C376	C377	C378	C379	C380	C381	C382	C383	C384	C385	C386	C387	C388	C389	C390	C391	C392	C393	C394	C395	C396	C397	C398	C399	C400

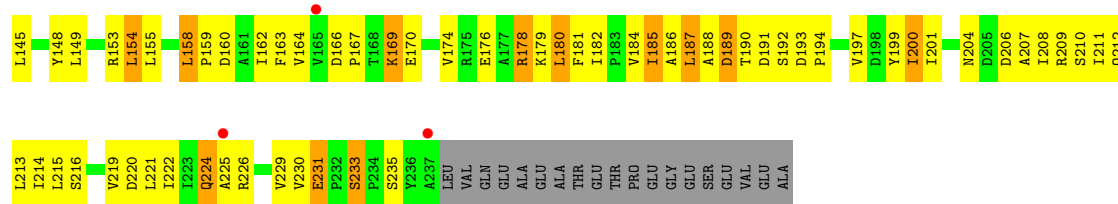


• Molecule 2: 30S Ribosomal Protein S2

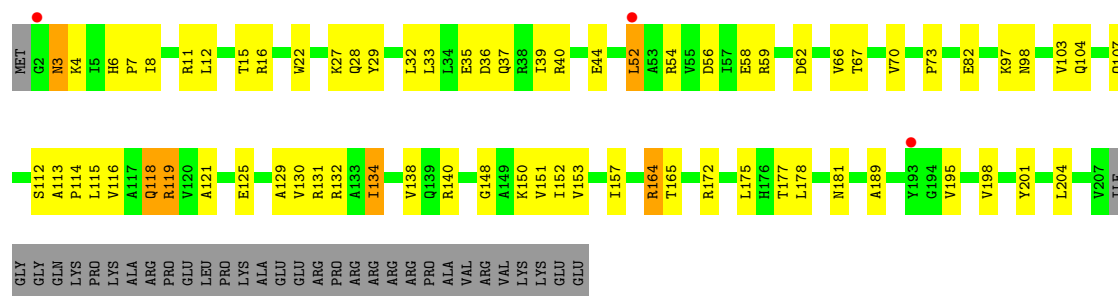


• Molecule 2: 30S Ribosomal Protein S2

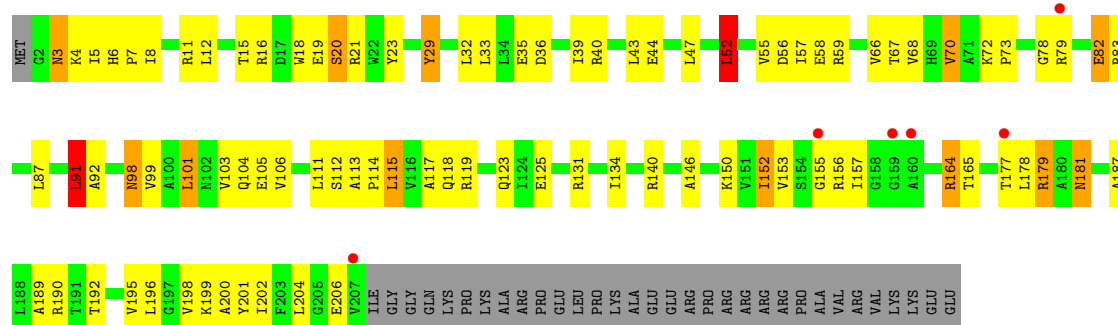




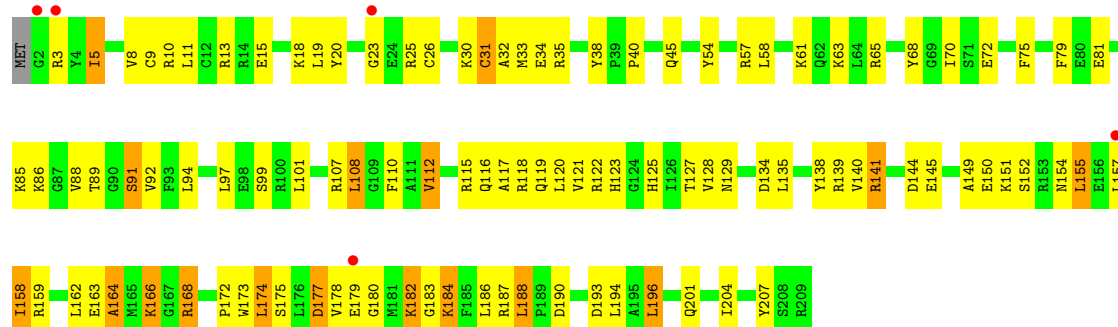
• Molecule 3: 30S Ribosomal Protein S3



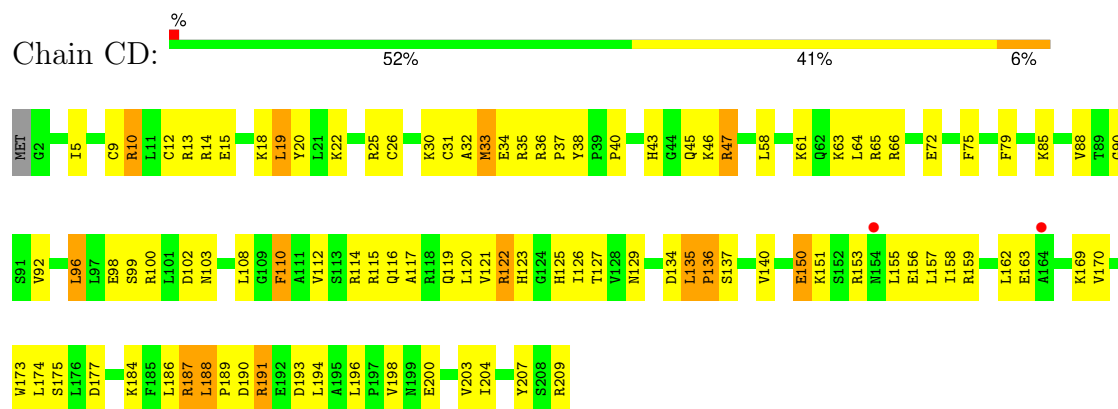
• Molecule 3: 30S Ribosomal Protein S3



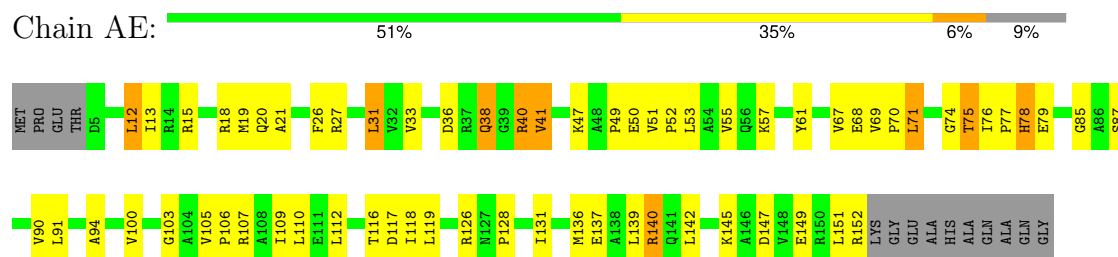
• Molecule 4: 30S Ribosomal Protein S4



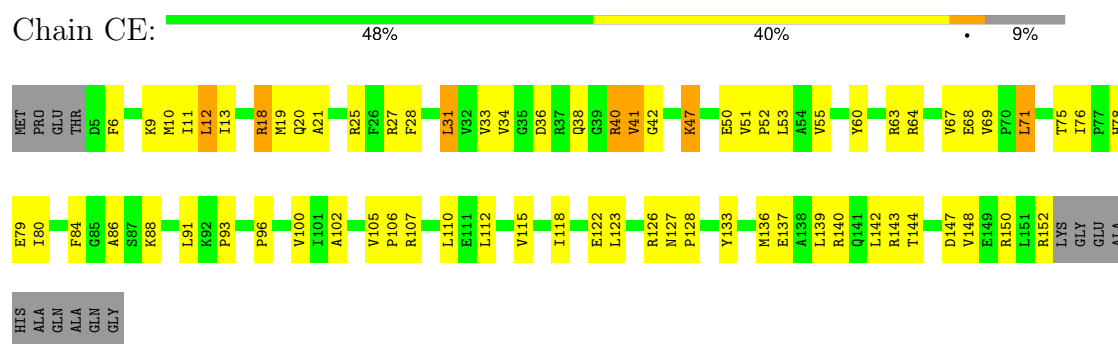
• Molecule 4: 30S Ribosomal Protein S4



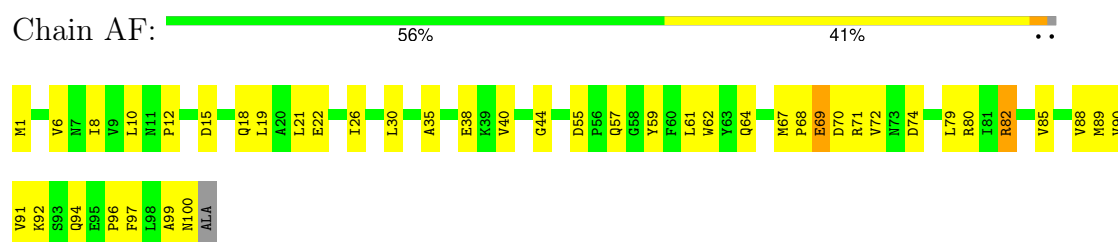
• Molecule 5: 30S Ribosomal Protein S5



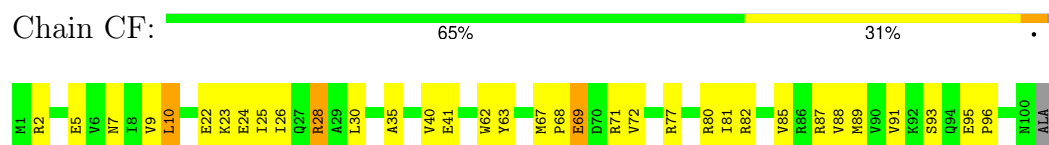
• Molecule 5: 30S Ribosomal Protein S5



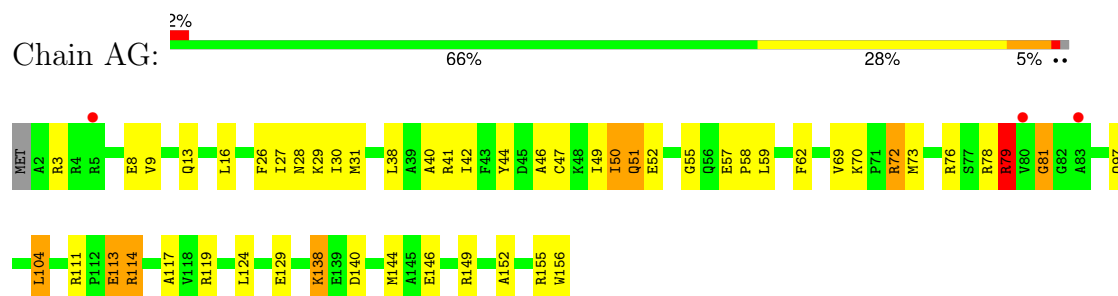
• Molecule 6: 30S Ribosomal Protein S6



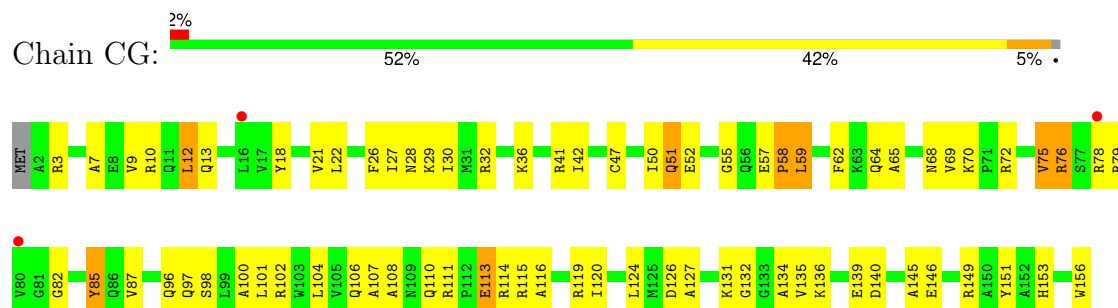
• Molecule 6: 30S Ribosomal Protein S6



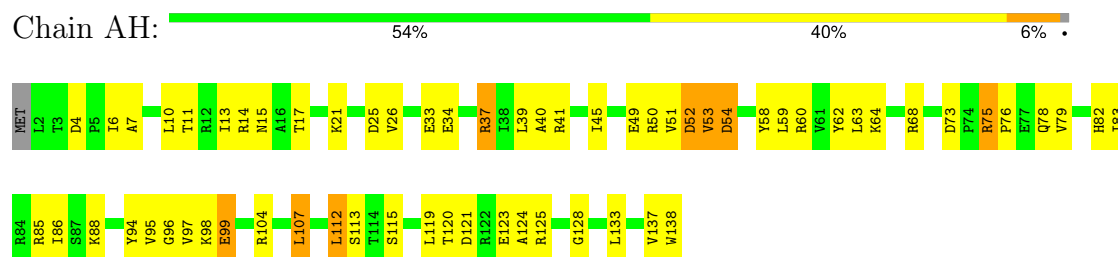
- Molecule 7: 30S Ribosomal Protein S7



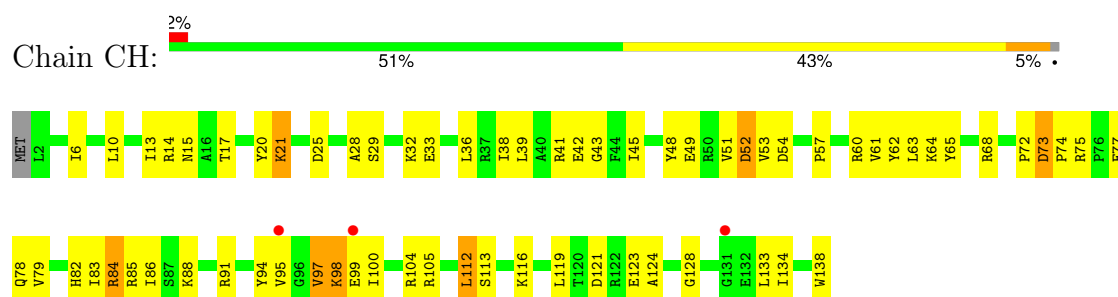
- Molecule 7: 30S Ribosomal Protein S7



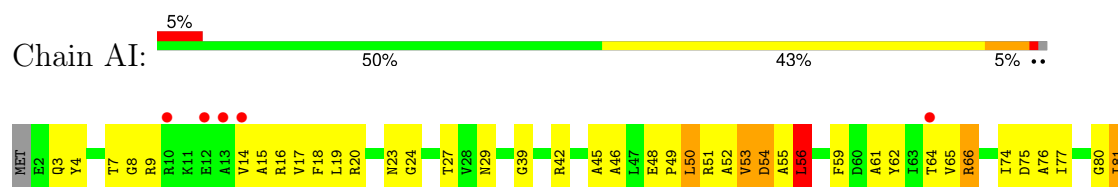
- Molecule 8: 30S Ribosomal Protein S8



- Molecule 8: 30S Ribosomal Protein S8

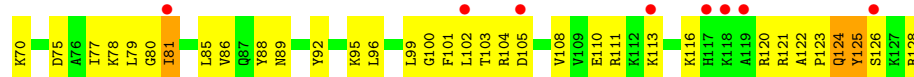
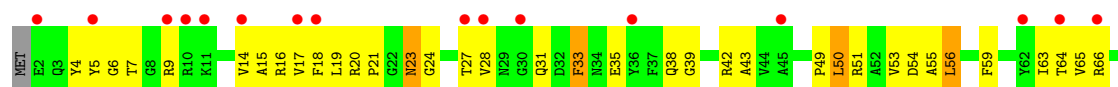


- Molecule 9: 30S Ribosomal Protein S9

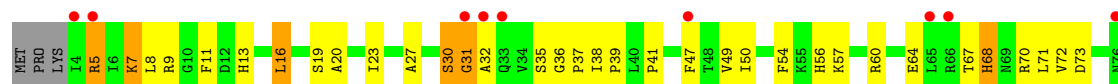




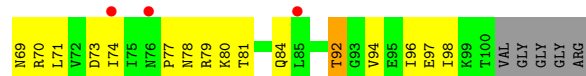
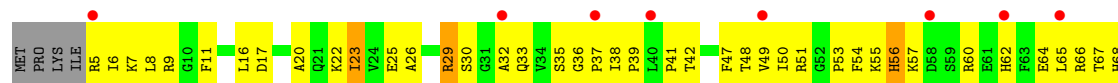
• Molecule 9: 30S Ribosomal Protein S9



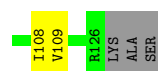
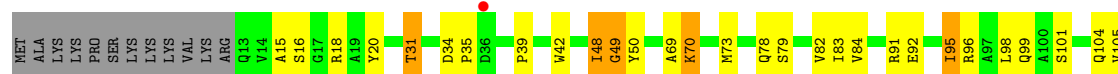
• Molecule 10: 30S Ribosomal Protein S10



• Molecule 10: 30S Ribosomal Protein S10

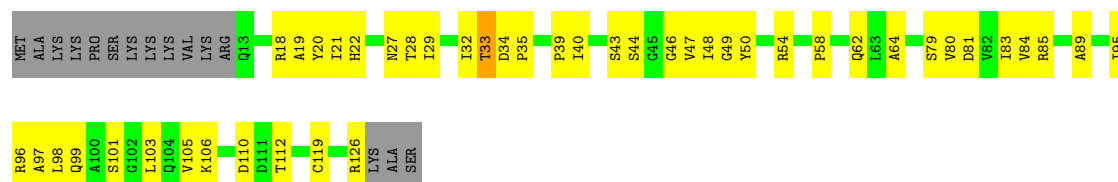


• Molecule 11: 30S Ribosomal Protein S11

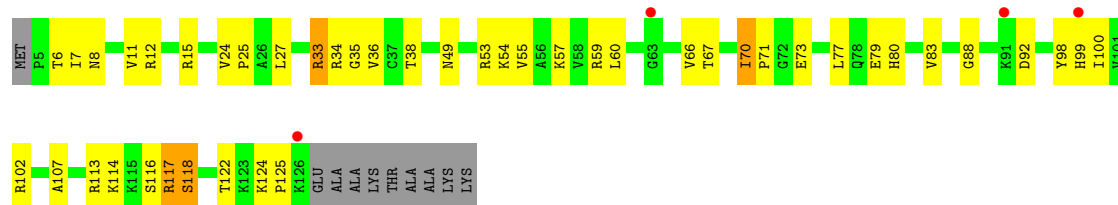


• Molecule 11: 30S Ribosomal Protein S11

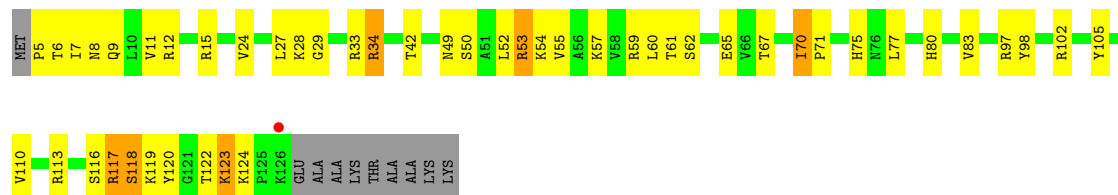




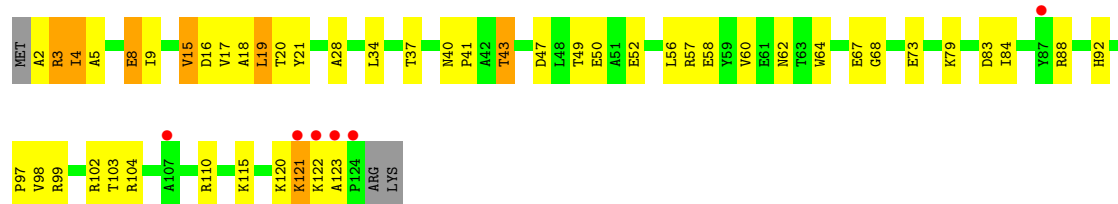
• Molecule 12: 30S Ribosomal Protein S12



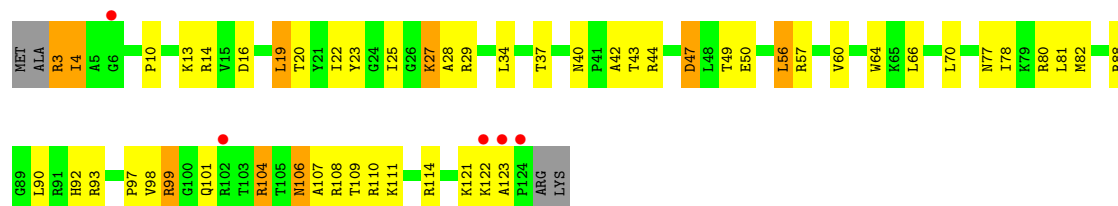
• Molecule 12: 30S Ribosomal Protein S12



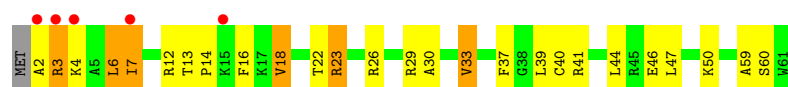
• Molecule 13: 30S Ribosomal Protein S13



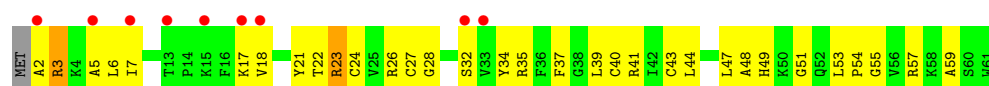
• Molecule 13: 30S Ribosomal Protein S13



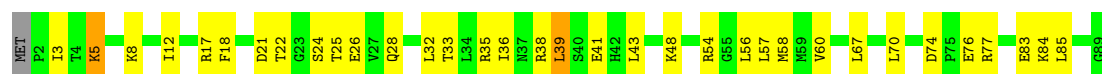
• Molecule 14: 30S Ribosomal Protein S14



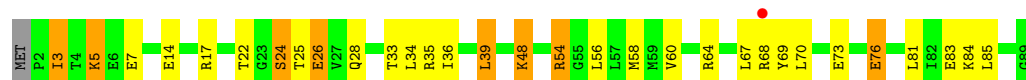
• Molecule 14: 30S Ribosomal Protein S14



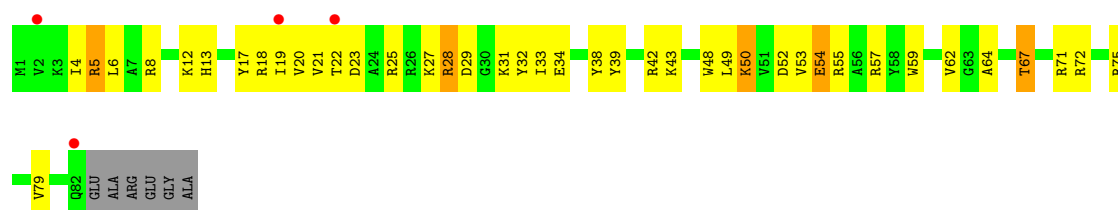
• Molecule 15: 30S Ribosomal Protein S15



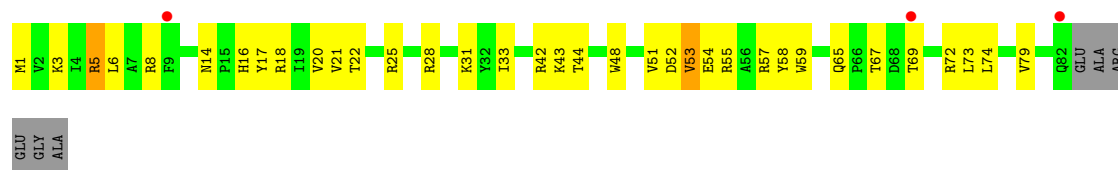
• Molecule 15: 30S Ribosomal Protein S15



• Molecule 16: 30S Ribosomal Protein S16



• Molecule 16: 30S Ribosomal Protein S16

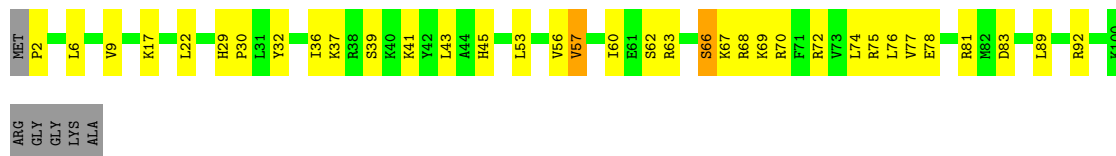


• Molecule 17: 30S Ribosomal Protein S17

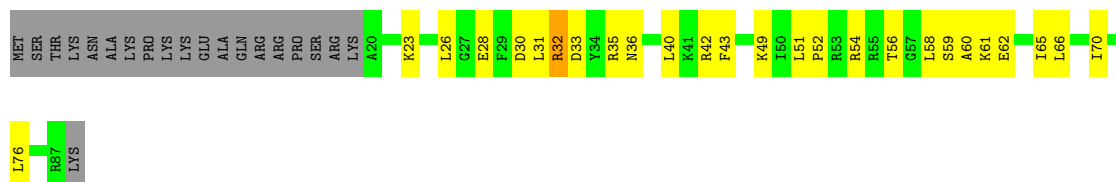




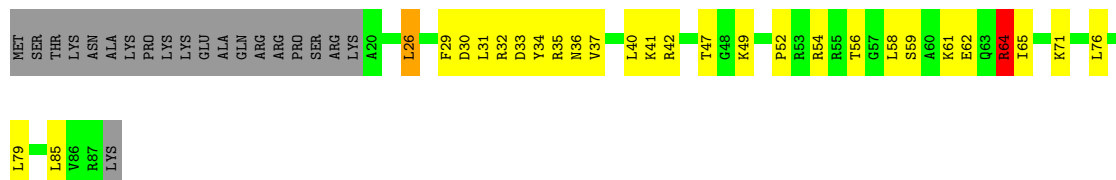
• Molecule 17: 30S Ribosomal Protein S17



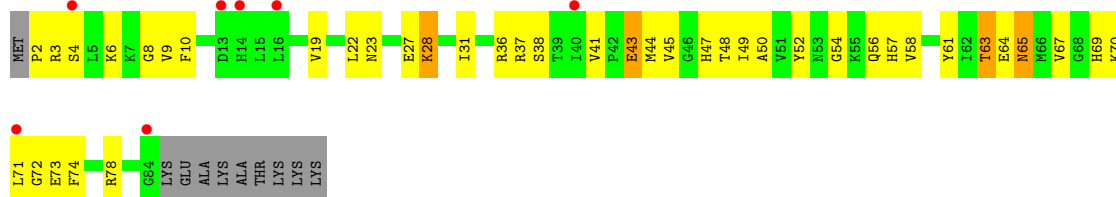
• Molecule 18: 30S Ribosomal Protein S18



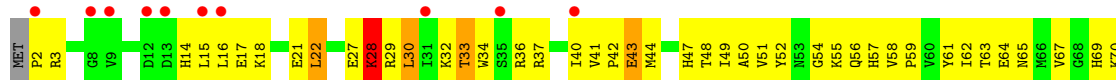
• Molecule 18: 30S Ribosomal Protein S18

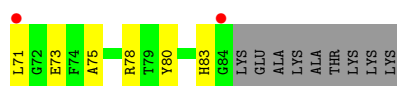


• Molecule 19: 30S Ribosomal Protein S19

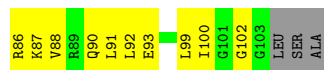


• Molecule 19: 30S Ribosomal Protein S19

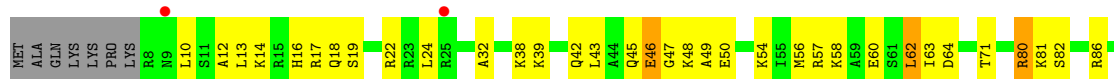




• Molecule 20: 30S Ribosomal Protein S20



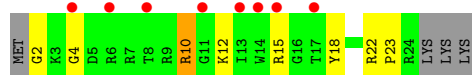
• Molecule 20: 30S Ribosomal Protein S20



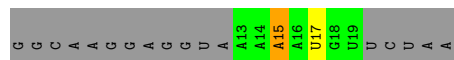
• Molecule 21: 30S Ribosomal Protein THX



• Molecule 21: 30S Ribosomal Protein THX

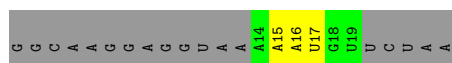


• Molecule 22: mRNA



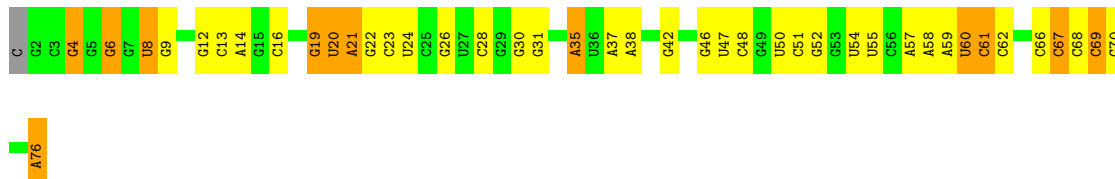
• Molecule 22: mRNA





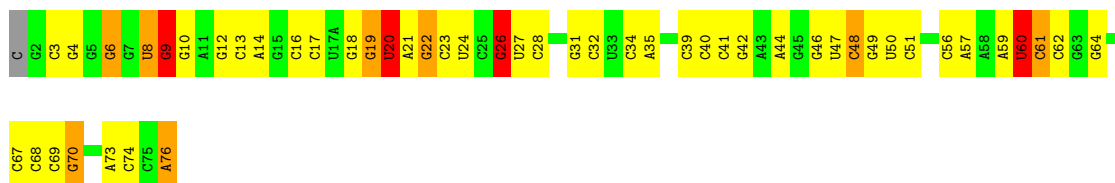
• Molecule 23: P-site tRNA

Chain AX: 44% 39% 16%



• Molecule 23: P-site tRNA

Chain CX: 34% 49% 10% 5%



• Molecule 24: Dityromycin

Chain AW: 40% 60%



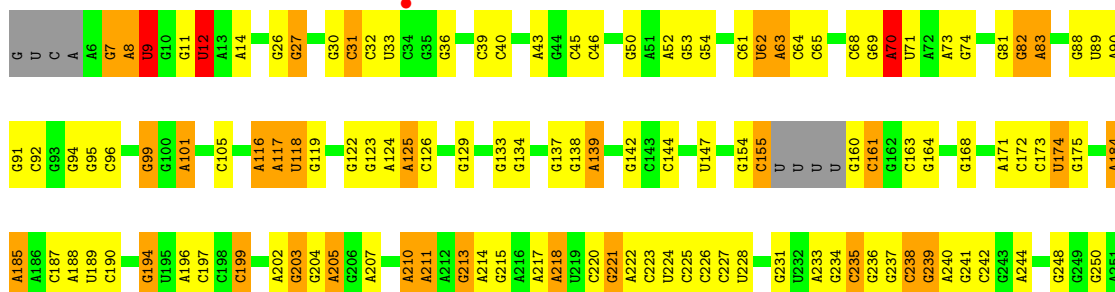
• Molecule 24: Dityromycin

Chain CW: 20% 80%



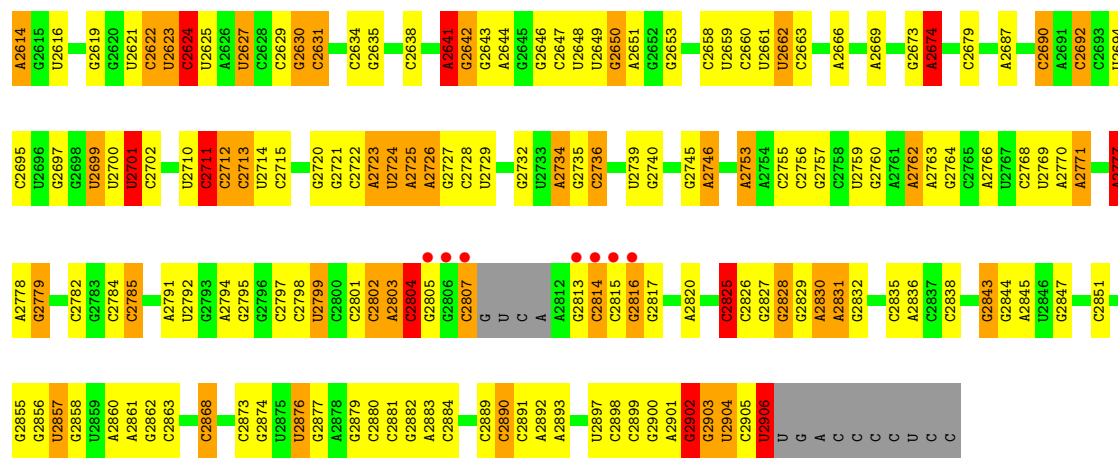
• Molecule 25: 23S Ribosomal RNA

Chain BA: 44% 34% 13% 6%



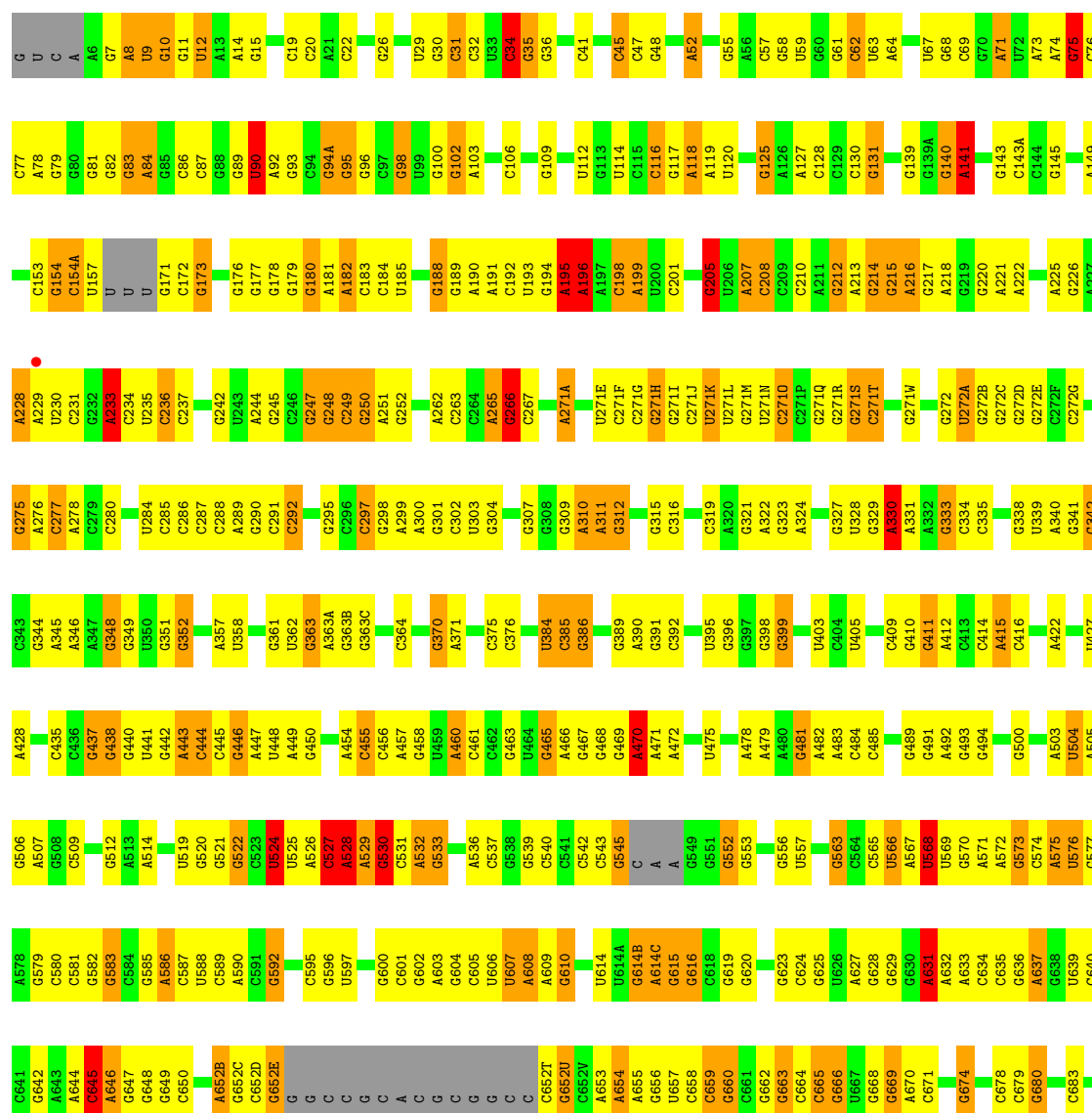
G1356	G1261	U1176	U	A1042	C954	G879	G807	G727	G581	G507	G423	A335	C252
U1359	G1262	C1180	A	G1043	A955	U880	A808	G733	G582	A508	G424	A339	C253
C1360	C1263	G1181	G	U1044	A956	C883	G810	G733	G582	A509	G425	G339	C254
C1361	G1264	G1182	A	U1045	G952	C884	G810	G733	G582	A510	G426	G342	G255
G1365	A1265	G1183	G	A1046	G952	C885	U814	G733	U858	C511	G427	A346	U265
G1366	G1269	G1184	C	A1047	G955	U886	G815	G733	C587	C512	A428	A346	C266
A1367	G1270	C1185	A	G1048	G955	U886	G815	G733	C587	C513	A428	A346	C267
A1368	G1270	C1186	A	G1048	G955	U886	G815	G733	C587	C514	A428	A346	G268
U1369	G1284	U1187	C	C1051	G973	G892	G817	G747	U589	G514	C431	G351	G269
G1370	U1285	A1188	C	A1055	G974	C893	G818	G748	G590	G515	U432	U352	C270
G1371	U1286	A1189	A	A1056	G977	U894	A821	G749	U591	G518	G433	G353	U271
U1372	A1287	U1190	U	A1057	A978	G895	G822	U750	U592	G519	G434	A354	U272
C1373	U1288	C1195	C	U1058	G991	A936	G823	A752	A594	G523	G435	A355	G273
C1376	A1289	G1199	C	C1059	U982	G902	A829	A753	A595	U524	G436	A355	U274
A1377	G1290	C1199	U	U1065	G983	C903	A830	G758	A596	G525	G437	A355	C275
G1378	G1290	U1200	U	A1066	G984	C904	A831	G758	A596	G526	G438	A355	C276
A1382	G1296	A1201	U	A1067	G985	U905	A832	G758	A596	A527	A439	A355	C277
G1385	U1297	A1202	A	G1068	G987	G906	C833	G762	A598	A528	U448	A355	G278
U1386	G1298	G1203	A	U1069	U988	U907	U834	G764	U599	U529	A449	A355	G279
G1386	A1299	C1204	G	G1070	G989	A908	A835	G764	G600	A530	A450	A355	C280
G1386	G1302	U1210	A	G1071	G990	G909	A836	G767	G605	G531	A455	A355	G281
G1386	G1302	U1211	G	U1072	G991	A910	C837	G768	G606	A532	A456	A355	G287
G1386	G1302	U1212	U	A1073	G991	A911	C838	A769	G607	G533	A456	A355	U288
G1386	G1302	U1213	U	A1074	G991	A911	C838	A769	G607	G534	A456	A355	G289
G1386	G1302	U1214	G	A1075	G991	A911	C838	A769	G607	G535	A456	A355	G290
G1386	G1302	U1215	C	A1076	G991	A911	C838	A769	G607	G536	A456	A355	C294
G1386	G1302	U1216	G	A1077	G991	A911	C838	A769	G607	G537	A456	A355	C295
G1386	G1302	U1217	U	A1078	G991	A911	C838	A769	G607	G538	A456	A355	U296
G1386	G1302	U1218	U	A1079	G991	A911	C838	A769	G607	G539	A456	A355	C297
G1386	G1302	U1219	U	A1080	G991	A911	C838	A769	G607	G540	A456	A355	G297
G1386	G1302	U1220	A	U1081	G991	A911	C838	A769	G607	G541	A456	A355	U382
G1386	G1302	U1221	A	U1082	G991	A911	C838	A769	G607	G542	A456	A355	A383
G1386	G1302	U1222	G	U1083	G991	A911	C838	A769	G607	G543	A456	A355	G384
G1386	G1302	U1223	C	U1084	G991	A911	C838	A769	G607	G544	A456	A355	U386
G1386	G1302	U1224	U	U1085	G991	A911	C838	A769	G607	G545	A456	A355	G387
G1386	G1302	U1225	U	U1086	G991	A911	C838	A769	G607	G546	A456	A355	A388
G1386	G1302	U1226	U	U1087	G991	A911	C838	A769	G607	G547	A456	A355	G389
G1386	G1302	U1227	U	U1088	G991	A911	C838	A769	G607	G548	A456	A355	A306
G1386	G1302	U1228	U	U1089	G991	A911	C838	A769	G607	G549	A456	A355	A307
G1386	G1302	U1229	U	U1090	G991	A911	C838	A769	G607	G550	A456	A355	C310
G1386	G1302	U1230	U	U1091	G991	A911	C838	A769	G607	G551	A456	A355	C311
G1386	G1302	U1231	U	U1092	G991	A911	C838	A769	G607	G552	A456	A355	C312
G1386	G1302	U1232	U	U1093	G991	A911	C838	A769	G607	G553	A456	A355	A313
G1386	G1302	U1233	U	U1094	G991	A911	C838	A769	G607	G554	A456	A355	C316
G1386	G1302	U1234	U	U1095	G991	A911	C838	A769	G607	G555	A456	A355	C319
G1386	G1302	U1235	U	U1096	G991	A911	C838	A769	G607	G556	A456	A355	A323
G1386	G1302	U1236	U	U1097	G991	A911	C838	A769	G607	G557	A456	A355	A324
G1386	G1302	U1237	U	U1098	G991	A911	C838	A769	G607	G558	A456	A355	G325
G1386	G1302	U1238	U	U1099	G991	A911	C838	A769	G607	G559	A456	A355	C326
G1386	G1302	U1239	U	U1100	G991	A911	C838	A769	G607	G560	A456	A355	U330
G1386	G1302	U1240	U	U1101	G991	A911	C838	A769	G607	G561	A456	A355	G331
G1386	G1302	U1241	U	U1102	G991	A911	C838	A769	G607	G562	A456	A355	A334
G1386	G1302	U1242	U	U1103	G991	A911	C838	A769	G607	G563	A456	A355	
G1386	G1302	U1243	U	U1104	G991	A911	C838	A769	G607	G564	A456	A355	
G1386	G1302	U1244	U	U1105	G991	A911	C838	A769	G607	G565	A456	A355	
G1386	G1302	U1245	U	U1106	G991	A911	C838	A769	G607	G566	A456	A355	
G1386	G1302	U1246	U	U1107	G991	A911	C838	A769	G607	G567	A456	A355	
G1386	G1302	U1247	U	U1108	G991	A911	C838	A769	G607	G568	A456	A355	
G1386	G1302	U1248	U	U1109	G991	A911	C838	A769	G607	G569	A456	A355	
G1386	G1302	U1249	U	U1110	G991	A911	C838	A769	G607	G570	A456	A355	
G1386	G1302	U1250	U	U1111	G991	A911	C838	A769	G607	G571	A456	A355	
G1386	G1302	U1251	U	U1112	G991	A911	C838	A769	G607	G572	A456	A355	
G1386	G1302	U1252	U	U1113	G991	A911	C838	A769	G607	G573	A456	A355	
G1386	G1302	U1253	U	U1114	G991	A911	C838	A769	G607	G574	A456	A355	
G1386	G1302	U1254	U	U1115	G991	A911	C838	A769	G607	G575	A456	A355	
G1386	G1302	U1255	U	U1116	G991	A911	C838	A769	G607	G576	A456	A355	
G1386	G1302	U1256	U	U1117	G991	A911	C838	A769	G607	G577	A456	A355	
G1386	G1302	U1257	U	U1118	G991	A911	C838	A769	G607	G578	A456	A355	
G1386	G1302	U1258	U	U1119	G991	A911	C838	A769	G607	G579	A456	A355	
G1386	G1302	U1259	U	U1120	G991	A911	C838	A769	G607	G580	A456	A355	
G1386	G1302	U1260	U	U1121	G991	A911	C838	A769	G607	G581	A456	A355	
G1386	G1302	U1261	U	U1122	G991	A911	C838	A769	G607	G582	A456	A355	
G1386	G1302	U1262	U	U1123	G991	A911	C838	A769	G607	G583	A456	A355	
G1386	G1302	U1263	U	U1124	G991	A911	C838	A769	G607	G584	A456	A355	
G1386	G1302	U1264	U	U1125	G991	A911	C838	A769	G607	G585	A456	A355	
G1386	G1302	U1265	U	U1126	G991	A911	C838	A769	G607	G586	A456	A355	
G1386	G1302	U1266	U	U1127	G991	A911	C838	A769	G607	G587	A456	A355	
G1386	G1302	U1267	U	U1128	G991	A911	C838	A769	G607	G588	A456	A355	
G1386	G1302	U1268	U	U1129	G991	A911	C838	A769	G607	G589	A456	A355	
G1386	G1302	U1269	U	U1130	G991	A911	C838	A769	G607	G590	A456	A355	
G1386	G1302	U1270	U	U1131	G991	A911	C838	A769	G607	G591	A456	A355	
G1386	G1302	U1271	U	U1132	G991	A911	C838	A769	G607	G592	A456	A355	
G1386	G1302	U1272	U	U1133	G991	A911	C838	A769	G607	G593	A456	A355	
G1386	G1302	U1273	U	U1134	G991	A911	C838	A769	G607	G594	A456	A355	
G1386	G1302	U1274	U	U1135	G991	A911	C838	A769	G607	G595	A456	A355	
G1386	G1302	U1275	U	U1136	G991	A911	C838	A769	G607	G596	A456	A355	
G1386	G1302	U1276	U	U1137	G991	A911	C838	A769	G607	G597	A456	A355	
G1386	G1302	U1277	U	U1138	G991	A911	C838	A769	G607	G598	A456	A355	
G1386	G1302	U1278	U	U1139	G991	A911	C838	A769	G607	G599	A456	A355	
G1386	G1302	U1279	U	U1140	G991	A911	C838	A769	G607	G600	A456	A355	
G1386	G1302	U1280	U	U1141	G991	A911	C838	A769	G607	G601	A456	A355	
G1386	G1302	U1281	U	U1142	G991	A911	C838	A769	G607	G602	A456	A355	
G1386	G1302	U1282	U	U1143	G991	A911	C838	A769	G607	G603	A456	A355	
G1386	G1302	U1283	U	U1144	G991	A911	C838	A769	G607	G604	A456	A355	
G1386	G1302	U1284	U	U1145	G991	A911	C838	A769	G607	G605	A456	A355	
G1386	G1302	U1285	U	U1146	G991	A911	C838	A769	G607	G606	A456	A355	
G1386	G1302	U1286	U	U1147	G991	A911	C838	A769	G607	G607	A456	A355	
G1386	G1302	U1287	U	U1148	G991	A911	C838	A769	G607	G608	A456	A355	
G1386	G1302	U1288	U	U1149	G991	A911	C838	A769	G607	G609	A456	A355	
G1386	G1302	U1289	U	U1150	G991	A911	C838	A769	G607	G610	A456	A355	
G1386	G1302	U1290	U	U1151	G991	A911	C838	A769	G607	G611	A456	A355	
G1386	G1302	U1291	U	U1152	G991	A911	C838	A769	G607	G612	A456	A355	
G1386	G1302	U1292	U	U1153	G991	A911	C838	A769	G607	G613	A456	A355	
G1386	G1302	U1293	U	U1154	G991	A911	C838	A769	G607	G614	A456	A355	
G1386													





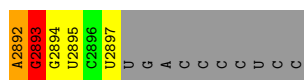
• Molecule 25: 23S Ribosomal RNA

Chain DA: 36% 41% 14% 7%



A1689	G1538	C1467	A1392	C1315	A1247	A	G	A981	C915	G854	G775	G686
U1692	G1539	G1468	A1393	G1319	A1248	U	G	C982	G916	G855	G776	C887
U1693	U1540	G1470	A1394	C1320	U1249	C	U	A983	A917	C856	A777	U688
	A1541	A1471	A1395	A1321	G1250	A	C	A984	A918	C857		
	C1542	A1472	U1396	A1322	C1251	A	G	U858	G919	A782	A783	C692
	A1543	G1473	U1397	U1323	G1252		G	C985	G920	A783	A784	C693
	A1544	G1474	C1398	U1324	A1253		C	C986	G921	G859		
	A1545	G1475	C1399	G1324	C1181		C	C987	U922	U860		
	A1546	G1476			A1182		C		G923	A861		
	A1554	G1477	C1403	C1327	U1255		A	A990	C924	G862		
	A1554	G1478	A1404	U1328	G1183		G	C991	A926	A863	G704	G705
	C1557	G1479	U1405	U1329	C1257		G	C994	G927	A788		
	A1558		U1406	C1330	G1187		A	C995	G928	C865	C790	A705
	G1559		C1407	A1331	U1188		G	A996	G932	A866	C791	C708
	G1563		C1408	G1332	G1259		G	C997	G933	C867	G792	U709
	G1563		G1410	C1333	G1260		U	C998	A933	U868	A793	G710
	G1564		C1411	U1334	C1261		U	C999	G940	G869	G794	
	C1565		G1487	U1335	G1191		G	U1000	G942	A870	C795	G717
	C1565		A1412	G1192	C1123		G		G943	U871	C796	A718
	U1566		G1413	U1193	G1124		C		U943	A872	C797	C719
	A1490			G1197	G1125		U		G944	C873	C798	C720
			G1416	A1126			U		G945	G874	G799	
			G1417				U		A946	C875	G799	
			G1418	U1198	U1198		A		G947	A800	G801	G723
	A1494		U1340	U1199	G1130		G		G948	C876	G801	U724
	A1495		U1341	C1200	G1131		A		G949	U877	G725	G725
	A1496		U1420	C1201	A1132		A		G950	A878	A802	G726
	U1497		G1421		U1133		G		C884	C879	G805	
	C1498			A1204	U1135		C		C885	G880	C806	C730
			C1345	U1205	G1136		C		C886	G881	U807	C731
			G1348	U1206	U1137		C		C887	G882	G808	C732
			C1349	C1208	G1138		C		C888	G883	G733	G733
			C1350	U1209	U1139		C		C889	A890	C816	G739
			C1351	A1210	G1139		C		C890	G892	C817	U740
			U1352	U1211	U1141		U		C891	G893	G818	U741
			A1353	A1212	U1142		C		C892	C894	A819	G742
			A1354	A1213	A1143		U		C893	A824	U747	G743
			C1432	A1214	G1144		U		C894	U826	G748	
			U1433	G1219			U		C895	C897	U827	
			A1358	U1285			A		C896	C898	U828	A752
			A1359	A1286			A		C897	A900	A829	C753
			A1360	U1287			U		C898	C902	G831	C755
			C1363	U1288			U		C899	C903		
			G1364	C1289			A		C900	C904	C837	G760
			A1365	C1290			G		C901	U905	G838	A761
			A1365	C1291			G		C902	G906	U839	U762
			G1368	U1292			U		C903	U907	C840	G763
			G1369	C1293			U		C904	C908	A764	G763
			C1370	U1300			U		C905	A909	G765	G765
			G1371	U1301			A		C906	U910	U847	
			U1372	A1301			A		C907	A911	G848	
			G1377	C1293			U		C908	C912	A849	
			A1378	G1235			A		C909	C913	G852	U773
			A1379	G1236			U		C910	C914	G853	A774
			G1380	G1237			U		C911			
			A1381	U1165			A		C912			
			G1380	G1166			G		C913			
			A1384	C1238			U		C914			
			G1385	G1239			C		C915			
			C1386	U1240			U		C916			
			C1387	G1168			C		C917			
			C1387	G1169			C		C918			
			C1387	G1170			A		C919			
			C1387	G1171			C		C920			
			C1387	G1171			U		C921			
			C1387	G1171			U		C922			
			C1387	G1171			U		C923			
			C1387	G1171			U		C924			
			C1387	G1171			U		C925			
			C1387	G1171			U		C926			
			C1387	G1171			U		C927			
			C1387	G1171			U		C928			
			C1387	G1171			U		C929			
			C1387	G1171			U		C930			
			C1387	G1171			U		C931			
			C1387	G1171			U		C932			
			C1387	G1171			U		C933			
			C1387	G1171			U		C934			
			C1387	G1171			U		C935			
			C1387	G1171			U		C936			
			C1387	G1171			U		C937			
			C1387	G1171			U		C938			
			C1387	G1171			U		C939			
			C1387	G1171			U		C940			
			C1387	G1171			U		C941			
			C1387	G1171			U		C942			
			C1387	G1171			U		C943			
			C1387	G1171			U		C944			
			C1387	G1171			U		C945			
			C1387	G1171			U		C946			
			C1387	G1171			U		C947			
			C1387	G1171			U		C948			
			C1387	G1171			U		C949			
			C1387	G1171			U		C950			
			C1387	G1171			U		C951			
			C1387	G1171			U		C952			
			C1387	G1171			U		C953			
			C1387	G1171			U		C954			
			C1387	G1171			U		C955			
			C1387	G1171			U		C956			
			C1387	G1171			U		C957			
			C1387	G1171			U		C958			
			C1387	G1171			U		C959			
			C1387	G1171			U		C960			
			C1387	G1171			U		C961			
			C1387	G1171			U		C962			
			C1387	G1171			U		C963			
			C1387	G1171			U		C964			
			C1387	G1171			U		C965			
			C1387	G1171			U		C966			
			C1387	G1171			U		C967			
			C1387	G1171			U		C968			
			C1387	G1171			U		C969			
			C1387	G1171			U		C970			
			C1387	G1171			U		C971			
			C1387	G1171			U		C972			
			C1387	G1171			U		C973			
			C1387	G1171			U		C974			
			C1387	G1171			U		C975			
			C1387	G1171			U		C976			
			C1387	G1171			U		C977			
			C1387	G1171			U		C978			
			C1387	G1171			U		C979			
			C1387	G1171			U		C980			
			C1387	G1171			U		C981			
			C1387	G1171			U		C982			
			C1387	G1171			U		C983			
			C1387	G1171			U		C984			
			C1387	G1171			U		C985			
			C1387	G1171			U		C986			
			C1387	G1171			U		C987			
			C1387	G1171			U		C988			
			C1387	G1171			U		C989			
			C1387	G1171			U		C990			
			C1387	G1171			U		C991			
			C1387	G1171			U		C992			
			C1387	G1171			U		C993			
			C1387	G1171			U		C994			
			C1387	G1171			U		C995			
			C1387	G1171			U		C996			
			C1387	G1171			U		C997			
			C1387	G1171			U		C998			
			C1387	G1171			U		C999			
			C1387	G1171			U		C1000			
			C1387	G1171			U		C1001			
			C1387	G1171			U		C1002			
			C1387	G1171			U		C1003			
			C1387	G1171			U		C1004			
			C1387	G1171			U		C1005			
			C1387	G1171			U		C1006			
			C1387	G1171			U		C1007			
			C1387	G1171			U		C10			

A2821	A2749	C2559	G2455	G2382	G2314	C2248	C	G2032	G1959	U1851	C1781
G2822	A2750	C2540	G2461	G2383	G2315	U2249	C	A2033	A1960	C1852	C1782
A2823	G2751	A2541	C2462	G2384	C2316	G2250	U	U2034	U1963	A1783	A1783
C2824	G2752	A2542	C2463	G2385	C2317	G2251	A	G2037	G1964	A1784	A1784
C2825	C2610	G2545	C2464	G2386	G2318	G2252	A	G2038	C1965	A1785	A1785
C2826	U2611	U2546		G2387	G2319	G2253	U	C2039	A1966	A1786	A1786
A2827	C2612			A2388	A2320	G2254	A	G2040	G1967	A1787	A1787
A2828				G2389	G2321	G2255	C	C2041	G1968	C1788	C1788
A2829	U2615	G2549	G2468	G2390	G2322	G2256	C	U2042	G1969	A1789	A1789
A2758	C2616	G2550	A2469	G2391	G2323	G2257	A	A2043	A1970	A1876	A1876
G2759	C2617	C2551	C2470	A2392	G2324	C2258	C	C2044	A1971	A1877	A1877
G2697	G2618	U2552	A2472	A2393	A2327	C2259	C	C2045	A1972	G1878	G1878
U2698		U2553	U2473	C2394	G2328	C2260	U	G2046	G1973		
C2699		U2554	C2474	A2395	G2329	C2261	A	G2047	G1974		
	G2625	U2555		G2396	G2330	U2262	G	U2048	C1975	A1885	A1885
C2703	C2628	U2556	A2475	G2397	G2331		U	G2049	G1976	C1886	C1886
C2704	A2629	C2557	C2476	U2398	G2332	U2265	G	C2050	U1977	A1889	A1889
A2705	G2630	G2558	A2478	G2399	A2333	A2266	C	A2051	A1978	A1890	A1890
	G2631	C2559		G2400	G2334	A2267	C	G2052	C1983	G1895	G1895
G2708	G2632	C2560	C2483	U2401	A2335	A2268	A		G1984	G1899	G1899
G2709		U2561		C2402	A2336		G	C2055	G1985	A1900	A1900
C2710	C2635	U2562	G2487	G2403	G2337	U2271	C	G2056	A1986	A1802	A1802
A2711	U2636	U2563	A2488	C2404	G2338	U2272	C			A1803	A1803
U2712		A2564	G2489	G2405	G2339	A2273	U			A1804	A1804
A2712A		U2565	G2490	U2406	G2342	A2274	C			U1805	U1805
A2713	A2639	A2566		G2407	C2343	C2275	U	A2059	U1991	G1806	G1806
G2714		C2567		U2408	U2344	C2276	G	A2060	G1992	G1807	G1807
U2715	G2643	C2568	G2494	G2409	C2345	G2277	A	G2061	U1993	A1810	A1810
U2716	G2644	G2569	G2495	G2410	G2346	G2280	C	A2062	G1996	G1811	G1811
G2717	G2645	G2570	A2497	G2411	A2347	G2281	C	C2063	C1997	A1812	A1812
G2718	G2646	G2571	C2498	G2412	U2348	G2282	C		G1998	G1813	G1813
G2719	U2647	C2572	C2499	G2413	U2349	G2283	C	G2069	G1999	G1814	G1814
U2720	C2648	A2573	U2500	G2414	U2350	G2284	C	G2070	G2000	A1815	A1815
A2721	U2649	C2574	G2501	C2420	A2352	G2285	C	G2071	G2003	G1816	G1816
G2722	U2650	G2575	C2502	G2421	C2355	A2286	G	G2072	A2004	G1817	G1817
C2723		C2576	U2503	A2422	C2356	A2287	C	U2074	G2005	U1818	U1818
C2724	U2653	U2577	U2504	A2423	C2357	A2288	U	U2075	C2006	A1819	A1819
A2725	A2654	G2578	G2505	A2424	U2357	A2289	C	U2076			
U2726			U2506	A2425	G2358	G2290	C		G2009	G1822	G1822
G2727	A2657	G2581	C2507	A2426	C2359	G2291	C	C2078	G2010	G1823	G1823
U2728	C2658	G2582	C2508	C2427	A2360	U2292	G	U2079	A1927	G1824	G1824
G2729	G2659	G2583	C2509	G2428	A2361	C2293	G	G2080	A1928	A1825	A1825
C2730	A2660	U2584	G2512	G2429	G2362	C2294	U	C2081	G1929	G1826	G1826
G2731	G2661	U2585		A2430	C2363	C2295	G	A2082	G1930	C1827	C1827
G2732	A2662	C2586		A2434	C2364	G2296	G	G2083	A1931	G1828	G1828
A2733	G2663	A2587	C2517	A2435	A2365	U2297	C	C2084	A1932	A1829	A1829
A2734		G2588	C2518	A2436	A2366	C2298	G	U2085	U2016	G1933	G1933
G2735	C2666	G2589	U2519	A2439	A2369	A2299	G	U2086	U2017	U1833	U1833
G2736	C2667	A2590	C2520	C2440	C2370	G2299	C		G2018	A1936	A1936
G2737	A2671	C2591	C2521	C2441	G2371	G2300	G	U2096	A2019	A1937	A1937
U2738	G2672	G2592		C2442	G2372	C2301	C	C2097	A2020	A1938	A1938
A2739			G2525	G2445	G2373	G2302	A	U2098	G2021	U1939	U1939
U2740	G2679	G2595	C2526	G2446	G2374	G2303	G	U2099	U2022	G1945	G1945
A2741	C2680	U2528	C2527	G2447	G2375	A2304	G	G2100	G2023	G1840	G1840
C2742	G2681	U2529	G2529	A2448	A2376	A2305	C	G2101	G2024	U1946	U1946
G2743	U2682	G2599	G2536		A2377	G2308	C	U	U2028	G1845	G1845
G2744	C2683	C2601	U2537	A2451	A2378	U2244	C	C	G2029	G1846	G1846
C2745	C2684	A2602	U2538	C2452	C2380	U2245	C	G	A2030	A1847	A1847
U2746	G2685	G2603	C2538		C2381	U2246	G	C	G1956	A1848	A1848
G2747		U2604				U2247	C	G	U1958		
A2748						U2248	C	G			



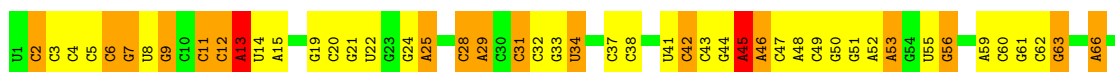
- Molecule 26: 5S Ribosomal RNA

Chain BB: 50% 38% 10% ..



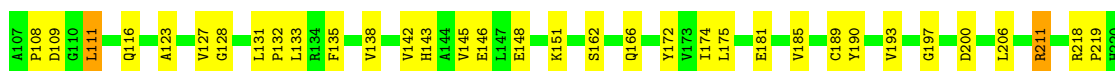
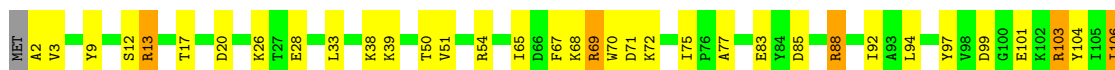
- Molecule 26: 5S Ribosomal RNA

Chain DB: 30% 47% 19% ..



- Molecule 27: 50S Ribosomal Protein L2

Chain BD: 69% 27% .

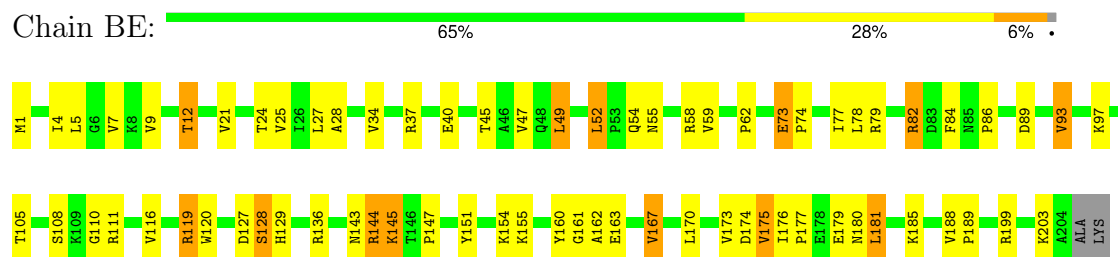


- Molecule 27: 50S Ribosomal Protein L2

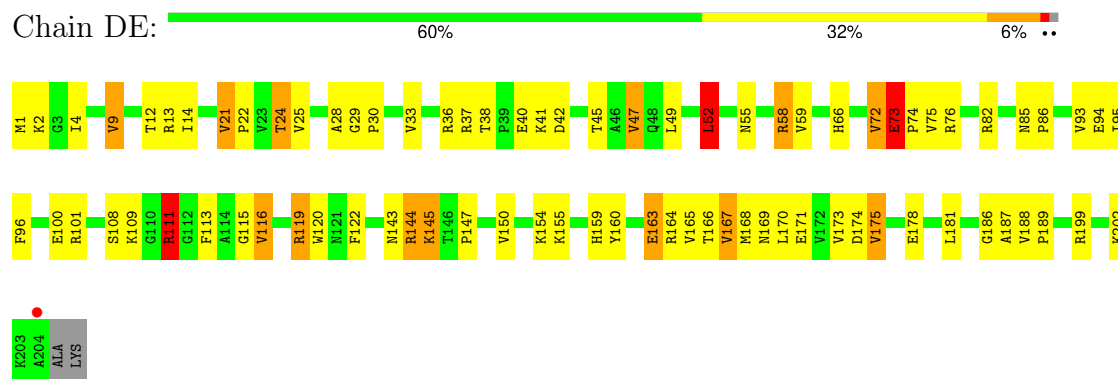
Chain DD: 67% 28% 5%



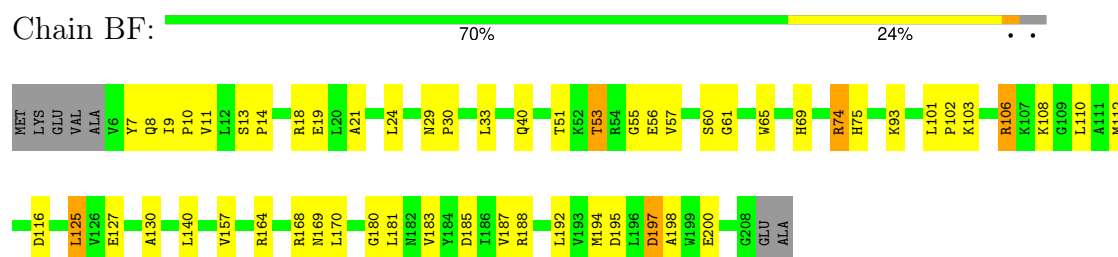
- Molecule 28: 50S Ribosomal Protein L3



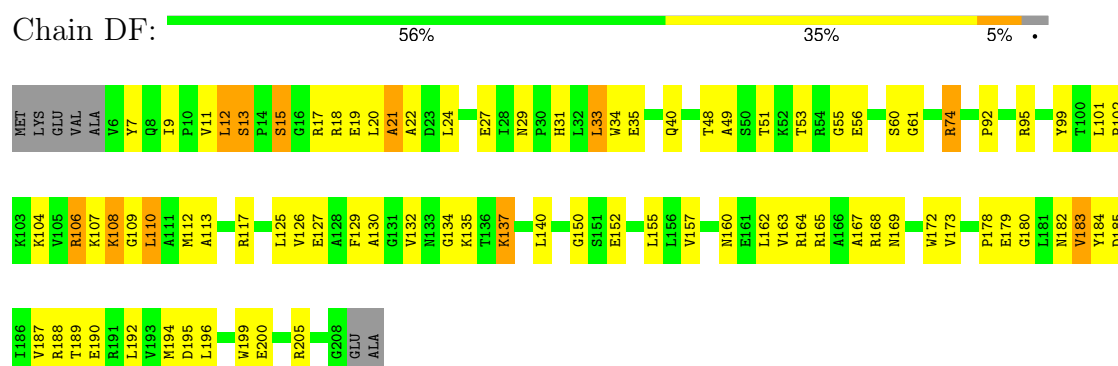
• Molecule 28: 50S Ribosomal Protein L3



• Molecule 29: 50S Ribosomal Protein L4

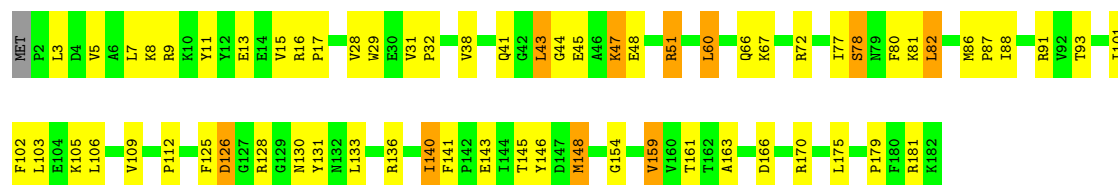


• Molecule 29: 50S Ribosomal Protein L4

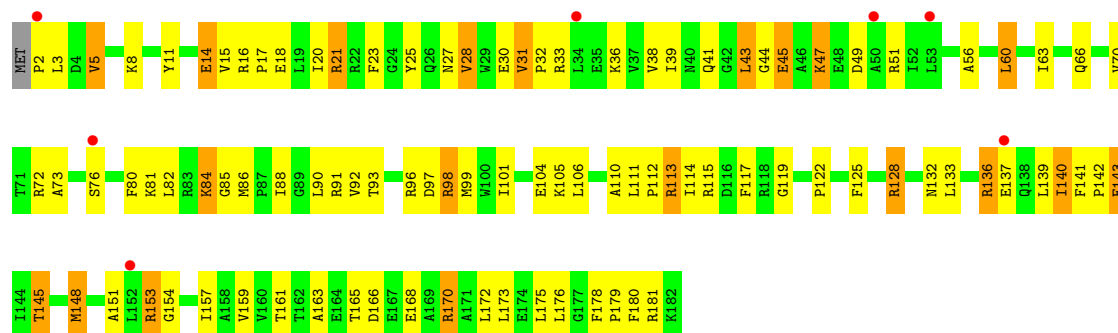


• Molecule 30: 50S Ribosomal Protein L5

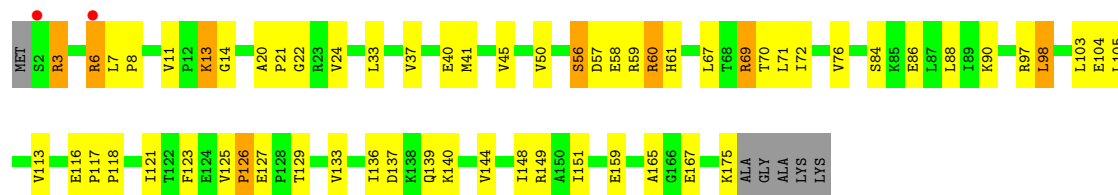




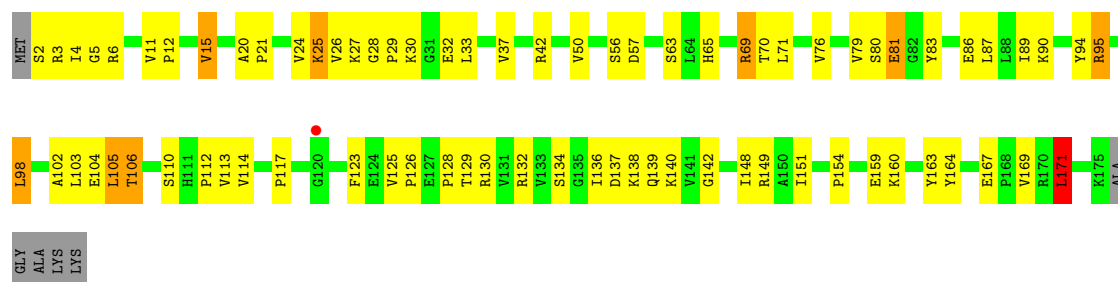
• Molecule 30: 50S Ribosomal Protein L5



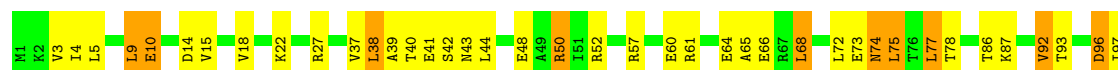
• Molecule 31: 50S Ribosomal Protein L6



• Molecule 31: 50S Ribosomal Protein L6



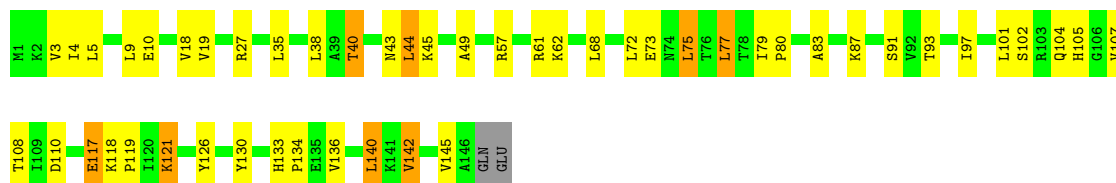
• Molecule 32: 50S Ribosomal Protein L9





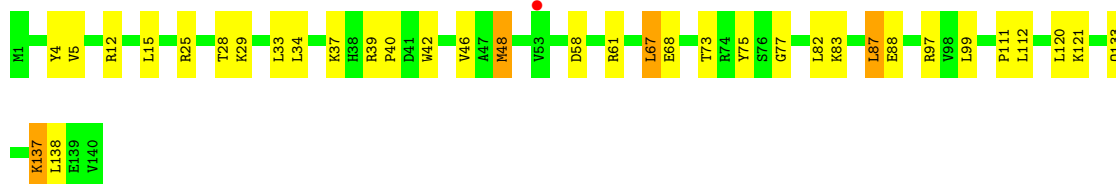
• Molecule 32: 50S Ribosomal Protein L9

Chain DI: 66% 28% 5% •



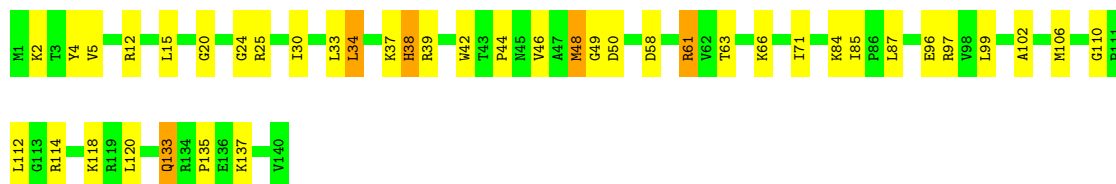
• Molecule 33: 50S Ribosomal Protein L13

Chain BN: 75% 22% •



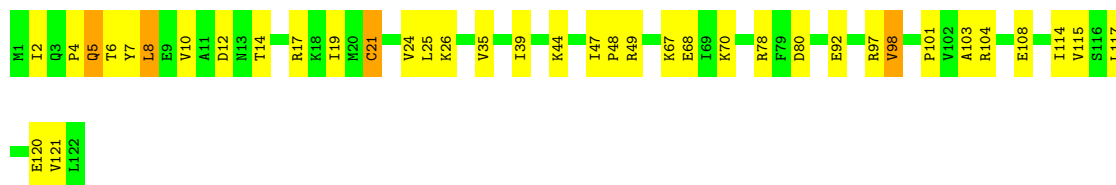
• Molecule 33: 50S Ribosomal Protein L13

Chain DN: 71% 26% •



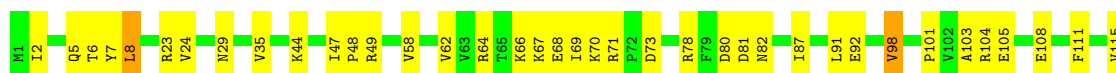
• Molecule 34: 50S Ribosomal Protein L14

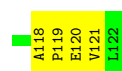
Chain BO: 69% 28% •



• Molecule 34: 50S Ribosomal Protein L14

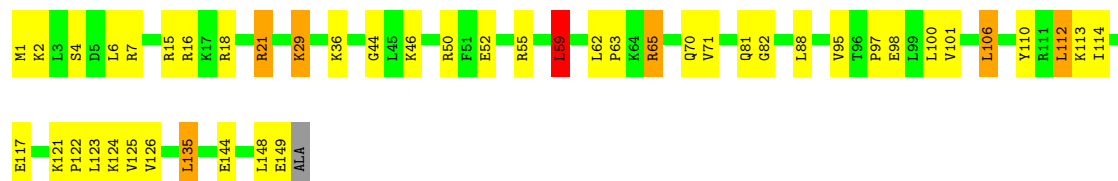
Chain DO: 66% 33% •





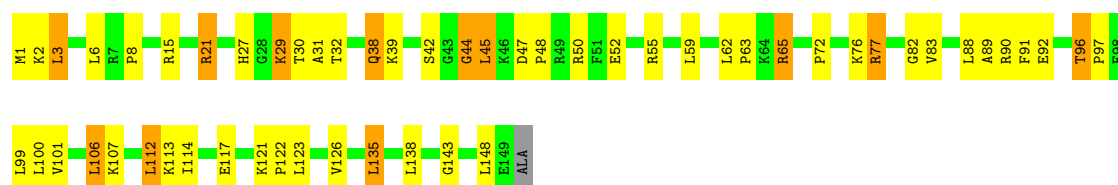
• Molecule 35: 50S Ribosomal Protein L15

Chain BP: 69% 26%



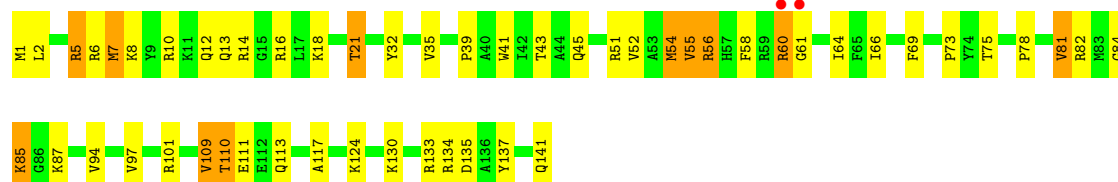
• Molecule 35: 50S Ribosomal Protein L15

Chain DP: 63% 29% 8%



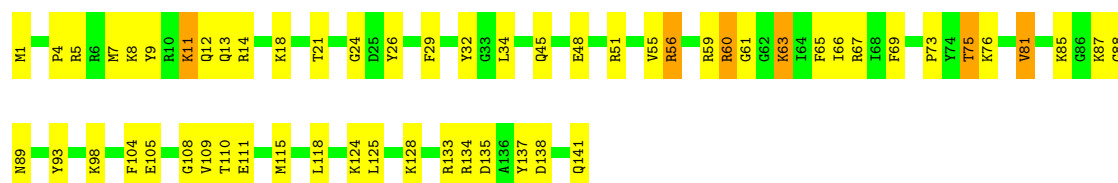
• Molecule 36: 50S Ribosomal Protein L16

Chain BQ: 62% 30% 8%



• Molecule 36: 50S Ribosomal Protein L16

Chain DQ: 60% 36%



• Molecule 37: 50S Ribosomal Protein L17

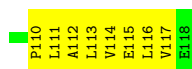
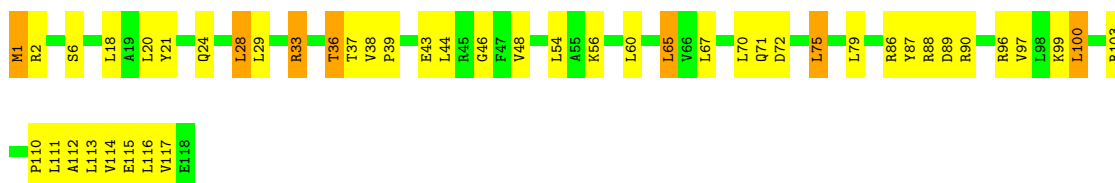
Chain BR: 68% 21% 11%





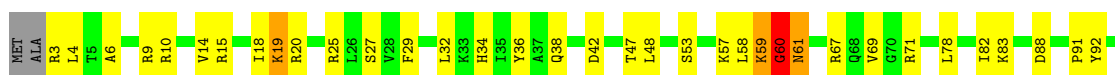
• Molecule 37: 50S Ribosomal Protein L17

Chain DR: 61% 33% 6%



• Molecule 38: 50S Ribosomal Protein L18

Chain BS: 64% 30% ...



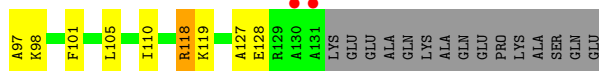
• Molecule 38: 50S Ribosomal Protein L18

Chain DS: 4% 48% 42% 8%



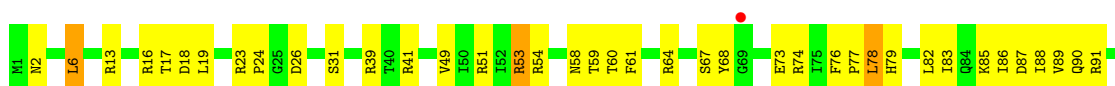
• Molecule 39: 50S Ribosomal Protein L19

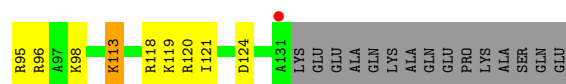
Chain BT: 60% 28% 10%



• Molecule 39: 50S Ribosomal Protein L19

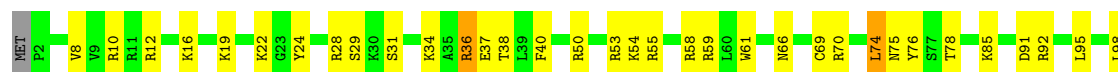
Chain DT: 57% 30% 10%





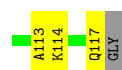
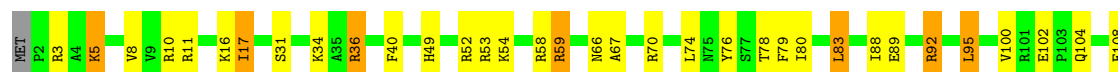
• Molecule 40: 50S Ribosomal Protein L20

Chain BU: 65% 31%



• Molecule 40: 50S Ribosomal Protein L20

Chain DU: 67% 25% 6%



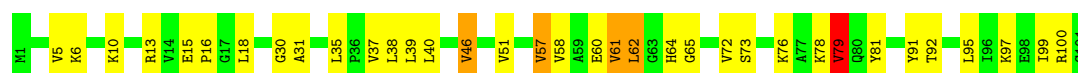
• Molecule 41: 50S Ribosomal Protein L21

Chain BV: 74% 20% 5%



• Molecule 41: 50S Ribosomal Protein L21

Chain DV: 65% 30%



• Molecule 42: 50S Ribosomal Protein L22

Chain BW: 77% 19%



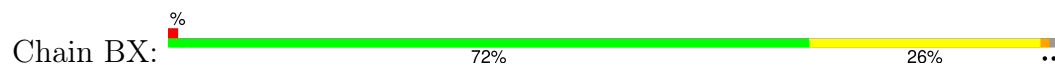
• Molecule 42: 50S Ribosomal Protein L22

Chain DW: 65% 32%

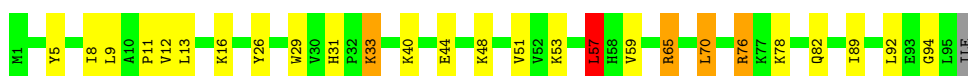




- Molecule 43: 50S Ribosomal Protein L23



- Molecule 43: 50S Ribosomal Protein L23



- Molecule 44: 50S Ribosomal Protein L24



- Molecule 44: 50S Ribosomal Protein L24

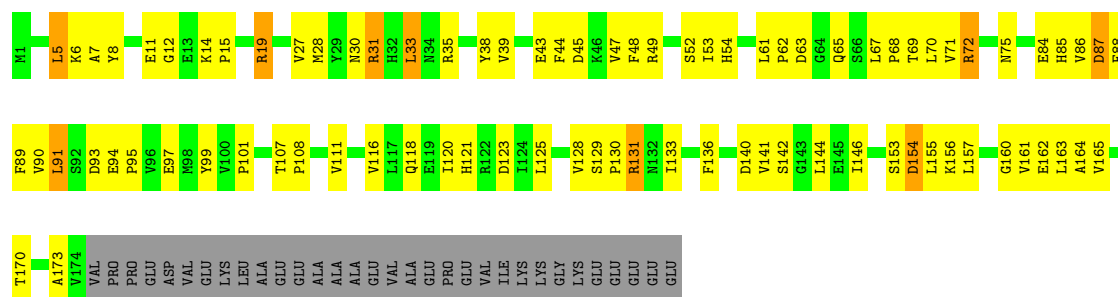


- Molecule 45: 50S Ribosomal Protein L25




- Molecule 45: 50S Ribosomal Protein L25

Chain DZ:  44% 36% 16%



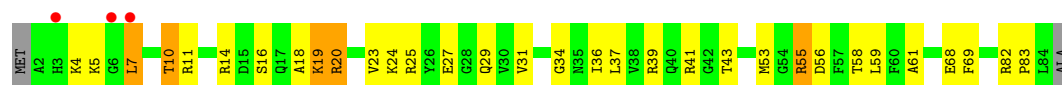
• Molecule 46: 50S Ribosomal Protein L27

Chain B0:  73% 19% 6%



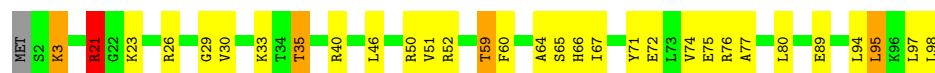
• Molecule 46: 50S Ribosomal Protein L27

Chain D0:  60% 32% 6%



• Molecule 47: 50S Ribosomal Protein L28

Chain B1:  67% 27% 6%



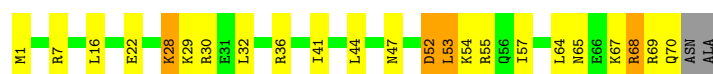
• Molecule 47: 50S Ribosomal Protein L28

Chain D1:  64% 29% 6%



• Molecule 48: 50S Ribosomal Protein L29

Chain B2:  65% 26% 6%

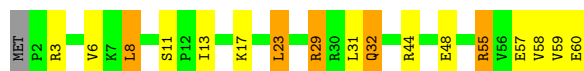


• Molecule 48: 50S Ribosomal Protein L29

Chain D2:  61% 29% 7%



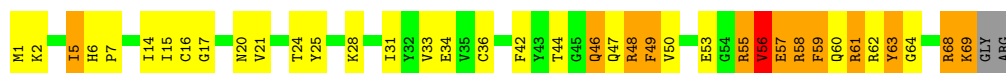
- Molecule 49: 50S Ribosomal Protein L30



- Molecule 49: 50S Ribosomal Protein L30



- Molecule 50: 50S Ribosomal Protein L31



- Molecule 50: 50S Ribosomal Protein L31



- Molecule 51: 50S Ribosomal Protein L32



- Molecule 51: 50S Ribosomal Protein L32

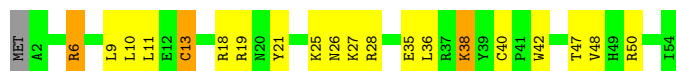


- Molecule 52: 50S Ribosomal Protein L33

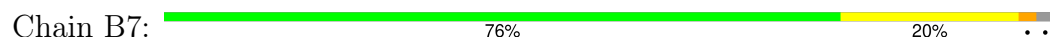




- Molecule 52: 50S Ribosomal Protein L33



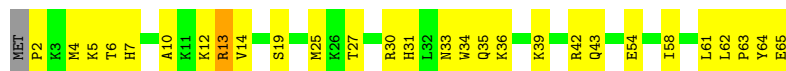
- Molecule 53: 50S Ribosomal Protein L34



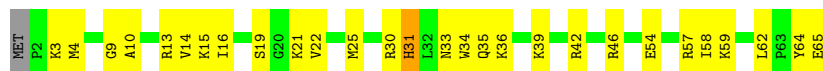
- Molecule 53: 50S Ribosomal Protein L34



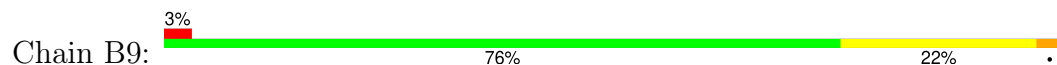
- Molecule 54: 50S Ribosomal Protein L35



- Molecule 54: 50S Ribosomal Protein L35

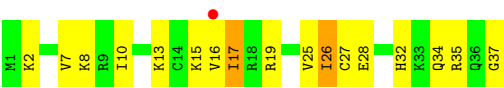


- Molecule 55: 50S Ribosomal Protein L36



- Molecule 55: 50S Ribosomal Protein L36





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.08Å 449.83Å 619.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 3.00 49.74 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.74-3.00) 98.8 (49.74-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.203 , 0.259 0.203 , 0.257	Depositor DCC
R_{free} test set	57319 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	286321	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2QY, MVA, K, MG, 2QZ, 2R3, SF4, ZN, FME, 2R1, 004

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	0.77	7/36038 (0.0%)	1.39	355/56244 (0.6%)
1	CA	0.76	13/36170 (0.0%)	1.43	365/56452 (0.6%)
2	AB	0.49	0/1881	0.77	0/2542
2	CB	0.56	0/1860	0.81	2/2518 (0.1%)
3	AC	0.48	0/1576	0.64	0/2130
3	CC	0.50	0/1566	0.72	2/2119 (0.1%)
4	AD	0.49	0/1689	0.76	1/2267 (0.0%)
4	CD	0.50	0/1704	0.71	0/2284
5	AE	0.47	0/1145	0.71	0/1543
5	CE	0.50	0/1149	0.76	0/1548
6	AF	0.48	0/819	0.69	0/1111
6	CF	0.53	0/829	0.76	0/1123
7	AG	0.48	0/1250	0.66	1/1679 (0.1%)
7	CG	0.50	0/1254	0.72	1/1683 (0.1%)
8	AH	0.46	0/1108	0.69	0/1494
8	CH	0.47	0/1108	0.71	0/1494
9	AI	0.47	0/1002	0.73	1/1346 (0.1%)
9	CI	0.56	0/997	0.75	2/1343 (0.1%)
10	AJ	0.47	0/722	0.67	0/982
10	CJ	0.53	0/727	0.69	0/988
11	AK	0.44	0/844	0.65	1/1145 (0.1%)
11	CK	0.46	0/848	0.67	0/1149
12	AL	0.50	0/946	0.73	0/1274
12	CL	0.52	0/946	0.74	0/1274
13	AM	0.48	0/969	0.68	0/1302
13	CM	0.48	0/961	0.66	0/1291
14	AN	0.48	0/501	0.71	0/664
14	CN	0.55	0/501	0.71	0/664
15	AO	0.49	0/739	0.76	0/985
15	CO	0.47	0/739	0.70	0/985
16	AP	0.47	0/697	0.73	0/939
16	CP	0.49	0/693	0.70	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.51	0/836	0.68	0/1117
17	CQ	0.51	0/836	0.70	0/1117
18	AR	0.48	0/560	0.73	0/746
18	CR	0.50	0/560	0.75	1/746 (0.1%)
19	AS	0.47	0/667	0.66	0/900
19	CS	0.50	0/661	0.80	1/893 (0.1%)
20	AT	0.48	0/730	0.77	0/965
20	CT	0.43	0/729	0.68	0/965
21	AU	0.47	0/203	0.62	0/266
21	CU	0.51	0/203	0.64	0/266
22	AV	0.99	0/127	1.42	2/198 (1.0%)
22	CV	0.82	0/126	1.39	1/195 (0.5%)
23	AX	0.88	8/1813 (0.4%)	1.62	47/2825 (1.7%)
23	CX	0.94	6/1813 (0.3%)	1.87	57/2825 (2.0%)
24	AW	0.46	0/20	0.84	0/23
24	CW	0.34	0/20	0.64	0/23
25	BA	1.07	33/65892 (0.1%)	1.49	877/102850 (0.9%)
25	DA	0.82	13/65466 (0.0%)	1.46	741/102184 (0.7%)
26	BB	0.83	0/2878	1.31	13/4490 (0.3%)
26	DB	0.93	2/2878 (0.1%)	1.50	45/4490 (1.0%)
27	BD	0.71	2/2186 (0.1%)	0.82	0/2944
27	DD	0.63	2/2186 (0.1%)	0.77	0/2944
28	BE	0.72	0/1592	0.77	0/2149
28	DE	0.57	0/1592	0.79	2/2149 (0.1%)
29	BF	0.73	0/1619	0.75	0/2193
29	DF	0.53	0/1615	0.80	2/2188 (0.1%)
30	BG	0.46	0/1450	0.71	0/1959
30	DG	0.54	0/1449	0.76	0/1958
31	BH	0.61	0/1356	0.72	0/1834
31	DH	0.54	0/1356	0.71	1/1834 (0.1%)
32	BI	0.51	0/1100	0.70	0/1501
32	DI	0.51	0/1076	0.74	0/1471
33	BN	0.67	0/1144	0.75	0/1543
33	DN	0.54	0/1144	0.74	0/1543
34	BO	0.66	0/943	0.78	1/1269 (0.1%)
34	DO	0.56	0/943	0.78	1/1269 (0.1%)
35	BP	0.64	0/1152	0.82	1/1533 (0.1%)
35	DP	0.55	0/1152	0.83	2/1533 (0.1%)
36	BQ	0.69	0/1143	0.81	0/1527
36	DQ	0.59	0/1143	0.77	0/1527
37	BR	0.62	0/982	0.86	0/1312
37	DR	0.51	0/982	0.70	0/1312
38	BS	0.55	0/887	0.78	1/1180 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DS	0.51	0/880	0.74	0/1172
39	BT	0.59	0/1105	0.79	0/1477
39	DT	0.53	0/1097	0.74	0/1468
40	BU	0.70	0/977	0.76	0/1301
40	DU	0.52	0/977	0.71	0/1301
41	BV	0.67	0/782	0.72	0/1049
41	DV	0.57	0/782	0.75	0/1049
42	BW	0.73	0/897	0.76	0/1205
42	DW	0.59	0/897	0.74	0/1205
43	BX	0.71	0/764	0.75	1/1025 (0.1%)
43	DX	0.56	0/764	0.80	2/1025 (0.2%)
44	BY	0.70	0/819	0.78	0/1095
44	DY	0.57	0/819	0.75	0/1095
45	BZ	0.55	0/1379	0.74	0/1873
45	DZ	0.54	0/1390	0.70	0/1890
46	B0	0.63	0/662	0.81	2/881 (0.2%)
46	D0	0.55	0/662	0.78	0/881
47	B1	0.66	0/762	0.81	3/1014 (0.3%)
47	D1	0.55	0/762	0.74	0/1014
48	B2	0.61	0/590	0.81	0/781
48	D2	0.47	0/590	0.67	0/781
49	B3	0.67	0/474	0.78	0/635
49	D3	0.50	0/469	0.70	0/630
50	B4	0.57	0/564	0.81	0/759
50	D4	0.59	0/544	0.89	1/735 (0.1%)
51	B5	0.72	0/469	0.84	1/635 (0.2%)
51	D5	0.59	0/469	0.73	1/635 (0.2%)
52	B6	0.66	0/460	0.66	0/613
52	D6	0.58	0/456	0.72	0/608
53	B7	0.74	0/426	0.82	0/561
53	D7	0.60	0/426	0.78	1/561 (0.2%)
54	B8	0.68	0/519	0.72	0/684
54	D8	0.58	0/525	0.73	0/691
55	B9	0.74	0/310	0.73	0/407
55	D9	0.61	0/310	0.80	0/407
All	All	0.81	86/305966 (0.0%)	1.30	2539/457396 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	3
4	CD	0	1
7	AG	0	1
9	AI	0	1
19	CS	0	1
23	CX	1	0
24	AW	0	1
24	CW	0	1
27	DD	0	1
38	BS	0	1
44	BY	0	1
45	BZ	0	1
50	B4	0	1
50	D4	0	1
All	All	1	15

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	C6-N1	-13.21	1.30	1.39
1	CA	1119	C	N3-C4	-13.12	1.24	1.33
1	AA	343	U	C4-O4	12.79	1.33	1.23
1	CA	1154	G	N1-C2	-12.44	1.27	1.37
23	CX	76	A	N7-C5	-12.26	1.31	1.39

The worst 5 of 2539 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1119	C	N1-C2-O2	40.38	143.13	118.90
1	CA	1154	G	C5-C6-O6	34.47	149.28	128.60
23	CX	76	A	O4'-C1'-N9	33.86	135.29	108.20
1	CA	1154	G	N3-C2-N2	29.11	140.27	119.90
1	CA	1154	G	N1-C2-N2	-27.03	91.87	116.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	CX	76	A	C1'

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	AB	8	LYS	Peptide
2	AB	9	GLU	Peptide
7	AG	79	ARG	Peptide
9	AI	52	ALA	Peptide

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32196	0	16250	907	0
1	CA	32312	0	16307	1000	0
2	AB	1846	0	1867	106	0
2	CB	1825	0	1828	118	0
3	AC	1552	0	1546	51	0
3	CC	1542	0	1517	81	0
4	AD	1659	0	1676	86	0
4	CD	1674	0	1714	83	0
5	AE	1129	0	1185	44	0
5	CE	1133	0	1191	57	0
6	AF	806	0	793	34	0
6	CF	816	0	808	24	0
7	AG	1231	0	1238	33	0
7	CG	1235	0	1249	53	0
8	AH	1088	0	1126	43	0
8	CH	1088	0	1126	56	0
9	AI	983	0	986	47	0
9	CI	978	0	966	55	0
10	AJ	709	0	650	41	0
10	CJ	714	0	672	58	0
11	AK	829	0	825	17	0
11	CK	833	0	836	27	0
12	AL	930	0	980	35	0
12	CL	930	0	980	40	0
13	AM	958	0	1002	35	0
13	CM	950	0	988	50	0
14	AN	492	0	529	27	0
14	CN	492	0	529	31	0
15	AO	728	0	760	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	728	0	760	26	0
16	AP	681	0	697	35	0
16	CP	677	0	686	30	0
17	AQ	823	0	891	21	0
17	CQ	823	0	891	27	0
18	AR	555	0	618	24	0
18	CR	555	0	618	19	0
19	AS	652	0	662	42	0
19	CS	646	0	644	49	0
20	AT	728	0	798	36	0
20	CT	727	0	796	26	0
21	AU	199	0	208	6	0
21	CU	199	0	208	8	0
22	AV	114	0	54	1	0
22	CV	113	0	54	1	0
23	AX	1623	0	823	23	0
23	CX	1623	0	823	22	0
24	AW	93	0	84	10	0
24	CW	93	0	84	10	0
25	BA	58834	0	29666	828	0
25	DA	58458	0	29481	1163	0
26	BB	2573	0	1306	33	0
26	DB	2573	0	1306	65	0
27	BD	2136	0	2218	62	0
27	DD	2136	0	2218	74	0
28	BE	1559	0	1618	55	0
28	DE	1559	0	1618	65	0
29	BF	1584	0	1625	38	0
29	DF	1580	0	1619	65	0
30	BG	1425	0	1443	41	0
30	DG	1424	0	1434	89	0
31	BH	1330	0	1407	37	0
31	DH	1330	0	1407	50	0
32	BI	1085	0	1114	42	0
32	DI	1061	0	1080	27	0
33	BN	1117	0	1183	18	0
33	DN	1117	0	1184	25	0
34	BO	933	0	996	26	0
34	DO	933	0	996	30	0
35	BP	1135	0	1212	42	0
35	DP	1135	0	1212	52	0
36	BQ	1122	0	1179	38	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DQ	1122	0	1179	38	0
37	BR	968	0	1033	24	0
37	DR	968	0	1032	28	0
38	BS	877	0	938	30	0
38	DS	870	0	923	45	0
39	BT	1091	0	1151	36	0
39	DT	1083	0	1136	38	0
40	BU	959	0	1019	28	0
40	DU	959	0	1019	26	0
41	BV	771	0	830	15	0
41	DV	771	0	830	23	0
42	BW	886	0	940	15	0
42	DW	886	0	940	25	0
43	BX	750	0	814	19	0
43	DX	750	0	814	22	0
44	BY	806	0	881	22	0
44	DY	806	0	881	27	0
45	BZ	1349	0	1355	44	0
45	DZ	1360	0	1363	55	0
46	B0	653	0	674	19	0
46	D0	653	0	674	31	0
47	B1	755	0	826	19	0
47	D1	755	0	826	20	0
48	B2	588	0	643	13	0
48	D2	588	0	643	18	0
49	B3	469	0	518	12	0
49	D3	464	0	514	10	0
50	B4	551	0	532	38	0
50	D4	531	0	502	38	0
51	B5	455	0	465	14	0
51	D5	455	0	465	8	0
52	B6	453	0	473	10	0
52	D6	449	0	469	13	0
53	B7	418	0	467	11	0
53	D7	418	0	467	8	0
54	B8	511	0	571	31	0
54	D8	517	0	582	24	0
55	B9	307	0	335	7	0
55	D9	307	0	335	14	0
56	AA	222	0	0	0	0
56	AD	1	0	0	0	0
56	AF	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AM	2	0	0	0	0
56	AN	1	0	0	0	0
56	AS	1	0	0	0	0
56	AV	1	0	0	0	0
56	AX	9	0	0	0	0
56	B0	6	0	0	0	0
56	B1	2	0	0	0	0
56	B2	1	0	0	0	0
56	B3	3	0	0	0	0
56	B5	1	0	0	0	0
56	B7	4	0	0	0	0
56	B8	2	0	0	0	0
56	B9	1	0	0	0	0
56	BA	739	0	0	0	0
56	BB	18	0	0	0	0
56	BD	12	0	0	0	0
56	BE	9	0	0	0	0
56	BF	6	0	0	0	0
56	BG	4	0	0	0	0
56	BN	6	0	0	0	0
56	BO	1	0	0	0	0
56	BP	4	0	0	0	0
56	BQ	4	0	0	0	0
56	BR	3	0	0	0	0
56	BU	9	0	0	0	0
56	BV	3	0	0	0	0
56	BW	5	0	0	0	0
56	BX	2	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	172	0	0	0	0
56	CE	2	0	0	0	0
56	CF	1	0	0	0	0
56	CN	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	3	0	0	0	0
56	D3	1	0	0	0	0
56	D5	2	0	0	0	0
56	D8	1	0	0	0	0
56	DA	657	0	0	0	0
56	DB	12	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DD	5	0	0	0	0
56	DE	6	0	0	0	0
56	DF	5	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	1	0	0	0	0
56	DP	2	0	0	0	0
56	DQ	4	0	0	0	0
56	DR	1	0	0	0	0
56	DU	2	0	0	0	0
56	DV	3	0	0	0	0
56	DW	2	0	0	0	0
56	DY	1	0	0	0	0
57	AD	8	0	0	1	0
57	CD	8	0	0	1	0
58	AN	1	0	0	0	0
58	B4	1	0	0	0	0
58	B5	1	0	0	0	0
58	B6	1	0	0	0	0
58	B9	1	0	0	0	0
58	BY	1	0	0	0	0
58	CN	1	0	0	0	0
58	D4	1	0	0	0	0
58	D5	1	0	0	0	0
58	D6	1	0	0	0	0
58	D9	1	0	0	0	0
58	DY	1	0	0	0	0
59	AX	10	0	10	1	0
59	CX	10	0	10	2	0
60	BA	1	0	0	0	0
60	DA	1	0	0	0	0
61	AA	147	0	0	23	0
61	AD	1	0	0	0	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	2	0	0	0	0
61	AO	2	0	0	0	0
61	AU	1	0	0	1	0
61	AV	2	0	0	0	0
61	AX	1	0	0	0	0
61	B0	4	0	0	0	0
61	B1	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B5	2	0	0	0	0
61	B7	1	0	0	1	0
61	B8	7	0	0	1	0
61	BA	1086	0	0	94	0
61	BB	26	0	0	2	0
61	BD	6	0	0	0	0
61	BE	13	0	0	3	0
61	BF	5	0	0	0	0
61	BG	1	0	0	0	0
61	BN	3	0	0	0	0
61	BO	2	0	0	0	0
61	BP	15	0	0	2	0
61	BQ	3	0	0	1	0
61	BR	1	0	0	0	0
61	BT	2	0	0	0	0
61	BU	5	0	0	0	0
61	BV	2	0	0	0	0
61	BW	4	0	0	0	0
61	BX	4	0	0	1	0
61	CA	186	0	0	24	0
61	CE	2	0	0	0	0
61	CN	1	0	0	0	0
61	CT	1	0	0	0	0
61	CX	2	0	0	0	0
61	D0	3	0	0	1	0
61	D1	1	0	0	0	0
61	D3	1	0	0	0	0
61	D7	1	0	0	0	0
61	D8	4	0	0	0	0
61	DA	906	0	0	116	0
61	DB	7	0	0	0	0
61	DD	10	0	0	0	0
61	DE	11	0	0	1	0
61	DF	4	0	0	0	0
61	DO	1	0	0	0	0
61	DP	14	0	0	2	0
61	DQ	3	0	0	1	0
61	DR	1	0	0	0	0
61	DU	4	0	0	0	0
61	DV	1	0	0	0	0
61	DX	2	0	0	1	0
61	DY	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	286321	0	191124	6684	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 6684 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1129:C:N4	1:AA:1143:G:H1	1.46	1.12
1:CA:1002:G:H1	1:CA:1038:C:N4	1.48	1.09
1:AA:348:G:H2'	1:AA:349:A:H5'	1.30	1.06
2:AB:185:ILE:HG22	2:AB:199:TYR:HB2	1.39	1.04
2:CB:16:HIS:HB2	2:CB:204:ASN:HB3	1.36	1.03

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	229/256 (90%)	201 (88%)	23 (10%)	5 (2%)	5	27
2	CB	229/256 (90%)	201 (88%)	21 (9%)	7 (3%)	3	19
3	AC	204/239 (85%)	182 (89%)	20 (10%)	2 (1%)	13	46
3	CC	204/239 (85%)	181 (89%)	21 (10%)	2 (1%)	13	46
4	AD	206/209 (99%)	184 (89%)	20 (10%)	2 (1%)	13	46
4	CD	206/209 (99%)	185 (90%)	18 (9%)	3 (2%)	8	36
5	AE	146/162 (90%)	136 (93%)	8 (6%)	2 (1%)	9	37
5	CE	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
6	AF	98/101 (97%)	94 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	CF	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
7	AG	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	19	54
7	CG	153/156 (98%)	139 (91%)	13 (8%)	1 (1%)	19	54
8	AH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
8	CH	135/138 (98%)	131 (97%)	3 (2%)	1 (1%)	19	54
9	AI	125/128 (98%)	112 (90%)	10 (8%)	3 (2%)	5	25
9	CI	125/128 (98%)	115 (92%)	8 (6%)	2 (2%)	8	34
10	AJ	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	3	19
10	CJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	5	28
11	AK	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	49
11	CK	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	49
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
13	AM	121/126 (96%)	113 (93%)	7 (6%)	1 (1%)	16	51
13	CM	120/126 (95%)	113 (94%)	6 (5%)	1 (1%)	16	51
14	AN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
14	CN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	AO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	CO	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	AP	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
16	CP	80/88 (91%)	73 (91%)	6 (8%)	1 (1%)	10	39
17	AQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
18	AR	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	8	36
18	CR	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
19	AS	81/93 (87%)	76 (94%)	5 (6%)	0	100	100
19	CS	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
20	AT	94/106 (89%)	84 (89%)	9 (10%)	1 (1%)	12	44
20	CT	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	3	19
21	AU	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
21	CU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	AW	3/10 (30%)	0	2 (67%)	1 (33%)	0	0
24	CW	3/10 (30%)	1 (33%)	1 (33%)	1 (33%)	0	0
27	BD	273/276 (99%)	260 (95%)	12 (4%)	1 (0%)	30	66
27	DD	273/276 (99%)	258 (94%)	13 (5%)	2 (1%)	19	54
28	BE	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	25	61
28	DE	202/206 (98%)	195 (96%)	4 (2%)	3 (2%)	8	36
29	BF	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	25	61
29	DF	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	13	46
30	BG	179/182 (98%)	167 (93%)	9 (5%)	3 (2%)	7	33
30	DG	179/182 (98%)	161 (90%)	14 (8%)	4 (2%)	5	27
31	BH	172/180 (96%)	165 (96%)	6 (4%)	1 (1%)	22	57
31	DH	172/180 (96%)	164 (95%)	7 (4%)	1 (1%)	22	57
32	BI	144/148 (97%)	124 (86%)	14 (10%)	6 (4%)	2	13
32	DI	144/148 (97%)	124 (86%)	17 (12%)	3 (2%)	5	28
33	BN	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
33	DN	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	19	54
34	BO	120/122 (98%)	116 (97%)	3 (2%)	1 (1%)	16	51
34	DO	120/122 (98%)	117 (98%)	2 (2%)	1 (1%)	16	51
35	BP	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	19	54
35	DP	147/150 (98%)	135 (92%)	9 (6%)	3 (2%)	6	29
36	BQ	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	19	54
36	DQ	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	19	54
37	BR	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14	49
37	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	BS	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	14	49
38	DS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	14	49
39	BT	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
39	DT	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
40	BU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
40	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
41	BV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	13	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	DV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	13	46
42	BW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
42	DW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
43	BX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
43	DX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	BY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
44	DY	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
45	BZ	169/206 (82%)	150 (89%)	18 (11%)	1 (1%)	22	57
45	DZ	172/206 (84%)	162 (94%)	10 (6%)	0	100	100
46	B0	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	11	41
46	D0	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	11	41
47	B1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	12	44
47	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	12	44
48	B2	68/72 (94%)	68 (100%)	0	0	100	100
48	D2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
49	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
49	D3	57/60 (95%)	57 (100%)	0	0	100	100
50	B4	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	4
50	D4	67/71 (94%)	52 (78%)	8 (12%)	7 (10%)	0	2
51	B5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
51	D5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
52	B6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
52	D6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
53	B7	46/49 (94%)	46 (100%)	0	0	100	100
53	D7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	5	27
54	B8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
54	D8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
55	B9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
55	D9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	11415/12148 (94%)	10659 (93%)	648 (6%)	108 (1%)	14	49

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	125	PRO
3	AC	107	GLN
4	AD	166	LYS
9	AI	54	ASP
10	AJ	31	GLY

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	192/220 (87%)	154 (80%)	38 (20%)	1	6
2	CB	187/220 (85%)	155 (83%)	32 (17%)	1	8
3	AC	143/188 (76%)	128 (90%)	15 (10%)	5	23
3	CC	140/188 (74%)	123 (88%)	17 (12%)	4	18
4	AD	170/181 (94%)	146 (86%)	24 (14%)	3	13
4	CD	173/181 (96%)	152 (88%)	21 (12%)	4	18
5	AE	113/123 (92%)	102 (90%)	11 (10%)	6	27
5	CE	114/123 (93%)	104 (91%)	10 (9%)	8	31
6	AF	83/90 (92%)	76 (92%)	7 (8%)	9	33
6	CF	85/90 (94%)	79 (93%)	6 (7%)	12	40
7	AG	119/127 (94%)	100 (84%)	19 (16%)	2	10
7	CG	120/127 (94%)	102 (85%)	18 (15%)	2	12
8	AH	114/119 (96%)	97 (85%)	17 (15%)	2	12
8	CH	114/119 (96%)	102 (90%)	12 (10%)	5	23
9	AI	90/99 (91%)	78 (87%)	12 (13%)	3	15
9	CI	89/99 (90%)	75 (84%)	14 (16%)	2	10
10	AJ	66/92 (72%)	59 (89%)	7 (11%)	5	23
10	CJ	69/92 (75%)	65 (94%)	4 (6%)	17	48
11	AK	82/99 (83%)	75 (92%)	7 (8%)	8	33
11	CK	83/99 (84%)	77 (93%)	6 (7%)	12	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	97/109 (89%)	87 (90%)	10 (10%)	6	24
12	CL	97/109 (89%)	83 (86%)	14 (14%)	2	13
13	AM	93/101 (92%)	81 (87%)	12 (13%)	3	16
13	CM	92/101 (91%)	78 (85%)	14 (15%)	2	11
14	AN	49/50 (98%)	41 (84%)	8 (16%)	2	9
14	CN	49/50 (98%)	41 (84%)	8 (16%)	2	9
15	AO	78/80 (98%)	68 (87%)	10 (13%)	3	16
15	CO	78/80 (98%)	66 (85%)	12 (15%)	2	11
16	AP	69/74 (93%)	61 (88%)	8 (12%)	4	20
16	CP	68/74 (92%)	64 (94%)	4 (6%)	16	47
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	14	44
17	CQ	94/97 (97%)	86 (92%)	8 (8%)	8	33
18	AR	59/77 (77%)	56 (95%)	3 (5%)	20	53
18	CR	59/77 (77%)	53 (90%)	6 (10%)	6	24
19	AS	69/80 (86%)	63 (91%)	6 (9%)	8	32
19	CS	67/80 (84%)	59 (88%)	8 (12%)	4	19
20	AT	70/82 (85%)	60 (86%)	10 (14%)	2	13
20	CT	70/82 (85%)	61 (87%)	9 (13%)	3	16
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2	9
21	CU	18/22 (82%)	16 (89%)	2 (11%)	5	21
24	AW	3/3 (100%)	2 (67%)	1 (33%)	0	1
24	CW	3/3 (100%)	2 (67%)	1 (33%)	0	1
27	BD	215/218 (99%)	193 (90%)	22 (10%)	6	24
27	DD	215/218 (99%)	195 (91%)	20 (9%)	7	29
28	BE	164/166 (99%)	140 (85%)	24 (15%)	2	12
28	DE	164/166 (99%)	140 (85%)	24 (15%)	2	12
29	BF	160/166 (96%)	145 (91%)	15 (9%)	7	28
29	DF	159/166 (96%)	142 (89%)	17 (11%)	5	22
30	BG	143/156 (92%)	124 (87%)	19 (13%)	3	15
30	DG	142/156 (91%)	117 (82%)	25 (18%)	1	8
31	BH	144/148 (97%)	128 (89%)	16 (11%)	5	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	DH	144/148 (97%)	131 (91%)	13 (9%)	8	30
32	BI	110/124 (89%)	85 (77%)	25 (23%)	0	3
32	DI	104/124 (84%)	90 (86%)	14 (14%)	3	14
33	BN	118/119 (99%)	100 (85%)	18 (15%)	2	11
33	DN	118/119 (99%)	102 (86%)	16 (14%)	3	14
34	BO	100/100 (100%)	95 (95%)	5 (5%)	20	53
34	DO	100/100 (100%)	92 (92%)	8 (8%)	10	35
35	BP	115/116 (99%)	103 (90%)	12 (10%)	5	23
35	DP	115/116 (99%)	102 (89%)	13 (11%)	4	21
36	BQ	111/111 (100%)	96 (86%)	15 (14%)	3	14
36	DQ	111/111 (100%)	97 (87%)	14 (13%)	3	17
37	BR	101/101 (100%)	83 (82%)	18 (18%)	1	8
37	DR	101/101 (100%)	84 (83%)	17 (17%)	1	9
38	BS	87/88 (99%)	78 (90%)	9 (10%)	6	24
38	DS	85/88 (97%)	73 (86%)	12 (14%)	3	13
39	BT	115/127 (91%)	103 (90%)	12 (10%)	5	23
39	DT	113/127 (89%)	103 (91%)	10 (9%)	8	31
40	BU	93/94 (99%)	85 (91%)	8 (9%)	8	32
40	DU	93/94 (99%)	79 (85%)	14 (15%)	2	12
41	BV	80/82 (98%)	68 (85%)	12 (15%)	2	12
41	DV	80/82 (98%)	70 (88%)	10 (12%)	3	17
42	BW	90/92 (98%)	83 (92%)	7 (8%)	10	36
42	DW	90/92 (98%)	82 (91%)	8 (9%)	8	31
43	BX	77/78 (99%)	74 (96%)	3 (4%)	27	61
43	DX	77/78 (99%)	73 (95%)	4 (5%)	19	52
44	BY	85/91 (93%)	76 (89%)	9 (11%)	5	23
44	DY	85/91 (93%)	77 (91%)	8 (9%)	7	28
45	BZ	145/179 (81%)	127 (88%)	18 (12%)	4	17
45	DZ	145/179 (81%)	128 (88%)	17 (12%)	4	19
46	B0	65/67 (97%)	62 (95%)	3 (5%)	23	56
46	D0	65/67 (97%)	60 (92%)	5 (8%)	10	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	B1	80/83 (96%)	70 (88%)	10 (12%)	3	17
47	D1	80/83 (96%)	69 (86%)	11 (14%)	3	14
48	B2	65/67 (97%)	56 (86%)	9 (14%)	3	14
48	D2	65/67 (97%)	57 (88%)	8 (12%)	4	18
49	B3	51/52 (98%)	44 (86%)	7 (14%)	3	14
49	D3	50/52 (96%)	42 (84%)	8 (16%)	2	10
50	B4	59/63 (94%)	47 (80%)	12 (20%)	1	5
50	D4	53/63 (84%)	44 (83%)	9 (17%)	1	9
51	B5	50/52 (96%)	45 (90%)	5 (10%)	6	25
51	D5	50/52 (96%)	45 (90%)	5 (10%)	6	25
52	B6	51/52 (98%)	47 (92%)	4 (8%)	10	36
52	D6	50/52 (96%)	43 (86%)	7 (14%)	3	13
53	B7	41/42 (98%)	39 (95%)	2 (5%)	21	54
53	D7	41/42 (98%)	38 (93%)	3 (7%)	11	39
54	B8	53/55 (96%)	50 (94%)	3 (6%)	17	49
54	D8	54/55 (98%)	52 (96%)	2 (4%)	29	63
55	B9	34/34 (100%)	33 (97%)	1 (3%)	37	70
55	D9	34/34 (100%)	31 (91%)	3 (9%)	8	31
All	All	9325/10072 (93%)	8217 (88%)	1108 (12%)	4	19

5 of 1108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	DP	65	ARG
37	DR	36	THR
35	DP	55	ARG
45	DZ	131	ARG
35	BP	135	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
55	B9	36	GLN
44	DY	43	ASN
5	CE	141	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	DX	31	HIS
32	DI	133	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1522 (98%)	421 (28%)	24 (1%)
1	CA	1501/1522 (98%)	421 (28%)	30 (1%)
22	AV	4/24 (16%)	1 (25%)	0
22	CV	4/24 (16%)	1 (25%)	0
23	AX	75/77 (97%)	18 (24%)	0
23	CX	75/77 (97%)	19 (25%)	0
25	BA	2722/2915 (93%)	527 (19%)	41 (1%)
25	DA	2704/2915 (92%)	526 (19%)	35 (1%)
26	BB	119/122 (97%)	21 (17%)	0
26	DB	119/122 (97%)	23 (19%)	1 (0%)
All	All	8818/9320 (94%)	1978 (22%)	131 (1%)

5 of 1978 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	15	G
1	AA	16	A
1	AA	22	G

5 of 131 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	DA	1427	A
25	DA	1608	A
26	DB	45	A
25	BA	1466	U
25	BA	1321	A

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

14 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
24	2QZ	CW	1	24	7,8,9	0.83	0	7,10,12	3.69	2 (28%)
24	004	AW	3	24	9,10,11	1.20	1 (11%)	9,12,14	1.16	0
24	2QY	CW	10	24	12,13,14	2.04	2 (16%)	14,16,18	3.56	3 (21%)
24	2R1	CW	6	24	10,10,11	1.82	3 (30%)	8,13,15	3.68	3 (37%)
24	2R3	CW	8	24	12,14,15	0.71	0	16,18,20	2.15	6 (37%)
24	2QZ	AW	1	24	7,8,9	0.41	0	7,10,12	2.50	1 (14%)
24	2R3	AW	8	24	12,14,15	0.81	0	16,18,20	2.05	7 (43%)
24	MVA	CW	5	24	6,7,8	0.81	0	6,8,10	1.51	2 (33%)
24	MVA	CW	9	24	6,7,8	0.89	0	6,8,10	1.10	0
24	2QY	AW	10	24	12,13,14	1.94	2 (16%)	14,16,18	3.62	6 (42%)
24	MVA	AW	9	24	6,7,8	0.38	0	6,8,10	0.94	1 (16%)
24	004	CW	3	24	9,10,11	1.35	1 (11%)	9,12,14	0.68	0
24	2R1	AW	6	24	10,10,11	2.43	4 (40%)	8,13,15	4.19	3 (37%)
24	MVA	AW	5	24	6,7,8	0.57	0	6,8,10	1.28	0

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
24	2QZ	CW	1	24	-	1/8/10/12	-
24	004	AW	3	24	-	1/4/6/8	0/1/1/1
24	2QY	CW	10	24	-	1/5/8/10	0/1/1/1
24	2R1	CW	6	24	-	0/2/14/16	0/1/1/1
24	2R3	CW	8	24	-	6/11/12/14	0/1/1/1
24	2QZ	AW	1	24	-	3/8/10/12	-
24	2R3	AW	8	24	-	6/11/12/14	0/1/1/1
24	MVA	CW	5	24	-	5/6/8/10	-
24	MVA	CW	9	24	-	5/6/8/10	-
24	2QY	AW	10	24	-	3/5/8/10	0/1/1/1
24	MVA	AW	9	24	-	5/6/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	004	CW	3	24	-	0/4/6/8	0/1/1/1
24	2R1	AW	6	24	-	1/2/14/16	0/1/1/1
24	MVA	AW	5	24	-	2/6/8/10	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CW	10	2QY	C-CA	6.08	1.53	1.43
24	AW	10	2QY	C-CA	5.76	1.53	1.43
24	AW	6	2R1	OD1-CG1	4.61	1.56	1.42
24	AW	6	2R1	CA-N	4.13	1.46	1.36
24	CW	6	2R1	CA-N	3.84	1.45	1.36

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AW	6	2R1	OD2-CG2-CB	-10.70	92.15	111.99
24	CW	10	2QY	CN-N-CA	-9.76	109.17	123.98
24	AW	10	2QY	CN-N-CA	-9.66	109.33	123.98
24	CW	1	2QZ	OG1-CB-CG2	9.20	137.20	109.68
24	CW	6	2R1	OD2-CG2-CB	-8.95	95.40	111.99

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AW	1	2QZ	N-CA-CB-OG1
24	AW	5	MVA	CB-CA-N-CN
24	AW	8	2R3	N-CA-CB-OB
24	AW	8	2R3	N-CA-CB-CG
24	AW	8	2R3	C-CA-CB-OB

There are no ring outliers.

14 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	CW	1	2QZ	3	0
24	AW	3	004	1	0
24	CW	10	2QY	4	0
24	CW	6	2R1	1	0
24	CW	8	2R3	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AW	1	2QZ	2	0
24	AW	8	2R3	4	0
24	CW	5	MVA	1	0
24	CW	9	MVA	3	0
24	AW	10	2QY	3	0
24	AW	9	MVA	3	0
24	CW	3	004	1	0
24	AW	6	2R1	3	0
24	AW	5	MVA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1991 ligands modelled in this entry, 1987 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	FME	AX	101	23	8,9,10	0.94	0	8,9,11	1.49	2 (25%)
57	SF4	AD	501	4	0,12,12	-	-	-		
57	SF4	CD	501	4	0,12,12	-	-	-		
59	FME	CX	101	23	8,9,10	0.82	0	8,9,11	1.37	1 (12%)

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
59	FME	AX	101	23	-	2/7/9/11	-
57	SF4	AD	501	4	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SF4	CD	501	4	-	-	0/6/5/5
59	FME	CX	101	23	-	1/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AX	101	FME	CA-N-CN	-2.47	119.03	122.82
59	CX	101	FME	CA-N-CN	-2.33	119.25	122.82
59	AX	101	FME	CB-CA-N	2.31	114.72	110.52

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AX	101	FME	O1-CN-N-CA
59	CX	101	FME	O1-CN-N-CA
59	AX	101	FME	CB-CG-SD-CE

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	AX	101	FME	1	0
57	AD	501	SF4	1	0
57	CD	501	SF4	1	0
59	CX	101	FME	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1498/1522 (98%)	-0.05	23 (1%) 71 50	39, 80, 103, 118	0
1	CA	1503/1522 (98%)	-0.05	19 (1%) 74 54	41, 80, 103, 119	0
2	AB	231/256 (90%)	0.32	4 (1%) 69 47	69, 86, 97, 105	0
2	CB	231/256 (90%)	0.40	8 (3%) 47 28	70, 88, 98, 107	0
3	AC	206/239 (86%)	0.30	3 (1%) 71 50	73, 87, 95, 104	0
3	CC	206/239 (86%)	0.47	6 (2%) 54 32	72, 89, 97, 104	0
4	AD	208/209 (99%)	0.41	5 (2%) 59 37	61, 80, 90, 97	0
4	CD	208/209 (99%)	0.28	2 (0%) 79 60	61, 79, 89, 97	0
5	AE	148/162 (91%)	-0.24	0 100 100	51, 73, 82, 93	0
5	CE	148/162 (91%)	0.04	0 100 100	53, 75, 84, 96	0
6	AF	100/101 (99%)	-0.04	0 100 100	63, 77, 87, 94	0
6	CF	100/101 (99%)	-0.00	0 100 100	62, 78, 87, 95	0
7	AG	155/156 (99%)	0.15	3 (1%) 66 44	74, 86, 99, 106	0
7	CG	155/156 (99%)	0.28	3 (1%) 66 44	75, 86, 99, 105	0
8	AH	137/138 (99%)	0.02	0 100 100	60, 74, 82, 89	0
8	CH	137/138 (99%)	0.17	3 (2%) 62 40	62, 75, 83, 89	0
9	AI	127/128 (99%)	0.66	6 (4%) 37 21	73, 91, 99, 101	0
9	CI	127/128 (99%)	1.18	24 (18%) 4 3	72, 93, 100, 102	0
10	AJ	97/105 (92%)	0.90	9 (9%) 16 9	73, 91, 100, 105	0
10	CJ	96/105 (91%)	1.05	11 (11%) 11 6	77, 93, 100, 104	0
11	AK	114/129 (88%)	-0.14	1 (0%) 81 63	53, 74, 87, 91	0
11	CK	114/129 (88%)	-0.12	0 100 100	55, 76, 87, 92	0
12	AL	122/132 (92%)	0.10	4 (3%) 49 29	53, 68, 80, 87	0
12	CL	122/132 (92%)	0.00	1 (0%) 82 66	53, 69, 80, 87	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	123/126 (97%)	0.26	6 (4%)	36	20	67, 85, 95, 105	0
13	CM	122/126 (96%)	0.61	5 (4%)	42	24	77, 92, 100, 109	0
14	AN	60/61 (98%)	0.71	5 (8%)	19	10	75, 87, 94, 103	0
14	CN	60/61 (98%)	1.17	9 (15%)	6	4	77, 89, 94, 100	0
15	AO	88/89 (98%)	0.03	0	100	100	55, 72, 85, 90	0
15	CO	88/89 (98%)	-0.06	1 (1%)	77	58	55, 72, 85, 91	0
16	AP	82/88 (93%)	0.52	4 (4%)	36	20	67, 78, 89, 94	0
16	CP	82/88 (93%)	0.44	3 (3%)	45	27	66, 76, 88, 94	0
17	AQ	99/105 (94%)	0.07	1 (1%)	79	60	59, 72, 83, 90	0
17	CQ	99/105 (94%)	0.04	0	100	100	58, 72, 83, 89	0
18	AR	68/88 (77%)	0.04	0	100	100	65, 73, 87, 91	0
18	CR	68/88 (77%)	-0.06	0	100	100	64, 75, 87, 91	0
19	AS	83/93 (89%)	0.64	7 (8%)	18	10	77, 92, 99, 106	0
19	CS	83/93 (89%)	1.00	12 (14%)	7	4	79, 92, 101, 106	0
20	AT	96/106 (90%)	0.49	5 (5%)	34	19	62, 76, 86, 90	0
20	CT	96/106 (90%)	0.18	3 (3%)	51	30	62, 74, 86, 92	0
21	AU	23/27 (85%)	1.19	2 (8%)	17	10	73, 88, 93, 94	0
21	CU	23/27 (85%)	1.66	8 (34%)	1	1	73, 89, 92, 94	0
22	AV	7/24 (29%)	0.27	0	100	100	65, 77, 102, 104	0
22	CV	6/24 (25%)	0.38	0	100	100	67, 78, 103, 103	0
23	AX	76/77 (98%)	-0.42	0	100	100	52, 80, 97, 105	0
23	CX	76/77 (98%)	-0.19	0	100	100	52, 82, 100, 106	0
24	AW	3/10 (30%)	0.35	0	100	100	67, 67, 82, 98	0
24	CW	3/10 (30%)	-0.46	0	100	100	67, 67, 78, 82	0
25	BA	2731/2915 (93%)	-0.73	12 (0%)	89	77	23, 44, 85, 111	0
25	DA	2714/2915 (93%)	-0.73	4 (0%)	92	88	26, 47, 85, 118	0
26	BB	120/122 (98%)	-0.32	0	100	100	42, 68, 80, 95	0
26	DB	120/122 (98%)	0.03	0	100	100	48, 74, 84, 97	0
27	BD	275/276 (99%)	-0.58	0	100	100	22, 42, 58, 77	0
27	DD	275/276 (99%)	-0.59	0	100	100	23, 44, 60, 79	0
28	BE	204/206 (99%)	-0.56	0	100	100	23, 45, 67, 88	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DE	204/206 (99%)	-0.54	1 (0%) 87 75	24, 47, 70, 88	0
29	BF	203/210 (96%)	-0.37	0 100 100	20, 51, 77, 94	0
29	DF	203/210 (96%)	-0.40	0 100 100	22, 54, 78, 93	0
30	BG	181/182 (99%)	0.04	0 100 100	59, 77, 90, 103	0
30	DG	181/182 (99%)	0.45	7 (3%) 44 26	63, 80, 92, 102	0
31	BH	174/180 (96%)	-0.02	2 (1%) 77 58	50, 66, 78, 84	0
31	DH	174/180 (96%)	0.16	1 (0%) 85 71	54, 71, 82, 87	0
32	BI	146/148 (98%)	-0.22	0 100 100	45, 75, 87, 92	0
32	DI	146/148 (98%)	0.03	0 100 100	48, 76, 86, 91	0
33	BN	140/140 (100%)	-0.30	1 (0%) 84 68	32, 49, 68, 80	0
33	DN	140/140 (100%)	-0.37	0 100 100	34, 53, 72, 81	0
34	BO	122/122 (100%)	-0.71	0 100 100	25, 39, 60, 78	0
34	DO	122/122 (100%)	-0.53	0 100 100	34, 52, 68, 79	0
35	BP	149/150 (99%)	-0.33	0 100 100	26, 54, 76, 84	0
35	DP	149/150 (99%)	-0.22	0 100 100	30, 57, 79, 86	0
36	BQ	141/141 (100%)	-0.19	2 (1%) 73 52	33, 51, 65, 79	0
36	DQ	141/141 (100%)	-0.30	0 100 100	35, 54, 70, 80	0
37	BR	118/118 (100%)	-0.67	0 100 100	22, 35, 51, 64	0
37	DR	118/118 (100%)	-0.40	0 100 100	36, 50, 64, 81	0
38	BS	110/112 (98%)	-0.45	0 100 100	38, 55, 69, 81	0
38	DS	110/112 (98%)	0.43	4 (3%) 46 27	66, 78, 90, 100	0
39	BT	131/146 (89%)	-0.44	2 (1%) 71 50	33, 45, 75, 91	0
39	DT	131/146 (89%)	-0.36	2 (1%) 71 50	44, 56, 80, 86	0
40	BU	116/118 (98%)	-0.85	0 100 100	19, 30, 50, 63	0
40	DU	116/118 (98%)	-0.24	0 100 100	39, 61, 79, 88	0
41	BV	101/101 (100%)	-0.44	0 100 100	29, 52, 70, 77	0
41	DV	101/101 (100%)	-0.45	0 100 100	32, 58, 74, 79	0
42	BW	112/113 (99%)	-0.61	0 100 100	27, 37, 61, 94	0
42	DW	112/113 (99%)	-0.57	0 100 100	31, 40, 63, 94	0
43	BX	95/96 (98%)	-0.30	1 (1%) 77 58	32, 46, 69, 82	0
43	DX	95/96 (98%)	-0.18	0 100 100	38, 50, 72, 83	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BY	107/110 (97%)	-0.03	2 (1%) 66 44	44, 59, 77, 82	0
44	DY	107/110 (97%)	0.16	3 (2%) 55 33	46, 63, 80, 85	0
45	BZ	171/206 (83%)	-0.03	2 (1%) 76 56	52, 71, 85, 93	0
45	DZ	174/206 (84%)	0.18	0 100 100	56, 74, 87, 95	0
46	B0	83/85 (97%)	-0.28	6 (7%) 23 13	22, 40, 75, 104	0
46	D0	83/85 (97%)	0.14	3 (3%) 46 27	45, 66, 87, 98	0
47	B1	97/98 (98%)	-0.55	0 100 100	25, 42, 71, 77	0
47	D1	97/98 (98%)	-0.31	1 (1%) 79 60	35, 56, 79, 85	0
48	B2	70/72 (97%)	-0.37	0 100 100	31, 48, 64, 77	0
48	D2	70/72 (97%)	-0.05	0 100 100	56, 73, 84, 86	0
49	B3	59/60 (98%)	-0.58	0 100 100	26, 38, 63, 86	0
49	D3	59/60 (98%)	-0.28	0 100 100	49, 62, 80, 93	0
50	B4	69/71 (97%)	0.13	0 100 100	64, 87, 101, 104	0
50	D4	69/71 (97%)	0.57	4 (5%) 30 17	85, 95, 104, 107	0
51	B5	59/60 (98%)	-0.89	0 100 100	14, 35, 55, 71	0
51	D5	59/60 (98%)	-0.49	0 100 100	29, 51, 70, 77	0
52	B6	53/54 (98%)	-0.53	0 100 100	40, 54, 68, 74	0
52	D6	53/54 (98%)	-0.44	0 100 100	42, 58, 68, 74	0
53	B7	48/49 (97%)	-0.53	0 100 100	26, 32, 67, 78	0
53	D7	48/49 (97%)	-0.41	1 (2%) 63 41	27, 34, 66, 79	0
54	B8	64/65 (98%)	-0.48	0 100 100	33, 43, 51, 56	0
54	D8	64/65 (98%)	-0.29	0 100 100	34, 46, 56, 60	0
55	B9	37/37 (100%)	0.00	1 (2%) 56 34	43, 52, 68, 77	0
55	D9	37/37 (100%)	0.12	1 (2%) 56 34	48, 57, 72, 78	0
All	All	20462/21468 (95%)	-0.23	269 (1%) 74 54	14, 65, 95, 119	0

The worst 5 of 269 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	6.4
13	AM	123	ALA	5.9
13	CM	123	ALA	5.7
9	CI	11	LYS	5.1
44	BY	1	MET	4.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	2R1	AW	6	10/11	0.76	0.14	66,72,84,91	0
24	MVA	AW	5	8/9	0.77	0.15	69,82,86,91	0
24	004	AW	3	10/11	0.81	0.12	67,87,95,97	0
24	2QY	CW	10	13/14	0.85	0.11	60,72,80,86	0
24	2R1	CW	6	10/11	0.86	0.12	68,82,90,91	0
24	2R3	AW	8	14/15	0.86	0.13	70,78,86,87	0
24	MVA	CW	5	8/9	0.87	0.12	76,88,91,99	0
24	MVA	CW	9	8/9	0.88	0.11	70,73,84,91	0
24	2QY	AW	10	13/14	0.90	0.10	49,70,87,100	0
24	MVA	AW	9	8/9	0.92	0.11	63,74,87,88	0
24	2QZ	AW	1	9/10	0.92	0.10	50,71,82,83	0
24	2R3	CW	8	14/15	0.93	0.08	62,69,77,78	0
24	2QZ	CW	1	9/10	0.94	0.10	63,71,80,101	0
24	004	CW	3	10/11	0.94	0.08	69,78,82,83	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	CA	3147	1/1	0.22	0.30	77,77,77,77	0
56	MG	CA	3139	1/1	0.53	0.22	76,76,76,76	0
56	MG	AA	3180	1/1	0.57	0.30	75,75,75,75	0
56	MG	BA	3661	1/1	0.60	0.22	69,69,69,69	0
56	MG	CA	3114	1/1	0.61	0.18	67,67,67,67	0
56	MG	CA	3053	1/1	0.62	0.52	87,87,87,87	0
56	MG	AA	3093	1/1	0.63	0.25	90,90,90,90	0
56	MG	AA	3129	1/1	0.63	0.26	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3030	1/1	0.67	0.43	74,74,74,74	0
56	MG	CA	3142	1/1	0.68	0.21	80,80,80,80	0
56	MG	CA	3161	1/1	0.68	0.15	71,71,71,71	0
56	MG	DA	3356	1/1	0.68	0.15	57,57,57,57	0
56	MG	DG	3001	1/1	0.68	0.16	68,68,68,68	0
56	MG	BA	3625	1/1	0.69	0.17	80,80,80,80	0
56	MG	AA	3164	1/1	0.69	0.29	61,61,61,61	0
56	MG	CA	3156	1/1	0.69	0.22	80,80,80,80	0
56	MG	BA	3203	1/1	0.70	0.17	45,45,45,45	0
56	MG	BB	3005	1/1	0.70	0.26	62,62,62,62	0
56	MG	AA	3076	1/1	0.70	0.38	74,74,74,74	0
56	MG	AA	3200	1/1	0.71	0.24	79,79,79,79	0
56	MG	AS	3001	1/1	0.71	0.17	79,79,79,79	0
56	MG	AA	3094	1/1	0.71	0.13	78,78,78,78	0
56	MG	AA	3072	1/1	0.71	0.20	69,69,69,69	0
56	MG	AX	108	1/1	0.72	0.27	66,66,66,66	0
56	MG	BA	3103	1/1	0.72	0.27	58,58,58,58	0
56	MG	DA	3619	1/1	0.73	0.17	67,67,67,67	0
56	MG	CA	3025	1/1	0.73	0.17	102,102,102,102	0
56	MG	CA	3070	1/1	0.74	0.21	59,59,59,59	0
56	MG	BA	3133	1/1	0.74	0.36	53,53,53,53	0
56	MG	AA	3022	1/1	0.74	0.20	56,56,56,56	0
56	MG	DA	3540	1/1	0.74	0.16	76,76,76,76	0
56	MG	DA	3602	1/1	0.74	0.20	63,63,63,63	0
56	MG	AA	3021	1/1	0.74	0.18	76,76,76,76	0
56	MG	AA	3133	1/1	0.74	0.43	71,71,71,71	0
56	MG	AA	3209	1/1	0.75	0.18	66,66,66,66	0
56	MG	DA	3464	1/1	0.75	0.11	51,51,51,51	0
56	MG	DA	3346	1/1	0.75	0.13	64,64,64,64	0
56	MG	CA	3164	1/1	0.76	0.17	43,43,43,43	0
56	MG	DA	3001	1/1	0.76	0.37	76,76,76,76	0
56	MG	DA	3296	1/1	0.76	0.21	65,65,65,65	0
56	MG	AA	3087	1/1	0.76	0.21	87,87,87,87	0
56	MG	CA	3119	1/1	0.76	0.29	73,73,73,73	0
56	MG	DA	3436	1/1	0.76	0.13	61,61,61,61	0
56	MG	BA	3582	1/1	0.76	0.16	52,52,52,52	0
56	MG	AA	3002	1/1	0.76	0.14	74,74,74,74	0
56	MG	DA	3568	1/1	0.76	0.19	58,58,58,58	0
56	MG	AA	3131	1/1	0.76	0.27	65,65,65,65	0
56	MG	DA	3603	1/1	0.76	0.17	66,66,66,66	0
56	MG	CA	3061	1/1	0.76	0.37	68,68,68,68	0
56	MG	DA	3630	1/1	0.76	0.12	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3639	1/1	0.76	0.24	55,55,55,55	0
56	MG	BA	3708	1/1	0.76	0.16	38,38,38,38	0
56	MG	CA	3056	1/1	0.77	0.20	63,63,63,63	0
56	MG	BD	304	1/1	0.77	0.23	41,41,41,41	0
56	MG	BA	3704	1/1	0.77	0.20	58,58,58,58	0
56	MG	CA	3027	1/1	0.77	0.14	64,64,64,64	0
56	MG	DA	3456	1/1	0.77	0.19	58,58,58,58	0
56	MG	AA	3114	1/1	0.77	0.19	73,73,73,73	0
56	MG	AA	3030	1/1	0.77	0.43	66,66,66,66	0
56	MG	AA	3063	1/1	0.78	0.18	57,57,57,57	0
56	MG	DA	3066	1/1	0.78	0.26	59,59,59,59	0
56	MG	DA	3567	1/1	0.78	0.15	68,68,68,68	0
56	MG	DA	3141	1/1	0.78	0.23	63,63,63,63	0
56	MG	CA	3144	1/1	0.78	0.27	84,84,84,84	0
56	MG	BA	3620	1/1	0.78	0.22	57,57,57,57	0
56	MG	CA	3117	1/1	0.78	0.12	58,58,58,58	0
56	MG	BA	3292	1/1	0.78	0.27	59,59,59,59	0
56	MG	BA	3740	1/1	0.78	0.26	57,57,57,57	0
56	MG	DB	3001	1/1	0.78	0.18	80,80,80,80	0
56	MG	DA	3462	1/1	0.78	0.19	71,71,71,71	0
56	MG	BA	3711	1/1	0.79	0.29	64,64,64,64	0
56	MG	AA	3067	1/1	0.79	0.29	76,76,76,76	0
56	MG	BA	3358	1/1	0.79	0.12	78,78,78,78	0
56	MG	DA	3441	1/1	0.79	0.12	46,46,46,46	0
56	MG	DA	3115	1/1	0.79	0.11	64,64,64,64	0
56	MG	AA	3184	1/1	0.79	0.16	81,81,81,81	0
56	MG	DA	3220	1/1	0.79	0.07	61,61,61,61	0
56	MG	DA	3500	1/1	0.79	0.33	66,66,66,66	0
56	MG	DB	3003	1/1	0.79	0.22	70,70,70,70	0
56	MG	AA	3115	1/1	0.79	0.27	67,67,67,67	0
56	MG	CA	3028	1/1	0.80	0.43	62,62,62,62	0
56	MG	DA	3123	1/1	0.80	0.14	61,61,61,61	0
56	MG	DA	3506	1/1	0.80	0.10	61,61,61,61	0
56	MG	DA	3131	1/1	0.80	0.09	60,60,60,60	0
56	MG	AA	3032	1/1	0.80	0.29	65,65,65,65	0
56	MG	DA	3169	1/1	0.80	0.24	58,58,58,58	0
56	MG	CA	3159	1/1	0.80	0.26	76,76,76,76	0
56	MG	AA	3136	1/1	0.80	0.14	68,68,68,68	0
56	MG	CA	3162	1/1	0.80	0.18	60,60,60,60	0
56	MG	DA	3627	1/1	0.80	0.14	52,52,52,52	0
56	MG	CA	3009	1/1	0.80	0.15	55,55,55,55	0
56	MG	AA	3189	1/1	0.80	0.13	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3642	1/1	0.80	0.22	67,67,67,67	0
56	MG	DA	3008	1/1	0.80	0.15	56,56,56,56	0
56	MG	AA	3117	1/1	0.80	0.18	64,64,64,64	0
56	MG	DA	3113	1/1	0.80	0.45	61,61,61,61	0
56	MG	CA	3152	1/1	0.81	0.22	45,45,45,45	0
56	MG	AX	104	1/1	0.81	0.12	62,62,62,62	0
56	MG	CA	3073	1/1	0.81	0.23	74,74,74,74	0
56	MG	CA	3110	1/1	0.81	0.15	93,93,93,93	0
56	MG	AA	3148	1/1	0.81	0.15	72,72,72,72	0
56	MG	BA	3705	1/1	0.81	0.15	64,64,64,64	0
56	MG	CA	3172	1/1	0.81	0.19	65,65,65,65	0
56	MG	BA	3510	1/1	0.81	0.24	66,66,66,66	0
56	MG	AA	3039	1/1	0.81	0.12	62,62,62,62	0
56	MG	AA	3112	1/1	0.81	0.14	53,53,53,53	0
56	MG	DA	3073	1/1	0.81	0.23	50,50,50,50	0
56	MG	DA	3096	1/1	0.81	0.15	68,68,68,68	0
56	MG	AA	3045	1/1	0.81	0.27	71,71,71,71	0
56	MG	BA	3636	1/1	0.81	0.12	54,54,54,54	0
56	MG	DA	3496	1/1	0.82	0.21	76,76,76,76	0
56	MG	BF	306	1/1	0.82	0.13	52,52,52,52	0
56	MG	CA	3067	1/1	0.82	0.17	66,66,66,66	0
56	MG	CA	3007	1/1	0.82	0.13	63,63,63,63	0
56	MG	DA	3549	1/1	0.82	0.20	73,73,73,73	0
56	MG	AA	3217	1/1	0.82	0.30	64,64,64,64	0
56	MG	CA	3091	1/1	0.82	0.12	95,95,95,95	0
56	MG	BA	3710	1/1	0.82	0.16	57,57,57,57	0
56	MG	DA	3241	1/1	0.82	0.07	74,74,74,74	0
56	MG	BA	3028	1/1	0.82	0.26	59,59,59,59	0
56	MG	BA	3716	1/1	0.82	0.20	77,77,77,77	0
56	MG	AD	502	1/1	0.82	0.31	56,56,56,56	0
56	MG	CA	3129	1/1	0.82	0.21	54,54,54,54	0
56	MG	CA	3136	1/1	0.82	0.25	70,70,70,70	0
56	MG	CA	3039	1/1	0.82	0.32	82,82,82,82	0
56	MG	AA	3171	1/1	0.82	0.15	77,77,77,77	0
56	MG	AA	3016	1/1	0.82	0.10	70,70,70,70	0
56	MG	CA	3065	1/1	0.83	0.17	81,81,81,81	0
56	MG	DA	3314	1/1	0.83	0.14	56,56,56,56	0
56	MG	BA	3247	1/1	0.83	0.26	58,58,58,58	0
56	MG	BB	3014	1/1	0.83	0.17	68,68,68,68	0
56	MG	DA	3414	1/1	0.83	0.20	59,59,59,59	0
56	MG	BB	3017	1/1	0.83	0.29	80,80,80,80	0
56	MG	BA	3638	1/1	0.83	0.14	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CX	103	1/1	0.83	0.08	57,57,57,57	0
56	MG	AA	3106	1/1	0.83	0.29	68,68,68,68	0
56	MG	BA	3686	1/1	0.83	0.26	65,65,65,65	0
56	MG	DA	3022	1/1	0.83	0.14	41,41,41,41	0
56	MG	BA	3693	1/1	0.83	0.22	57,57,57,57	0
56	MG	BA	3701	1/1	0.83	0.12	69,69,69,69	0
56	MG	BA	3294	1/1	0.83	0.21	59,59,59,59	0
56	MG	DA	3108	1/1	0.83	0.11	50,50,50,50	0
56	MG	DA	3554	1/1	0.83	0.07	62,62,62,62	0
56	MG	BA	3338	1/1	0.83	0.18	62,62,62,62	0
56	MG	BA	3068	1/1	0.83	0.30	43,43,43,43	0
56	MG	DA	3122	1/1	0.83	0.11	60,60,60,60	0
56	MG	CA	3141	1/1	0.83	0.40	85,85,85,85	0
56	MG	DA	3617	1/1	0.83	0.12	51,51,51,51	0
56	MG	AA	3079	1/1	0.83	0.27	65,65,65,65	0
56	MG	DA	3620	1/1	0.83	0.16	66,66,66,66	0
56	MG	AA	3127	1/1	0.83	0.20	50,50,50,50	0
56	MG	BA	3177	1/1	0.83	0.48	35,35,35,35	0
56	MG	DA	3171	1/1	0.83	0.26	58,58,58,58	0
56	MG	DA	3189	1/1	0.83	0.21	55,55,55,55	0
56	MG	CA	3060	1/1	0.83	0.29	59,59,59,59	0
56	MG	AA	3089	1/1	0.83	0.24	80,80,80,80	0
56	MG	DA	3246	1/1	0.83	0.10	55,55,55,55	0
56	MG	DQ	3004	1/1	0.83	0.13	52,52,52,52	0
59	FME	CX	101	10/11	0.83	0.25	59,80,100,106	0
56	MG	AA	3068	1/1	0.84	0.21	67,67,67,67	0
56	MG	DA	3418	1/1	0.84	0.14	57,57,57,57	0
56	MG	BA	3071	1/1	0.84	0.20	55,55,55,55	0
56	MG	AA	3196	1/1	0.84	0.32	78,78,78,78	0
56	MG	AA	3029	1/1	0.84	0.33	60,60,60,60	0
56	MG	BA	3651	1/1	0.84	0.23	52,52,52,52	0
56	MG	DA	3098	1/1	0.84	0.34	45,45,45,45	0
56	MG	AA	3098	1/1	0.84	0.37	76,76,76,76	0
56	MG	AA	3023	1/1	0.84	0.14	56,56,56,56	0
56	MG	AA	3028	1/1	0.84	0.23	72,72,72,72	0
56	MG	DA	3537	1/1	0.84	0.15	74,74,74,74	0
56	MG	BA	3272	1/1	0.84	0.21	49,49,49,49	0
56	MG	CA	3032	1/1	0.84	0.21	44,44,44,44	0
56	MG	DA	3124	1/1	0.84	0.17	66,66,66,66	0
56	MG	CA	3033	1/1	0.84	0.14	64,64,64,64	0
56	MG	AA	3064	1/1	0.84	0.07	65,65,65,65	0
56	MG	DA	3586	1/1	0.84	0.12	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3162	1/1	0.84	0.20	69,69,69,69	0
56	MG	CA	3041	1/1	0.84	0.32	71,71,71,71	0
56	MG	DA	3608	1/1	0.84	0.23	63,63,63,63	0
56	MG	DA	3613	1/1	0.84	0.21	64,64,64,64	0
56	MG	CA	3153	1/1	0.84	0.15	85,85,85,85	0
56	MG	AA	3033	1/1	0.84	0.23	68,68,68,68	0
56	MG	AA	3090	1/1	0.84	0.24	64,64,64,64	0
56	MG	BA	3022	1/1	0.84	0.24	66,66,66,66	0
56	MG	DA	3243	1/1	0.84	0.21	49,49,49,49	0
56	MG	BA	3465	1/1	0.84	0.12	51,51,51,51	0
56	MG	DA	3263	1/1	0.84	0.14	48,48,48,48	0
56	MG	BA	3467	1/1	0.84	0.09	44,44,44,44	0
56	MG	BA	3027	1/1	0.84	0.14	53,53,53,53	0
56	MG	AA	3092	1/1	0.84	0.27	59,59,59,59	0
56	MG	BA	3616	1/1	0.84	0.18	73,73,73,73	0
56	MG	DA	3405	1/1	0.84	0.26	53,53,53,53	0
56	MG	DA	3060	1/1	0.85	0.07	51,51,51,51	0
56	MG	DA	3062	1/1	0.85	0.24	58,58,58,58	0
56	MG	AA	3037	1/1	0.85	0.17	53,53,53,53	0
56	MG	AA	3061	1/1	0.85	0.11	57,57,57,57	0
56	MG	DA	3086	1/1	0.85	0.20	43,43,43,43	0
56	MG	CA	3029	1/1	0.85	0.17	54,54,54,54	0
56	MG	CA	3127	1/1	0.85	0.12	72,72,72,72	0
56	MG	AA	3162	1/1	0.85	0.17	79,79,79,79	0
56	MG	DA	3109	1/1	0.85	0.15	55,55,55,55	0
56	MG	DA	3112	1/1	0.85	0.23	49,49,49,49	0
56	MG	BA	3596	1/1	0.85	0.12	79,79,79,79	0
56	MG	BA	3601	1/1	0.85	0.18	61,61,61,61	0
56	MG	BA	3248	1/1	0.85	0.34	68,68,68,68	0
56	MG	BA	3257	1/1	0.85	0.22	56,56,56,56	0
56	MG	BA	3739	1/1	0.85	0.10	50,50,50,50	0
56	MG	DA	3566	1/1	0.85	0.18	55,55,55,55	0
56	MG	AA	3017	1/1	0.85	0.25	57,57,57,57	0
56	MG	BA	3060	1/1	0.85	0.32	64,64,64,64	0
56	MG	DA	3155	1/1	0.85	0.15	50,50,50,50	0
56	MG	DA	3596	1/1	0.85	0.21	68,68,68,68	0
56	MG	AA	3070	1/1	0.85	0.15	68,68,68,68	0
56	MG	BA	3648	1/1	0.85	0.14	54,54,54,54	0
56	MG	DA	3606	1/1	0.85	0.14	58,58,58,58	0
56	MG	BA	3301	1/1	0.85	0.18	44,44,44,44	0
56	MG	AA	3178	1/1	0.85	0.17	63,63,63,63	0
56	MG	CA	3071	1/1	0.85	0.26	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3667	1/1	0.85	0.18	72,72,72,72	0
56	MG	CA	3074	1/1	0.85	0.19	56,56,56,56	0
56	MG	CE	3001	1/1	0.85	0.19	66,66,66,66	0
56	MG	DA	3251	1/1	0.85	0.21	50,50,50,50	0
56	MG	CA	3081	1/1	0.85	0.14	72,72,72,72	0
56	MG	AA	3132	1/1	0.85	0.17	59,59,59,59	0
56	MG	DA	3306	1/1	0.85	0.11	51,51,51,51	0
56	MG	DA	3005	1/1	0.85	0.09	50,50,50,50	0
56	MG	DB	3010	1/1	0.85	0.17	66,66,66,66	0
56	MG	DF	304	1/1	0.85	0.25	39,39,39,39	0
56	MG	CA	3103	1/1	0.85	0.14	101,101,101,101	0
56	MG	AA	3088	1/1	0.85	0.25	53,53,53,53	0
59	FME	AX	101	10/11	0.85	0.22	55,74,92,107	0
56	MG	DA	3361	1/1	0.85	0.17	58,58,58,58	0
56	MG	BA	3088	1/1	0.86	0.10	55,55,55,55	0
56	MG	DA	3514	1/1	0.86	0.18	60,60,60,60	0
56	MG	DA	3524	1/1	0.86	0.10	51,51,51,51	0
56	MG	DA	3529	1/1	0.86	0.23	72,72,72,72	0
56	MG	DA	3532	1/1	0.86	0.14	60,60,60,60	0
56	MG	CA	3125	1/1	0.86	0.17	64,64,64,64	0
56	MG	BA	3641	1/1	0.86	0.10	33,33,33,33	0
56	MG	CA	3048	1/1	0.86	0.32	70,70,70,70	0
56	MG	DA	3212	1/1	0.86	0.18	48,48,48,48	0
56	MG	DA	3035	1/1	0.86	0.16	58,58,58,58	0
56	MG	DA	3057	1/1	0.86	0.19	57,57,57,57	0
56	MG	CA	3135	1/1	0.86	0.20	61,61,61,61	0
56	MG	AA	3025	1/1	0.86	0.11	78,78,78,78	0
56	MG	DA	3587	1/1	0.86	0.17	57,57,57,57	0
56	MG	DA	3589	1/1	0.86	0.14	65,65,65,65	0
56	MG	BA	3014	1/1	0.86	0.30	48,48,48,48	0
56	MG	BA	3021	1/1	0.86	0.17	62,62,62,62	0
56	MG	DA	3289	1/1	0.86	0.21	64,64,64,64	0
56	MG	DA	3084	1/1	0.86	0.10	55,55,55,55	0
56	MG	AA	3082	1/1	0.86	0.26	52,52,52,52	0
56	MG	BA	3223	1/1	0.86	0.23	49,49,49,49	0
56	MG	DA	3333	1/1	0.86	0.09	61,61,61,61	0
56	MG	BW	3001	1/1	0.86	0.13	55,55,55,55	0
56	MG	B7	101	1/1	0.86	0.16	45,45,45,45	0
56	MG	BA	3567	1/1	0.86	0.07	54,54,54,54	0
56	MG	AA	3053	1/1	0.86	0.20	56,56,56,56	0
56	MG	BA	3702	1/1	0.86	0.11	56,56,56,56	0
56	MG	AF	3001	1/1	0.86	0.16	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3134	1/1	0.86	0.31	70,70,70,70	0
56	MG	BA	3066	1/1	0.86	0.20	49,49,49,49	0
56	MG	CA	3168	1/1	0.86	0.30	79,79,79,79	0
56	MG	DB	3011	1/1	0.86	0.18	49,49,49,49	0
56	MG	AA	3097	1/1	0.86	0.32	53,53,53,53	0
56	MG	BA	3293	1/1	0.86	0.31	69,69,69,69	0
56	MG	DA	3491	1/1	0.86	0.25	55,55,55,55	0
56	MG	D3	101	1/1	0.86	0.12	54,54,54,54	0
56	MG	DA	3153	1/1	0.86	0.21	51,51,51,51	0
56	MG	AX	105	1/1	0.86	0.20	72,72,72,72	0
60	K	BA	3304	1/1	0.86	0.19	93,93,93,93	0
56	MG	DA	3367	1/1	0.87	0.19	55,55,55,55	0
56	MG	DA	3391	1/1	0.87	0.10	54,54,54,54	0
56	MG	CA	3042	1/1	0.87	0.28	69,69,69,69	0
56	MG	BA	3262	1/1	0.87	0.33	44,44,44,44	0
56	MG	BA	3267	1/1	0.87	0.18	56,56,56,56	0
56	MG	AA	3078	1/1	0.87	0.31	55,55,55,55	0
56	MG	AA	3203	1/1	0.87	0.12	76,76,76,76	0
56	MG	DA	3448	1/1	0.87	0.22	67,67,67,67	0
56	MG	BA	3694	1/1	0.87	0.16	48,48,48,48	0
56	MG	AA	3143	1/1	0.87	0.15	67,67,67,67	0
56	MG	BA	3107	1/1	0.87	0.23	60,60,60,60	0
56	MG	BA	3119	1/1	0.87	0.12	56,56,56,56	0
56	MG	BA	3122	1/1	0.87	0.12	68,68,68,68	0
56	MG	DA	3074	1/1	0.87	0.26	60,60,60,60	0
56	MG	BA	3123	1/1	0.87	0.12	47,47,47,47	0
56	MG	BA	3709	1/1	0.87	0.15	77,77,77,77	0
56	MG	BA	3433	1/1	0.87	0.25	46,46,46,46	0
56	MG	DA	3525	1/1	0.87	0.12	56,56,56,56	0
56	MG	AA	3215	1/1	0.87	0.32	77,77,77,77	0
56	MG	DA	3531	1/1	0.87	0.08	44,44,44,44	0
56	MG	BA	3137	1/1	0.87	0.16	59,59,59,59	0
56	MG	CA	3109	1/1	0.87	0.17	79,79,79,79	0
56	MG	BA	3722	1/1	0.87	0.10	49,49,49,49	0
56	MG	CA	3111	1/1	0.87	0.16	69,69,69,69	0
56	MG	BA	3732	1/1	0.87	0.21	56,56,56,56	0
56	MG	BA	3156	1/1	0.87	0.25	61,61,61,61	0
56	MG	BA	3514	1/1	0.87	0.13	49,49,49,49	0
56	MG	CA	3122	1/1	0.87	0.18	70,70,70,70	0
56	MG	DA	3585	1/1	0.87	0.26	62,62,62,62	0
56	MG	CA	3124	1/1	0.87	0.12	64,64,64,64	0
56	MG	BA	3530	1/1	0.87	0.14	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3538	1/1	0.87	0.13	29,29,29,29	0
56	MG	BA	3563	1/1	0.87	0.40	66,66,66,66	0
56	MG	BA	3565	1/1	0.87	0.13	75,75,75,75	0
56	MG	AA	3147	1/1	0.87	0.14	51,51,51,51	0
56	MG	DA	3170	1/1	0.87	0.10	45,45,45,45	0
56	MG	DA	3607	1/1	0.87	0.21	68,68,68,68	0
56	MG	BA	3180	1/1	0.87	0.28	48,48,48,48	0
56	MG	BX	102	1/1	0.87	0.22	60,60,60,60	0
56	MG	BA	3183	1/1	0.87	0.13	40,40,40,40	0
56	MG	CA	3004	1/1	0.87	0.14	88,88,88,88	0
56	MG	DA	3224	1/1	0.87	0.23	53,53,53,53	0
56	MG	DA	3621	1/1	0.87	0.15	46,46,46,46	0
56	MG	CA	3146	1/1	0.87	0.16	61,61,61,61	0
56	MG	BA	3597	1/1	0.87	0.14	46,46,46,46	0
56	MG	CA	3008	1/1	0.87	0.37	59,59,59,59	0
56	MG	BA	3184	1/1	0.87	0.24	51,51,51,51	0
56	MG	DA	3645	1/1	0.87	0.22	57,57,57,57	0
56	MG	BA	3186	1/1	0.87	0.19	50,50,50,50	0
56	MG	AA	3074	1/1	0.87	0.22	40,40,40,40	0
56	MG	DB	3006	1/1	0.87	0.11	54,54,54,54	0
56	MG	BA	3212	1/1	0.87	0.22	47,47,47,47	0
56	MG	AA	3081	1/1	0.87	0.27	46,46,46,46	0
56	MG	BA	3637	1/1	0.87	0.59	52,52,52,52	0
56	MG	DA	3323	1/1	0.87	0.10	60,60,60,60	0
56	MG	DA	3326	1/1	0.87	0.17	61,61,61,61	0
56	MG	BA	3240	1/1	0.87	0.26	54,54,54,54	0
56	MG	AA	3194	1/1	0.87	0.17	50,50,50,50	0
56	MG	AX	103	1/1	0.87	0.06	57,57,57,57	0
56	MG	AA	3020	1/1	0.87	0.10	80,80,80,80	0
56	MG	DA	3344	1/1	0.88	0.08	48,48,48,48	0
56	MG	CA	3160	1/1	0.88	0.13	49,49,49,49	0
56	MG	DA	3351	1/1	0.88	0.13	58,58,58,58	0
56	MG	BA	3681	1/1	0.88	0.26	54,54,54,54	0
56	MG	BA	3172	1/1	0.88	0.13	54,54,54,54	0
56	MG	CA	3034	1/1	0.88	0.27	66,66,66,66	0
56	MG	DA	3373	1/1	0.88	0.15	52,52,52,52	0
56	MG	CA	3038	1/1	0.88	0.10	54,54,54,54	0
56	MG	DA	3392	1/1	0.88	0.11	60,60,60,60	0
56	MG	CA	3171	1/1	0.88	0.16	61,61,61,61	0
56	MG	AA	3122	1/1	0.88	0.35	40,40,40,40	0
56	MG	BA	3369	1/1	0.88	0.14	49,49,49,49	0
56	MG	BA	3178	1/1	0.88	0.17	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3043	1/1	0.88	0.15	62,62,62,62	0
56	MG	AA	3207	1/1	0.88	0.15	51,51,51,51	0
56	MG	CA	3050	1/1	0.88	0.23	54,54,54,54	0
56	MG	DA	3457	1/1	0.88	0.09	44,44,44,44	0
56	MG	DA	3460	1/1	0.88	0.14	47,47,47,47	0
56	MG	AA	3080	1/1	0.88	0.22	58,58,58,58	0
56	MG	BA	3469	1/1	0.88	0.12	60,60,60,60	0
56	MG	DA	3468	1/1	0.88	0.14	47,47,47,47	0
56	MG	DA	3039	1/1	0.88	0.25	46,46,46,46	0
56	MG	DA	3040	1/1	0.88	0.15	45,45,45,45	0
56	MG	DA	3043	1/1	0.88	0.27	56,56,56,56	0
56	MG	DA	3504	1/1	0.88	0.11	46,46,46,46	0
56	MG	BA	3485	1/1	0.88	0.13	67,67,67,67	0
56	MG	AA	3046	1/1	0.88	0.20	60,60,60,60	0
56	MG	CA	3064	1/1	0.88	0.12	74,74,74,74	0
56	MG	BA	3064	1/1	0.88	0.10	49,49,49,49	0
56	MG	AA	3003	1/1	0.88	0.13	70,70,70,70	0
56	MG	BA	3204	1/1	0.88	0.12	48,48,48,48	0
56	MG	BA	3717	1/1	0.88	0.13	51,51,51,51	0
56	MG	DA	3534	1/1	0.88	0.13	62,62,62,62	0
56	MG	AA	3218	1/1	0.88	0.14	73,73,73,73	0
56	MG	DA	3089	1/1	0.88	0.08	51,51,51,51	0
56	MG	DA	3095	1/1	0.88	0.22	53,53,53,53	0
56	MG	BA	3213	1/1	0.88	0.15	63,63,63,63	0
56	MG	DA	3557	1/1	0.88	0.14	74,74,74,74	0
56	MG	DA	3563	1/1	0.88	0.16	49,49,49,49	0
56	MG	AA	3219	1/1	0.88	0.16	54,54,54,54	0
56	MG	DA	3102	1/1	0.88	0.11	49,49,49,49	0
56	MG	CA	3084	1/1	0.88	0.22	80,80,80,80	0
56	MG	CA	3086	1/1	0.88	0.20	70,70,70,70	0
56	MG	BA	3224	1/1	0.88	0.18	48,48,48,48	0
56	MG	BB	3001	1/1	0.88	0.17	56,56,56,56	0
56	MG	CA	3107	1/1	0.88	0.23	71,71,71,71	0
56	MG	AA	3174	1/1	0.88	0.19	49,49,49,49	0
56	MG	AA	3176	1/1	0.88	0.16	60,60,60,60	0
56	MG	AA	3086	1/1	0.88	0.13	65,65,65,65	0
56	MG	BB	3018	1/1	0.88	0.16	54,54,54,54	0
56	MG	CA	3116	1/1	0.88	0.16	76,76,76,76	0
56	MG	AA	3027	1/1	0.88	0.11	67,67,67,67	0
56	MG	BD	309	1/1	0.88	0.18	43,43,43,43	0
56	MG	AA	3005	1/1	0.88	0.35	66,66,66,66	0
56	MG	BG	3003	1/1	0.88	0.13	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BQ	3002	1/1	0.88	0.10	51,51,51,51	0
56	MG	AA	3018	1/1	0.88	0.20	51,51,51,51	0
56	MG	AA	3141	1/1	0.88	0.18	51,51,51,51	0
56	MG	DA	3628	1/1	0.88	0.11	38,38,38,38	0
56	MG	BA	3289	1/1	0.88	0.19	53,53,53,53	0
56	MG	DA	3637	1/1	0.88	0.20	59,59,59,59	0
56	MG	CA	3003	1/1	0.88	0.13	69,69,69,69	0
56	MG	BA	3291	1/1	0.88	0.17	44,44,44,44	0
56	MG	DA	3230	1/1	0.88	0.19	61,61,61,61	0
56	MG	AA	3065	1/1	0.88	0.25	50,50,50,50	0
56	MG	BA	3644	1/1	0.88	0.13	38,38,38,38	0
56	MG	BA	3155	1/1	0.88	0.08	56,56,56,56	0
56	MG	CA	3022	1/1	0.88	0.09	67,67,67,67	0
56	MG	AA	3019	1/1	0.88	0.16	64,64,64,64	0
56	MG	CA	3150	1/1	0.88	0.12	63,63,63,63	0
56	MG	BA	3158	1/1	0.88	0.29	43,43,43,43	0
56	MG	DQ	3003	1/1	0.88	0.18	58,58,58,58	0
56	MG	BA	3335	1/1	0.88	0.19	51,51,51,51	0
56	MG	DY	502	1/1	0.88	0.13	66,66,66,66	0
56	MG	BA	3671	1/1	0.88	0.13	44,44,44,44	0
56	MG	CA	3157	1/1	0.88	0.11	56,56,56,56	0
56	MG	CA	3158	1/1	0.88	0.12	64,64,64,64	0
56	MG	BA	3674	1/1	0.88	0.17	67,67,67,67	0
56	MG	DA	3425	1/1	0.89	0.17	51,51,51,51	0
56	MG	BA	3238	1/1	0.89	0.15	48,48,48,48	0
56	MG	BA	3473	1/1	0.89	0.14	55,55,55,55	0
56	MG	BA	3149	1/1	0.89	0.13	58,58,58,58	0
56	MG	AA	3077	1/1	0.89	0.31	67,67,67,67	0
56	MG	DA	3099	1/1	0.89	0.20	39,39,39,39	0
56	MG	AM	3002	1/1	0.89	0.25	60,60,60,60	0
56	MG	BA	3520	1/1	0.89	0.12	69,69,69,69	0
56	MG	AA	3071	1/1	0.89	0.24	60,60,60,60	0
56	MG	DA	3465	1/1	0.89	0.08	41,41,41,41	0
56	MG	DA	3110	1/1	0.89	0.15	46,46,46,46	0
56	MG	DA	3475	1/1	0.89	0.11	35,35,35,35	0
56	MG	AA	3015	1/1	0.89	0.13	74,74,74,74	0
56	MG	BA	3173	1/1	0.89	0.18	41,41,41,41	0
56	MG	CA	3145	1/1	0.89	0.08	67,67,67,67	0
56	MG	DA	3119	1/1	0.89	0.11	44,44,44,44	0
56	MG	DA	3121	1/1	0.89	0.10	46,46,46,46	0
56	MG	AA	3121	1/1	0.89	0.23	52,52,52,52	0
56	MG	AA	3073	1/1	0.89	0.12	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3094	1/1	0.89	0.19	62,62,62,62	0
56	MG	DA	3528	1/1	0.89	0.10	33,33,33,33	0
56	MG	DA	3128	1/1	0.89	0.16	54,54,54,54	0
56	MG	BA	3583	1/1	0.89	0.20	57,57,57,57	0
56	MG	AA	3139	1/1	0.89	0.18	58,58,58,58	0
56	MG	CA	3054	1/1	0.89	0.23	74,74,74,74	0
56	MG	DA	3536	1/1	0.89	0.10	57,57,57,57	0
56	MG	AA	3216	1/1	0.89	0.20	60,60,60,60	0
56	MG	DA	3157	1/1	0.89	0.29	56,56,56,56	0
56	MG	BA	3111	1/1	0.89	0.17	43,43,43,43	0
56	MG	DA	3166	1/1	0.89	0.07	37,37,37,37	0
56	MG	BA	3604	1/1	0.89	0.19	64,64,64,64	0
56	MG	BA	3296	1/1	0.89	0.24	69,69,69,69	0
56	MG	BA	3202	1/1	0.89	0.25	29,29,29,29	0
56	MG	BA	3317	1/1	0.89	0.16	40,40,40,40	0
56	MG	DA	3190	1/1	0.89	0.09	54,54,54,54	0
56	MG	DA	3196	1/1	0.89	0.17	54,54,54,54	0
56	MG	BA	3631	1/1	0.89	0.13	41,41,41,41	0
56	MG	BA	3634	1/1	0.89	0.15	77,77,77,77	0
56	MG	BA	3328	1/1	0.89	0.15	41,41,41,41	0
56	MG	DA	3591	1/1	0.89	0.14	67,67,67,67	0
56	MG	BD	305	1/1	0.89	0.18	41,41,41,41	0
56	MG	DA	3598	1/1	0.89	0.09	45,45,45,45	0
56	MG	DA	3240	1/1	0.89	0.24	58,58,58,58	0
56	MG	AA	3126	1/1	0.89	0.22	54,54,54,54	0
56	MG	CN	502	1/1	0.89	0.17	70,70,70,70	0
56	MG	AA	3056	1/1	0.89	0.27	61,61,61,61	0
56	MG	BA	3640	1/1	0.89	0.15	31,31,31,31	0
56	MG	DA	3255	1/1	0.89	0.17	46,46,46,46	0
56	MG	BA	3208	1/1	0.89	0.18	50,50,50,50	0
56	MG	DA	3618	1/1	0.89	0.18	61,61,61,61	0
56	MG	DA	3281	1/1	0.89	0.09	33,33,33,33	0
56	MG	DA	3282	1/1	0.89	0.14	58,58,58,58	0
56	MG	DA	3287	1/1	0.89	0.09	53,53,53,53	0
56	MG	AA	3128	1/1	0.89	0.23	64,64,64,64	0
56	MG	DA	3020	1/1	0.89	0.18	45,45,45,45	0
56	MG	CA	3106	1/1	0.89	0.23	72,72,72,72	0
56	MG	DA	3029	1/1	0.89	0.17	62,62,62,62	0
56	MG	BA	3373	1/1	0.89	0.07	48,48,48,48	0
56	MG	BA	3429	1/1	0.89	0.21	55,55,55,55	0
56	MG	AA	3004	1/1	0.89	0.17	50,50,50,50	0
56	MG	DA	3336	1/1	0.89	0.12	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3663	1/1	0.89	0.25	73,73,73,73	0
56	MG	CA	3112	1/1	0.89	0.20	69,69,69,69	0
56	MG	BA	3447	1/1	0.89	0.10	76,76,76,76	0
56	MG	BA	3669	1/1	0.89	0.12	61,61,61,61	0
56	MG	BA	3460	1/1	0.89	0.17	66,66,66,66	0
56	MG	DA	3069	1/1	0.89	0.17	49,49,49,49	0
56	MG	BA	3039	1/1	0.89	0.16	44,44,44,44	0
56	MG	CA	3121	1/1	0.89	0.29	59,59,59,59	0
56	MG	DV	202	1/1	0.89	0.21	45,45,45,45	0
56	MG	DW	202	1/1	0.89	0.11	53,53,53,53	0
56	MG	DA	3078	1/1	0.89	0.14	49,49,49,49	0
56	MG	BA	3675	1/1	0.89	0.29	68,68,68,68	0
56	MG	BA	3143	1/1	0.89	0.38	41,41,41,41	0
56	MG	DA	3087	1/1	0.89	0.15	43,43,43,43	0
56	MG	DA	3424	1/1	0.89	0.14	58,58,58,58	0
60	K	DA	3234	1/1	0.89	0.21	102,102,102,102	0
56	MG	BA	3549	1/1	0.90	0.25	49,49,49,49	0
56	MG	BA	3714	1/1	0.90	0.12	72,72,72,72	0
56	MG	CA	3069	1/1	0.90	0.21	63,63,63,63	0
56	MG	DA	3393	1/1	0.90	0.20	35,35,35,35	0
56	MG	AX	106	1/1	0.90	0.10	64,64,64,64	0
56	MG	DA	3068	1/1	0.90	0.12	52,52,52,52	0
56	MG	AA	3099	1/1	0.90	0.20	49,49,49,49	0
56	MG	CA	3072	1/1	0.90	0.20	57,57,57,57	0
56	MG	BA	3283	1/1	0.90	0.23	61,61,61,61	0
56	MG	BA	3571	1/1	0.90	0.12	48,48,48,48	0
56	MG	DA	3079	1/1	0.90	0.09	44,44,44,44	0
56	MG	DA	3444	1/1	0.90	0.18	43,43,43,43	0
56	MG	DA	3445	1/1	0.90	0.34	60,60,60,60	0
56	MG	DA	3447	1/1	0.90	0.13	56,56,56,56	0
56	MG	BA	3006	1/1	0.90	0.10	46,46,46,46	0
56	MG	DA	3452	1/1	0.90	0.22	64,64,64,64	0
56	MG	BA	3105	1/1	0.90	0.28	54,54,54,54	0
56	MG	BA	3591	1/1	0.90	0.13	38,38,38,38	0
56	MG	BB	3003	1/1	0.90	0.14	40,40,40,40	0
56	MG	DA	3093	1/1	0.90	0.14	51,51,51,51	0
56	MG	AA	3100	1/1	0.90	0.19	43,43,43,43	0
56	MG	BB	3006	1/1	0.90	0.21	34,34,34,34	0
56	MG	AA	3102	1/1	0.90	0.20	68,68,68,68	0
56	MG	CA	3108	1/1	0.90	0.11	45,45,45,45	0
56	MG	BA	3114	1/1	0.90	0.25	46,46,46,46	0
56	MG	DA	3495	1/1	0.90	0.09	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3106	1/1	0.90	0.28	45,45,45,45	0
56	MG	BA	3118	1/1	0.90	0.22	53,53,53,53	0
56	MG	BA	3299	1/1	0.90	0.25	56,56,56,56	0
56	MG	BA	3300	1/1	0.90	0.18	48,48,48,48	0
56	MG	DA	3513	1/1	0.90	0.12	58,58,58,58	0
56	MG	AA	3013	1/1	0.90	0.07	75,75,75,75	0
56	MG	DA	3523	1/1	0.90	0.08	47,47,47,47	0
56	MG	BD	311	1/1	0.90	0.29	53,53,53,53	0
56	MG	BF	303	1/1	0.90	0.18	42,42,42,42	0
56	MG	AA	3107	1/1	0.90	0.21	44,44,44,44	0
56	MG	BA	3632	1/1	0.90	0.13	55,55,55,55	0
56	MG	BG	3004	1/1	0.90	0.14	53,53,53,53	0
56	MG	AA	3001	1/1	0.90	0.19	74,74,74,74	0
56	MG	BU	202	1/1	0.90	0.48	41,41,41,41	0
56	MG	CA	3126	1/1	0.90	0.11	56,56,56,56	0
56	MG	BA	3331	1/1	0.90	0.12	61,61,61,61	0
56	MG	DA	3134	1/1	0.90	0.14	37,37,37,37	0
56	MG	DA	3135	1/1	0.90	0.15	58,58,58,58	0
56	MG	BW	3005	1/1	0.90	0.16	38,38,38,38	0
56	MG	AA	3113	1/1	0.90	0.16	56,56,56,56	0
56	MG	B1	3001	1/1	0.90	0.46	63,63,63,63	0
56	MG	B2	101	1/1	0.90	0.09	34,34,34,34	0
56	MG	BA	3209	1/1	0.90	0.23	39,39,39,39	0
56	MG	BA	3357	1/1	0.90	0.16	45,45,45,45	0
56	MG	DA	3571	1/1	0.90	0.17	57,57,57,57	0
56	MG	BA	3135	1/1	0.90	0.23	57,57,57,57	0
56	MG	BA	3643	1/1	0.90	0.11	59,59,59,59	0
56	MG	AA	3009	1/1	0.90	0.29	71,71,71,71	0
56	MG	DA	3172	1/1	0.90	0.21	46,46,46,46	0
56	MG	DA	3175	1/1	0.90	0.20	52,52,52,52	0
56	MG	DA	3595	1/1	0.90	0.14	53,53,53,53	0
56	MG	DA	3180	1/1	0.90	0.25	47,47,47,47	0
56	MG	BA	3214	1/1	0.90	0.17	37,37,37,37	0
56	MG	DA	3600	1/1	0.90	0.13	73,73,73,73	0
56	MG	CA	3015	1/1	0.90	0.15	53,53,53,53	0
56	MG	BA	3376	1/1	0.90	0.20	35,35,35,35	0
56	MG	DA	3205	1/1	0.90	0.15	41,41,41,41	0
56	MG	AX	102	1/1	0.90	0.14	66,66,66,66	0
56	MG	CA	3155	1/1	0.90	0.08	71,71,71,71	0
56	MG	BA	3144	1/1	0.90	0.11	52,52,52,52	0
56	MG	BA	3230	1/1	0.90	0.30	70,70,70,70	0
56	MG	DA	3236	1/1	0.90	0.08	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3047	1/1	0.90	0.23	59,59,59,59	0
56	MG	AA	3085	1/1	0.90	0.24	57,57,57,57	0
56	MG	CA	3031	1/1	0.90	0.34	55,55,55,55	0
56	MG	BA	3070	1/1	0.90	0.10	46,46,46,46	0
56	MG	AA	3135	1/1	0.90	0.17	49,49,49,49	0
56	MG	BA	3676	1/1	0.90	0.09	63,63,63,63	0
56	MG	DA	3256	1/1	0.90	0.14	41,41,41,41	0
56	MG	CA	3036	1/1	0.90	0.12	56,56,56,56	0
56	MG	DA	3278	1/1	0.90	0.08	39,39,39,39	0
56	MG	CA	3037	1/1	0.90	0.13	45,45,45,45	0
56	MG	DA	3646	1/1	0.90	0.09	42,42,42,42	0
56	MG	BA	3251	1/1	0.90	0.07	45,45,45,45	0
56	MG	DB	3002	1/1	0.90	0.23	72,72,72,72	0
56	MG	BA	3477	1/1	0.90	0.18	52,52,52,52	0
56	MG	DB	3004	1/1	0.90	0.14	56,56,56,56	0
56	MG	BA	3252	1/1	0.90	0.28	65,65,65,65	0
56	MG	BA	3499	1/1	0.90	0.23	50,50,50,50	0
56	MG	BA	3696	1/1	0.90	0.13	36,36,36,36	0
56	MG	DB	3012	1/1	0.90	0.23	50,50,50,50	0
56	MG	DE	303	1/1	0.90	0.14	36,36,36,36	0
56	MG	CA	3047	1/1	0.90	0.14	56,56,56,56	0
56	MG	BA	3697	1/1	0.90	0.14	63,63,63,63	0
56	MG	BA	3253	1/1	0.90	0.31	63,63,63,63	0
56	MG	BA	3512	1/1	0.90	0.13	42,42,42,42	0
56	MG	BA	3255	1/1	0.90	0.18	53,53,53,53	0
56	MG	BA	3164	1/1	0.90	0.18	57,57,57,57	0
56	MG	DA	3036	1/1	0.90	0.11	35,35,35,35	0
56	MG	BA	3261	1/1	0.90	0.25	45,45,45,45	0
56	MG	D8	5001	1/1	0.90	0.21	53,53,53,53	0
56	MG	DA	3353	1/1	0.90	0.16	54,54,54,54	0
56	MG	BA	3535	1/1	0.90	0.16	42,42,42,42	0
56	MG	BA	3167	1/1	0.90	0.42	50,50,50,50	0
56	MG	DA	3055	1/1	0.90	0.21	55,55,55,55	0
56	MG	AA	3048	1/1	0.91	0.11	52,52,52,52	0
56	MG	BA	3672	1/1	0.91	0.15	63,63,63,63	0
56	MG	DA	3012	1/1	0.91	0.18	52,52,52,52	0
56	MG	AA	3130	1/1	0.91	0.20	55,55,55,55	0
56	MG	BA	3231	1/1	0.91	0.18	50,50,50,50	0
56	MG	DA	3354	1/1	0.91	0.06	39,39,39,39	0
56	MG	DA	3023	1/1	0.91	0.36	64,64,64,64	0
56	MG	DA	3024	1/1	0.91	0.30	59,59,59,59	0
56	MG	DA	3363	1/1	0.91	0.16	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3139	1/1	0.91	0.22	50,50,50,50	0
56	MG	AA	3191	1/1	0.91	0.10	56,56,56,56	0
56	MG	BA	3466	1/1	0.91	0.09	53,53,53,53	0
56	MG	BA	3242	1/1	0.91	0.23	45,45,45,45	0
56	MG	AA	3118	1/1	0.91	0.27	39,39,39,39	0
56	MG	AA	3150	1/1	0.91	0.27	67,67,67,67	0
56	MG	DA	3054	1/1	0.91	0.13	34,34,34,34	0
56	MG	DA	3416	1/1	0.91	0.19	34,34,34,34	0
56	MG	BA	3150	1/1	0.91	0.20	42,42,42,42	0
56	MG	DA	3419	1/1	0.91	0.09	53,53,53,53	0
56	MG	BA	3478	1/1	0.91	0.20	36,36,36,36	0
56	MG	BA	3154	1/1	0.91	0.17	55,55,55,55	0
56	MG	DA	3432	1/1	0.91	0.17	37,37,37,37	0
56	MG	DA	3435	1/1	0.91	0.12	56,56,56,56	0
56	MG	DA	3061	1/1	0.91	0.21	47,47,47,47	0
56	MG	DA	3437	1/1	0.91	0.20	46,46,46,46	0
56	MG	AA	3197	1/1	0.91	0.17	64,64,64,64	0
56	MG	CA	3058	1/1	0.91	0.08	36,36,36,36	0
56	MG	BA	3072	1/1	0.91	0.27	45,45,45,45	0
56	MG	BA	3082	1/1	0.91	0.21	54,54,54,54	0
56	MG	DA	3071	1/1	0.91	0.30	46,46,46,46	0
56	MG	CA	3062	1/1	0.91	0.33	67,67,67,67	0
56	MG	CA	3063	1/1	0.91	0.08	57,57,57,57	0
56	MG	DA	3077	1/1	0.91	0.13	48,48,48,48	0
56	MG	DA	3458	1/1	0.91	0.12	47,47,47,47	0
56	MG	BA	3163	1/1	0.91	0.14	50,50,50,50	0
56	MG	AA	3120	1/1	0.91	0.23	53,53,53,53	0
56	MG	BA	3263	1/1	0.91	0.33	35,35,35,35	0
56	MG	AA	3042	1/1	0.91	0.18	50,50,50,50	0
56	MG	BA	3099	1/1	0.91	0.33	55,55,55,55	0
56	MG	BA	3279	1/1	0.91	0.23	60,60,60,60	0
56	MG	DA	3477	1/1	0.91	0.28	35,35,35,35	0
56	MG	DA	3483	1/1	0.91	0.13	55,55,55,55	0
56	MG	DA	3485	1/1	0.91	0.09	44,44,44,44	0
56	MG	DA	3487	1/1	0.91	0.07	44,44,44,44	0
56	MG	BA	3718	1/1	0.91	0.12	52,52,52,52	0
56	MG	BA	3552	1/1	0.91	0.18	30,30,30,30	0
56	MG	BA	3725	1/1	0.91	0.07	29,29,29,29	0
56	MG	DA	3498	1/1	0.91	0.15	75,75,75,75	0
56	MG	DA	3097	1/1	0.91	0.15	58,58,58,58	0
56	MG	CA	3075	1/1	0.91	0.26	76,76,76,76	0
56	MG	BA	3561	1/1	0.91	0.16	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3507	1/1	0.91	0.17	53,53,53,53	0
56	MG	BA	3280	1/1	0.91	0.26	44,44,44,44	0
56	MG	AA	3168	1/1	0.91	0.16	80,80,80,80	0
56	MG	DA	3515	1/1	0.91	0.14	57,57,57,57	0
56	MG	DA	3521	1/1	0.91	0.11	46,46,46,46	0
56	MG	CA	3088	1/1	0.91	0.10	49,49,49,49	0
56	MG	BA	3174	1/1	0.91	0.07	52,52,52,52	0
56	MG	CA	3099	1/1	0.91	0.21	64,64,64,64	0
56	MG	DA	3111	1/1	0.91	0.21	67,67,67,67	0
56	MG	AA	3083	1/1	0.91	0.16	56,56,56,56	0
56	MG	BB	3004	1/1	0.91	0.22	57,57,57,57	0
56	MG	BA	3007	1/1	0.91	0.13	55,55,55,55	0
56	MG	BA	3109	1/1	0.91	0.38	62,62,62,62	0
56	MG	BA	3181	1/1	0.91	0.11	37,37,37,37	0
56	MG	BA	3182	1/1	0.91	0.19	43,43,43,43	0
56	MG	AA	3125	1/1	0.91	0.14	56,56,56,56	0
56	MG	DA	3542	1/1	0.91	0.10	44,44,44,44	0
56	MG	DA	3543	1/1	0.91	0.11	52,52,52,52	0
56	MG	DA	3547	1/1	0.91	0.11	47,47,47,47	0
56	MG	BA	3112	1/1	0.91	0.21	46,46,46,46	0
56	MG	CA	3113	1/1	0.91	0.23	84,84,84,84	0
56	MG	BA	3185	1/1	0.91	0.16	40,40,40,40	0
56	MG	DA	3558	1/1	0.91	0.16	77,77,77,77	0
56	MG	DA	3559	1/1	0.91	0.12	47,47,47,47	0
56	MG	BA	3612	1/1	0.91	0.14	41,41,41,41	0
56	MG	BA	3614	1/1	0.91	0.10	48,48,48,48	0
56	MG	BA	3311	1/1	0.91	0.26	52,52,52,52	0
56	MG	DA	3146	1/1	0.91	0.22	34,34,34,34	0
56	MG	DA	3152	1/1	0.91	0.15	43,43,43,43	0
56	MG	AA	3084	1/1	0.91	0.20	71,71,71,71	0
56	MG	BA	3621	1/1	0.91	0.11	57,57,57,57	0
56	MG	BA	3318	1/1	0.91	0.13	30,30,30,30	0
56	MG	BN	3001	1/1	0.91	0.13	65,65,65,65	0
56	MG	BA	3627	1/1	0.91	0.21	50,50,50,50	0
56	MG	DA	3594	1/1	0.91	0.14	63,63,63,63	0
56	MG	BA	3629	1/1	0.91	0.08	51,51,51,51	0
56	MG	BU	208	1/1	0.91	0.14	42,42,42,42	0
56	MG	BA	3324	1/1	0.91	0.19	54,54,54,54	0
56	MG	BA	3116	1/1	0.91	0.23	30,30,30,30	0
56	MG	BA	3633	1/1	0.91	0.21	54,54,54,54	0
56	MG	BZ	3001	1/1	0.91	0.12	47,47,47,47	0
56	MG	BA	3117	1/1	0.91	0.14	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3075	1/1	0.91	0.11	50,50,50,50	0
56	MG	AA	3026	1/1	0.91	0.17	52,52,52,52	0
56	MG	DA	3197	1/1	0.91	0.23	43,43,43,43	0
56	MG	DA	3198	1/1	0.91	0.18	34,34,34,34	0
56	MG	DA	3201	1/1	0.91	0.09	43,43,43,43	0
56	MG	DA	3203	1/1	0.91	0.06	48,48,48,48	0
56	MG	B7	104	1/1	0.91	0.17	55,55,55,55	0
56	MG	DA	3209	1/1	0.91	0.11	44,44,44,44	0
56	MG	DA	3622	1/1	0.91	0.10	40,40,40,40	0
56	MG	B8	5001	1/1	0.91	0.09	62,62,62,62	0
56	MG	CA	3149	1/1	0.91	0.10	81,81,81,81	0
56	MG	DA	3222	1/1	0.91	0.09	45,45,45,45	0
56	MG	DA	3636	1/1	0.91	0.18	64,64,64,64	0
56	MG	BA	3342	1/1	0.91	0.19	46,46,46,46	0
56	MG	BA	3343	1/1	0.91	0.09	37,37,37,37	0
56	MG	AA	3181	1/1	0.91	0.18	46,46,46,46	0
56	MG	AA	3182	1/1	0.91	0.09	48,48,48,48	0
56	MG	BA	3368	1/1	0.91	0.12	22,22,22,22	0
56	MG	DA	3655	1/1	0.91	0.20	62,62,62,62	0
56	MG	BA	3126	1/1	0.91	0.18	47,47,47,47	0
56	MG	CA	3018	1/1	0.91	0.07	55,55,55,55	0
56	MG	CA	3019	1/1	0.91	0.09	62,62,62,62	0
56	MG	CA	3021	1/1	0.91	0.18	54,54,54,54	0
56	MG	BA	3649	1/1	0.91	0.22	43,43,43,43	0
56	MG	CA	3024	1/1	0.91	0.27	57,57,57,57	0
56	MG	DA	3273	1/1	0.91	0.14	32,32,32,32	0
56	MG	CA	3163	1/1	0.91	0.08	60,60,60,60	0
56	MG	BA	3131	1/1	0.91	0.09	31,31,31,31	0
56	MG	DE	305	1/1	0.91	0.18	68,68,68,68	0
56	MG	BA	3654	1/1	0.91	0.17	49,49,49,49	0
56	MG	DA	3285	1/1	0.91	0.11	41,41,41,41	0
56	MG	DP	202	1/1	0.91	0.18	54,54,54,54	0
56	MG	DQ	3002	1/1	0.91	0.17	51,51,51,51	0
56	MG	CA	3169	1/1	0.91	0.16	52,52,52,52	0
56	MG	BA	3656	1/1	0.91	0.12	70,70,70,70	0
56	MG	BA	3047	1/1	0.91	0.22	30,30,30,30	0
56	MG	DA	3299	1/1	0.91	0.08	35,35,35,35	0
56	MG	BA	3390	1/1	0.91	0.12	40,40,40,40	0
56	MG	BA	3666	1/1	0.91	0.33	54,54,54,54	0
56	MG	DA	3318	1/1	0.91	0.13	47,47,47,47	0
56	MG	BA	3394	1/1	0.91	0.20	45,45,45,45	0
56	MG	BA	3395	1/1	0.91	0.22	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3331	1/1	0.91	0.11	27,27,27,27	0
56	MG	DA	3003	1/1	0.91	0.08	43,43,43,43	0
56	MG	BA	3309	1/1	0.92	0.18	43,43,43,43	0
56	MG	BA	3310	1/1	0.92	0.14	59,59,59,59	0
56	MG	CA	3079	1/1	0.92	0.07	37,37,37,37	0
56	MG	DA	3431	1/1	0.92	0.16	56,56,56,56	0
56	MG	BA	3074	1/1	0.92	0.06	38,38,38,38	0
56	MG	BA	3313	1/1	0.92	0.14	56,56,56,56	0
56	MG	DA	3090	1/1	0.92	0.19	59,59,59,59	0
56	MG	DA	3092	1/1	0.92	0.19	48,48,48,48	0
56	MG	BA	3315	1/1	0.92	0.21	43,43,43,43	0
56	MG	BA	3001	1/1	0.92	0.23	52,52,52,52	0
56	MG	BA	3145	1/1	0.92	0.14	40,40,40,40	0
56	MG	BB	3016	1/1	0.92	0.14	24,24,24,24	0
56	MG	BA	3599	1/1	0.92	0.09	56,56,56,56	0
56	MG	DA	3449	1/1	0.92	0.25	46,46,46,46	0
56	MG	CA	3104	1/1	0.92	0.16	60,60,60,60	0
56	MG	DA	3454	1/1	0.92	0.08	52,52,52,52	0
56	MG	DA	3455	1/1	0.92	0.14	53,53,53,53	0
56	MG	BA	3600	1/1	0.92	0.12	54,54,54,54	0
56	MG	BA	3084	1/1	0.92	0.35	47,47,47,47	0
56	MG	BA	3004	1/1	0.92	0.18	45,45,45,45	0
56	MG	BA	3610	1/1	0.92	0.61	49,49,49,49	0
56	MG	DA	3461	1/1	0.92	0.09	40,40,40,40	0
56	MG	AA	3038	1/1	0.92	0.37	64,64,64,64	0
56	MG	AA	3187	1/1	0.92	0.08	72,72,72,72	0
56	MG	AA	3108	1/1	0.92	0.15	72,72,72,72	0
56	MG	BA	3340	1/1	0.92	0.17	57,57,57,57	0
56	MG	AA	3111	1/1	0.92	0.08	70,70,70,70	0
56	MG	BA	3235	1/1	0.92	0.26	44,44,44,44	0
56	MG	BN	3002	1/1	0.92	0.10	52,52,52,52	0
56	MG	DA	3484	1/1	0.92	0.09	47,47,47,47	0
56	MG	BN	3005	1/1	0.92	0.31	63,63,63,63	0
56	MG	BP	203	1/1	0.92	0.58	39,39,39,39	0
56	MG	BA	3161	1/1	0.92	0.13	50,50,50,50	0
56	MG	DA	3126	1/1	0.92	0.14	61,61,61,61	0
56	MG	BR	201	1/1	0.92	0.14	44,44,44,44	0
56	MG	BR	203	1/1	0.92	0.15	48,48,48,48	0
56	MG	AA	3222	1/1	0.92	0.20	64,64,64,64	0
56	MG	DA	3502	1/1	0.92	0.16	48,48,48,48	0
56	MG	BA	3026	1/1	0.92	0.07	36,36,36,36	0
56	MG	BV	3002	1/1	0.92	0.28	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3246	1/1	0.92	0.22	38,38,38,38	0
56	MG	BW	3002	1/1	0.92	0.16	34,34,34,34	0
56	MG	BA	3371	1/1	0.92	0.13	38,38,38,38	0
56	MG	BA	3166	1/1	0.92	0.11	41,41,41,41	0
56	MG	DA	3517	1/1	0.92	0.10	47,47,47,47	0
56	MG	AA	3140	1/1	0.92	0.10	65,65,65,65	0
56	MG	AA	3173	1/1	0.92	0.07	37,37,37,37	0
56	MG	AA	3069	1/1	0.92	0.11	77,77,77,77	0
56	MG	BA	3043	1/1	0.92	0.20	33,33,33,33	0
56	MG	BA	3405	1/1	0.92	0.11	57,57,57,57	0
56	MG	BA	3425	1/1	0.92	0.15	42,42,42,42	0
56	MG	DA	3530	1/1	0.92	0.12	57,57,57,57	0
56	MG	BA	3254	1/1	0.92	0.11	40,40,40,40	0
56	MG	CA	3151	1/1	0.92	0.10	80,80,80,80	0
56	MG	DA	3179	1/1	0.92	0.24	36,36,36,36	0
56	MG	BA	3044	1/1	0.92	0.20	32,32,32,32	0
56	MG	BA	3046	1/1	0.92	0.13	52,52,52,52	0
56	MG	BA	3453	1/1	0.92	0.21	54,54,54,54	0
56	MG	DA	3194	1/1	0.92	0.37	65,65,65,65	0
56	MG	DA	3195	1/1	0.92	0.13	51,51,51,51	0
56	MG	DA	3544	1/1	0.92	0.32	42,42,42,42	0
56	MG	BA	3455	1/1	0.92	0.17	47,47,47,47	0
56	MG	CA	3014	1/1	0.92	0.23	56,56,56,56	0
56	MG	BA	3179	1/1	0.92	0.31	53,53,53,53	0
56	MG	DA	3200	1/1	0.92	0.22	48,48,48,48	0
56	MG	BA	3658	1/1	0.92	0.17	62,62,62,62	0
56	MG	BA	3660	1/1	0.92	0.16	58,58,58,58	0
56	MG	AA	3198	1/1	0.92	0.09	73,73,73,73	0
56	MG	AA	3095	1/1	0.92	0.23	54,54,54,54	0
56	MG	BA	3664	1/1	0.92	0.19	63,63,63,63	0
56	MG	BA	3665	1/1	0.92	0.22	39,39,39,39	0
56	MG	DA	3570	1/1	0.92	0.17	67,67,67,67	0
56	MG	BA	3061	1/1	0.92	0.22	44,44,44,44	0
56	MG	AA	3123	1/1	0.92	0.26	38,38,38,38	0
56	MG	DA	3225	1/1	0.92	0.17	64,64,64,64	0
56	MG	BA	3470	1/1	0.92	0.11	44,44,44,44	0
56	MG	DA	3231	1/1	0.92	0.09	45,45,45,45	0
56	MG	DA	3235	1/1	0.92	0.18	46,46,46,46	0
56	MG	BA	3273	1/1	0.92	0.30	35,35,35,35	0
56	MG	BA	3476	1/1	0.92	0.08	47,47,47,47	0
56	MG	AA	3204	1/1	0.92	0.13	70,70,70,70	0
56	MG	CT	3001	1/1	0.92	0.19	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3096	1/1	0.92	0.21	52,52,52,52	0
56	MG	DA	3250	1/1	0.92	0.11	42,42,42,42	0
56	MG	BA	3481	1/1	0.92	0.15	41,41,41,41	0
56	MG	DA	3604	1/1	0.92	0.07	50,50,50,50	0
56	MG	DA	3252	1/1	0.92	0.21	36,36,36,36	0
56	MG	DA	3254	1/1	0.92	0.12	52,52,52,52	0
56	MG	BA	3677	1/1	0.92	0.14	47,47,47,47	0
56	MG	DA	3609	1/1	0.92	0.14	49,49,49,49	0
56	MG	DA	3611	1/1	0.92	0.16	51,51,51,51	0
56	MG	DA	3612	1/1	0.92	0.17	46,46,46,46	0
56	MG	AA	3012	1/1	0.92	0.13	58,58,58,58	0
56	MG	DA	3615	1/1	0.92	0.08	57,57,57,57	0
56	MG	BA	3682	1/1	0.92	0.28	50,50,50,50	0
56	MG	DA	3268	1/1	0.92	0.13	42,42,42,42	0
56	MG	DA	3270	1/1	0.92	0.14	55,55,55,55	0
56	MG	BA	3487	1/1	0.92	0.18	47,47,47,47	0
56	MG	DA	3015	1/1	0.92	0.18	54,54,54,54	0
56	MG	DA	3018	1/1	0.92	0.17	41,41,41,41	0
56	MG	BA	3284	1/1	0.92	0.43	76,76,76,76	0
56	MG	BA	3502	1/1	0.92	0.17	59,59,59,59	0
56	MG	BA	3503	1/1	0.92	0.14	56,56,56,56	0
56	MG	DA	3631	1/1	0.92	0.18	49,49,49,49	0
56	MG	DA	3634	1/1	0.92	0.13	33,33,33,33	0
56	MG	CA	3045	1/1	0.92	0.23	60,60,60,60	0
56	MG	BA	3505	1/1	0.92	0.12	45,45,45,45	0
56	MG	DA	3030	1/1	0.92	0.16	49,49,49,49	0
56	MG	DA	3033	1/1	0.92	0.15	41,41,41,41	0
56	MG	DA	3310	1/1	0.92	0.17	30,30,30,30	0
56	MG	BA	3288	1/1	0.92	0.11	45,45,45,45	0
56	MG	DA	3648	1/1	0.92	0.12	43,43,43,43	0
56	MG	CA	3049	1/1	0.92	0.18	51,51,51,51	0
56	MG	BA	3187	1/1	0.92	0.11	53,53,53,53	0
56	MG	DA	3325	1/1	0.92	0.16	31,31,31,31	0
56	MG	BA	3190	1/1	0.92	0.08	42,42,42,42	0
56	MG	BA	3518	1/1	0.92	0.09	52,52,52,52	0
56	MG	DA	3048	1/1	0.92	0.21	29,29,29,29	0
56	MG	DA	3049	1/1	0.92	0.13	56,56,56,56	0
56	MG	BA	3191	1/1	0.92	0.09	56,56,56,56	0
56	MG	BA	3524	1/1	0.92	0.09	50,50,50,50	0
56	MG	BA	3195	1/1	0.92	0.17	37,37,37,37	0
56	MG	DE	304	1/1	0.92	0.10	30,30,30,30	0
56	MG	BA	3196	1/1	0.92	0.17	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3295	1/1	0.92	0.08	30,30,30,30	0
56	MG	BA	3540	1/1	0.92	0.18	29,29,29,29	0
56	MG	DN	5001	1/1	0.92	0.07	71,71,71,71	0
56	MG	DA	3064	1/1	0.92	0.10	55,55,55,55	0
56	MG	BA	3546	1/1	0.92	0.17	46,46,46,46	0
56	MG	AX	107	1/1	0.92	0.08	82,82,82,82	0
56	MG	BA	3721	1/1	0.92	0.22	56,56,56,56	0
56	MG	DU	3001	1/1	0.92	0.19	61,61,61,61	0
56	MG	DA	3378	1/1	0.92	0.08	38,38,38,38	0
56	MG	DA	3380	1/1	0.92	0.07	40,40,40,40	0
56	MG	DA	3070	1/1	0.92	0.24	51,51,51,51	0
56	MG	BA	3297	1/1	0.92	0.13	43,43,43,43	0
56	MG	BA	3138	1/1	0.92	0.23	54,54,54,54	0
56	MG	AA	3154	1/1	0.92	0.12	60,60,60,60	0
56	MG	DA	3075	1/1	0.92	0.17	45,45,45,45	0
56	MG	BA	3737	1/1	0.92	0.11	39,39,39,39	0
56	MG	BA	3207	1/1	0.92	0.22	44,44,44,44	0
56	MG	BA	3680	1/1	0.93	0.15	62,62,62,62	0
56	MG	CA	3010	1/1	0.93	0.12	34,34,34,34	0
56	MG	DA	3129	1/1	0.93	0.10	45,45,45,45	0
56	MG	AA	3159	1/1	0.93	0.17	57,57,57,57	0
56	MG	DA	3132	1/1	0.93	0.21	47,47,47,47	0
56	MG	BA	3550	1/1	0.93	0.11	32,32,32,32	0
56	MG	CA	3016	1/1	0.93	0.14	72,72,72,72	0
56	MG	BA	3359	1/1	0.93	0.12	63,63,63,63	0
56	MG	BA	3687	1/1	0.93	0.14	59,59,59,59	0
56	MG	DA	3149	1/1	0.93	0.08	47,47,47,47	0
56	MG	AA	3007	1/1	0.93	0.09	68,68,68,68	0
56	MG	AA	3188	1/1	0.93	0.18	52,52,52,52	0
56	MG	DA	3154	1/1	0.93	0.31	45,45,45,45	0
56	MG	AA	3055	1/1	0.93	0.23	56,56,56,56	0
56	MG	DA	3472	1/1	0.93	0.09	38,38,38,38	0
56	MG	DA	3473	1/1	0.93	0.17	50,50,50,50	0
56	MG	DA	3156	1/1	0.93	0.32	38,38,38,38	0
56	MG	BA	3134	1/1	0.93	0.13	34,34,34,34	0
56	MG	DA	3478	1/1	0.93	0.06	58,58,58,58	0
56	MG	DA	3161	1/1	0.93	0.18	51,51,51,51	0
56	MG	BA	3375	1/1	0.93	0.08	44,44,44,44	0
56	MG	DA	3163	1/1	0.93	0.15	52,52,52,52	0
56	MG	BA	3008	1/1	0.93	0.14	30,30,30,30	0
56	MG	BA	3012	1/1	0.93	0.07	34,34,34,34	0
56	MG	DA	3493	1/1	0.93	0.12	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3590	1/1	0.93	0.12	23,23,23,23	0
56	MG	BA	3392	1/1	0.93	0.13	53,53,53,53	0
56	MG	BA	3593	1/1	0.93	0.08	51,51,51,51	0
56	MG	DA	3499	1/1	0.93	0.19	44,44,44,44	0
56	MG	BA	3277	1/1	0.93	0.27	45,45,45,45	0
56	MG	AA	3166	1/1	0.93	0.14	55,55,55,55	0
56	MG	BA	3075	1/1	0.93	0.20	36,36,36,36	0
56	MG	DA	3184	1/1	0.93	0.15	54,54,54,54	0
56	MG	BA	3199	1/1	0.93	0.15	31,31,31,31	0
56	MG	DA	3509	1/1	0.93	0.07	57,57,57,57	0
56	MG	BA	3201	1/1	0.93	0.21	36,36,36,36	0
56	MG	CE	3002	1/1	0.93	0.08	69,69,69,69	0
56	MG	BA	3286	1/1	0.93	0.18	42,42,42,42	0
56	MG	DA	3516	1/1	0.93	0.23	54,54,54,54	0
56	MG	BA	3607	1/1	0.93	0.15	74,74,74,74	0
56	MG	DA	3519	1/1	0.93	0.07	39,39,39,39	0
56	MG	DA	3520	1/1	0.93	0.08	38,38,38,38	0
56	MG	BA	3435	1/1	0.93	0.11	59,59,59,59	0
56	MG	BA	3444	1/1	0.93	0.15	29,29,29,29	0
56	MG	DA	3002	1/1	0.93	0.20	47,47,47,47	0
56	MG	CA	3044	1/1	0.93	0.14	52,52,52,52	0
56	MG	DA	3527	1/1	0.93	0.15	58,58,58,58	0
56	MG	BA	3141	1/1	0.93	0.26	43,43,43,43	0
56	MG	BA	3734	1/1	0.93	0.14	42,42,42,42	0
56	MG	BA	3735	1/1	0.93	0.08	47,47,47,47	0
56	MG	BA	3142	1/1	0.93	0.15	57,57,57,57	0
56	MG	DA	3214	1/1	0.93	0.13	48,48,48,48	0
56	MG	DA	3215	1/1	0.93	0.25	43,43,43,43	0
56	MG	DA	3216	1/1	0.93	0.11	47,47,47,47	0
56	MG	DA	3017	1/1	0.93	0.09	51,51,51,51	0
56	MG	BA	3618	1/1	0.93	0.18	37,37,37,37	0
56	MG	DA	3541	1/1	0.93	0.09	55,55,55,55	0
56	MG	DA	3223	1/1	0.93	0.09	41,41,41,41	0
56	MG	BA	3619	1/1	0.93	0.18	42,42,42,42	0
56	MG	BA	3081	1/1	0.93	0.21	44,44,44,44	0
56	MG	DA	3227	1/1	0.93	0.10	40,40,40,40	0
56	MG	BB	3002	1/1	0.93	0.16	49,49,49,49	0
56	MG	DA	3551	1/1	0.93	0.07	43,43,43,43	0
56	MG	CA	3057	1/1	0.93	0.14	40,40,40,40	0
56	MG	DA	3555	1/1	0.93	0.13	43,43,43,43	0
56	MG	BA	3458	1/1	0.93	0.14	46,46,46,46	0
56	MG	BA	3622	1/1	0.93	0.18	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3031	1/1	0.93	0.15	60,60,60,60	0
56	MG	DA	3032	1/1	0.93	0.06	36,36,36,36	0
56	MG	BA	3624	1/1	0.93	0.11	73,73,73,73	0
56	MG	BA	3017	1/1	0.93	0.21	38,38,38,38	0
56	MG	DA	3249	1/1	0.93	0.10	25,25,25,25	0
56	MG	DA	3569	1/1	0.93	0.07	54,54,54,54	0
56	MG	BB	3009	1/1	0.93	0.12	49,49,49,49	0
56	MG	BB	3011	1/1	0.93	0.13	45,45,45,45	0
56	MG	DA	3575	1/1	0.93	0.16	51,51,51,51	0
56	MG	DA	3578	1/1	0.93	0.21	68,68,68,68	0
56	MG	BA	3083	1/1	0.93	0.14	33,33,33,33	0
56	MG	DA	3041	1/1	0.93	0.20	54,54,54,54	0
56	MG	BA	3018	1/1	0.93	0.10	54,54,54,54	0
56	MG	AA	3036	1/1	0.93	0.14	69,69,69,69	0
56	MG	DA	3259	1/1	0.93	0.09	45,45,45,45	0
56	MG	BA	3468	1/1	0.93	0.19	45,45,45,45	0
56	MG	BA	3093	1/1	0.93	0.35	52,52,52,52	0
56	MG	AA	3169	1/1	0.93	0.08	62,62,62,62	0
56	MG	BA	3217	1/1	0.93	0.10	59,59,59,59	0
56	MG	DA	3276	1/1	0.93	0.07	26,26,26,26	0
56	MG	DA	3601	1/1	0.93	0.11	50,50,50,50	0
56	MG	DA	3058	1/1	0.93	0.15	56,56,56,56	0
56	MG	BA	3098	1/1	0.93	0.25	42,42,42,42	0
56	MG	BD	312	1/1	0.93	0.31	72,72,72,72	0
56	MG	DA	3284	1/1	0.93	0.12	45,45,45,45	0
56	MG	BE	307	1/1	0.93	0.20	51,51,51,51	0
56	MG	AA	3006	1/1	0.93	0.10	84,84,84,84	0
56	MG	DA	3288	1/1	0.93	0.10	68,68,68,68	0
56	MG	DA	3065	1/1	0.93	0.14	40,40,40,40	0
56	MG	BA	3305	1/1	0.93	0.10	48,48,48,48	0
56	MG	BA	3229	1/1	0.93	0.11	50,50,50,50	0
56	MG	DA	3302	1/1	0.93	0.12	42,42,42,42	0
56	MG	BA	3482	1/1	0.93	0.11	59,59,59,59	0
56	MG	BA	3100	1/1	0.93	0.15	42,42,42,42	0
56	MG	BA	3647	1/1	0.93	0.08	40,40,40,40	0
56	MG	BN	3003	1/1	0.93	0.14	67,67,67,67	0
56	MG	BA	3101	1/1	0.93	0.31	47,47,47,47	0
56	MG	CA	3105	1/1	0.93	0.10	59,59,59,59	0
56	MG	DA	3624	1/1	0.93	0.09	54,54,54,54	0
56	MG	DA	3625	1/1	0.93	0.07	48,48,48,48	0
56	MG	AN	101	1/1	0.93	0.08	64,64,64,64	0
56	MG	AA	3101	1/1	0.93	0.20	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BQ	3004	1/1	0.93	0.11	41,41,41,41	0
56	MG	DA	3081	1/1	0.93	0.20	56,56,56,56	0
56	MG	BA	3316	1/1	0.93	0.14	51,51,51,51	0
56	MG	BA	3504	1/1	0.93	0.18	54,54,54,54	0
56	MG	BA	3657	1/1	0.93	0.11	29,29,29,29	0
56	MG	BA	3037	1/1	0.93	0.24	39,39,39,39	0
56	MG	BA	3038	1/1	0.93	0.20	51,51,51,51	0
56	MG	DA	3091	1/1	0.93	0.41	50,50,50,50	0
56	MG	AA	3146	1/1	0.93	0.08	55,55,55,55	0
56	MG	BA	3042	1/1	0.93	0.20	50,50,50,50	0
56	MG	DA	3651	1/1	0.93	0.09	48,48,48,48	0
56	MG	DA	3364	1/1	0.93	0.11	40,40,40,40	0
56	MG	BW	3004	1/1	0.93	0.27	46,46,46,46	0
56	MG	DA	3370	1/1	0.93	0.20	40,40,40,40	0
56	MG	AA	3043	1/1	0.93	0.28	63,63,63,63	0
56	MG	BA	3250	1/1	0.93	0.30	61,61,61,61	0
56	MG	BA	3336	1/1	0.93	0.14	46,46,46,46	0
56	MG	DB	3009	1/1	0.93	0.29	41,41,41,41	0
56	MG	DA	3381	1/1	0.93	0.14	68,68,68,68	0
56	MG	CA	3123	1/1	0.93	0.14	75,75,75,75	0
56	MG	DA	3100	1/1	0.93	0.13	55,55,55,55	0
56	MG	DD	303	1/1	0.93	0.54	48,48,48,48	0
56	MG	DE	302	1/1	0.93	0.15	46,46,46,46	0
56	MG	B0	106	1/1	0.93	0.06	43,43,43,43	0
56	MG	DA	3395	1/1	0.93	0.07	40,40,40,40	0
56	MG	DA	3103	1/1	0.93	0.12	52,52,52,52	0
56	MG	DA	3409	1/1	0.93	0.07	54,54,54,54	0
56	MG	AA	3124	1/1	0.93	0.17	61,61,61,61	0
56	MG	BA	3533	1/1	0.93	0.15	30,30,30,30	0
56	MG	DP	201	1/1	0.93	0.09	52,52,52,52	0
56	MG	B3	3403	1/1	0.93	0.12	37,37,37,37	0
56	MG	AA	3052	1/1	0.93	0.20	58,58,58,58	0
56	MG	CA	3130	1/1	0.93	0.12	59,59,59,59	0
56	MG	CA	3132	1/1	0.93	0.12	66,66,66,66	0
56	MG	B7	103	1/1	0.93	0.16	46,46,46,46	0
56	MG	AA	3116	1/1	0.93	0.33	62,62,62,62	0
56	MG	DV	203	1/1	0.93	0.18	41,41,41,41	0
56	MG	DA	3116	1/1	0.93	0.13	43,43,43,43	0
56	MG	DA	3117	1/1	0.93	0.08	46,46,46,46	0
56	MG	BA	3673	1/1	0.93	0.18	60,60,60,60	0
56	MG	BA	3539	1/1	0.93	0.11	23,23,23,23	0
58	ZN	B4	501	1/1	0.93	0.10	152,152,152,152	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3442	1/1	0.93	0.18	58,58,58,58	0
56	MG	AA	3211	1/1	0.93	0.10	58,58,58,58	0
56	MG	BA	3544	1/1	0.93	0.12	35,35,35,35	0
56	MG	AA	3155	1/1	0.93	0.15	54,54,54,54	0
56	MG	AA	3193	1/1	0.94	0.16	65,65,65,65	0
56	MG	DA	3164	1/1	0.94	0.06	40,40,40,40	0
56	MG	BA	3211	1/1	0.94	0.08	43,43,43,43	0
56	MG	DA	3167	1/1	0.94	0.19	46,46,46,46	0
56	MG	DA	3463	1/1	0.94	0.08	32,32,32,32	0
56	MG	DA	3168	1/1	0.94	0.34	46,46,46,46	0
56	MG	AA	3153	1/1	0.94	0.14	46,46,46,46	0
56	MG	CF	3001	1/1	0.94	0.10	56,56,56,56	0
56	MG	BA	3152	1/1	0.94	0.11	52,52,52,52	0
56	MG	AA	3195	1/1	0.94	0.20	58,58,58,58	0
56	MG	DA	3173	1/1	0.94	0.12	50,50,50,50	0
56	MG	CA	3046	1/1	0.94	0.23	52,52,52,52	0
56	MG	AM	3001	1/1	0.94	0.05	76,76,76,76	0
56	MG	DA	3481	1/1	0.94	0.09	59,59,59,59	0
56	MG	DA	3482	1/1	0.94	0.06	45,45,45,45	0
56	MG	BA	3219	1/1	0.94	0.24	36,36,36,36	0
56	MG	BA	3221	1/1	0.94	0.26	55,55,55,55	0
56	MG	DA	3187	1/1	0.94	0.18	52,52,52,52	0
56	MG	DA	3486	1/1	0.94	0.07	52,52,52,52	0
56	MG	DA	3188	1/1	0.94	0.26	52,52,52,52	0
56	MG	BB	3015	1/1	0.94	0.08	35,35,35,35	0
56	MG	CA	3051	1/1	0.94	0.11	77,77,77,77	0
56	MG	DA	3192	1/1	0.94	0.16	48,48,48,48	0
56	MG	CA	3052	1/1	0.94	0.13	47,47,47,47	0
56	MG	DA	3014	1/1	0.94	0.09	38,38,38,38	0
56	MG	BA	3030	1/1	0.94	0.32	26,26,26,26	0
56	MG	BA	3157	1/1	0.94	0.08	52,52,52,52	0
56	MG	BA	3635	1/1	0.94	0.07	52,52,52,52	0
56	MG	DA	3503	1/1	0.94	0.08	41,41,41,41	0
56	MG	DA	3019	1/1	0.94	0.12	32,32,32,32	0
56	MG	BD	303	1/1	0.94	0.09	35,35,35,35	0
56	MG	BA	3479	1/1	0.94	0.14	44,44,44,44	0
56	MG	AA	3109	1/1	0.94	0.13	59,59,59,59	0
56	MG	DA	3511	1/1	0.94	0.09	47,47,47,47	0
56	MG	DA	3206	1/1	0.94	0.24	36,36,36,36	0
56	MG	BA	3102	1/1	0.94	0.17	45,45,45,45	0
56	MG	AA	3175	1/1	0.94	0.13	70,70,70,70	0
56	MG	BA	3234	1/1	0.94	0.20	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BE	306	1/1	0.94	0.24	38,38,38,38	0
56	MG	DA	3518	1/1	0.94	0.07	40,40,40,40	0
56	MG	BA	3104	1/1	0.94	0.25	34,34,34,34	0
56	MG	DA	3218	1/1	0.94	0.12	31,31,31,31	0
56	MG	AA	3110	1/1	0.94	0.12	41,41,41,41	0
56	MG	DA	3221	1/1	0.94	0.19	56,56,56,56	0
56	MG	DA	3034	1/1	0.94	0.18	40,40,40,40	0
56	MG	CA	3068	1/1	0.94	0.16	47,47,47,47	0
56	MG	AA	3142	1/1	0.94	0.17	60,60,60,60	0
56	MG	DA	3037	1/1	0.94	0.20	37,37,37,37	0
56	MG	BG	3002	1/1	0.94	0.17	51,51,51,51	0
56	MG	DA	3229	1/1	0.94	0.13	44,44,44,44	0
56	MG	BA	3326	1/1	0.94	0.17	15,15,15,15	0
56	MG	BA	3171	1/1	0.94	0.25	42,42,42,42	0
56	MG	BA	3507	1/1	0.94	0.09	37,37,37,37	0
56	MG	DA	3535	1/1	0.94	0.09	58,58,58,58	0
56	MG	BA	3509	1/1	0.94	0.14	29,29,29,29	0
56	MG	DA	3238	1/1	0.94	0.07	37,37,37,37	0
56	MG	AA	3201	1/1	0.94	0.12	76,76,76,76	0
56	MG	DA	3053	1/1	0.94	0.14	47,47,47,47	0
56	MG	CA	3078	1/1	0.94	0.11	51,51,51,51	0
56	MG	DA	3244	1/1	0.94	0.15	23,23,23,23	0
56	MG	BN	3004	1/1	0.94	0.19	69,69,69,69	0
56	MG	DA	3248	1/1	0.94	0.15	30,30,30,30	0
56	MG	DA	3056	1/1	0.94	0.16	37,37,37,37	0
56	MG	AA	3202	1/1	0.94	0.14	72,72,72,72	0
56	MG	AA	3011	1/1	0.94	0.34	44,44,44,44	0
56	MG	BQ	3001	1/1	0.94	0.21	38,38,38,38	0
56	MG	CA	3087	1/1	0.94	0.09	40,40,40,40	0
56	MG	BA	3113	1/1	0.94	0.20	48,48,48,48	0
56	MG	CA	3090	1/1	0.94	0.11	63,63,63,63	0
56	MG	BA	3339	1/1	0.94	0.15	47,47,47,47	0
56	MG	DA	3565	1/1	0.94	0.13	48,48,48,48	0
56	MG	CA	3092	1/1	0.94	0.12	56,56,56,56	0
56	MG	DA	3067	1/1	0.94	0.20	35,35,35,35	0
56	MG	AA	3059	1/1	0.94	0.17	49,49,49,49	0
56	MG	CA	3100	1/1	0.94	0.14	72,72,72,72	0
56	MG	BA	3051	1/1	0.94	0.18	34,34,34,34	0
56	MG	AA	3206	1/1	0.94	0.17	79,79,79,79	0
56	MG	BA	3352	1/1	0.94	0.08	58,58,58,58	0
56	MG	BV	3001	1/1	0.94	0.11	42,42,42,42	0
56	MG	DA	3582	1/1	0.94	0.17	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3356	1/1	0.94	0.09	33,33,33,33	0
56	MG	AA	3044	1/1	0.94	0.15	60,60,60,60	0
56	MG	AA	3208	1/1	0.94	0.14	38,38,38,38	0
56	MG	DA	3588	1/1	0.94	0.11	47,47,47,47	0
56	MG	BA	3256	1/1	0.94	0.22	60,60,60,60	0
56	MG	BA	3545	1/1	0.94	0.11	20,20,20,20	0
56	MG	DA	3593	1/1	0.94	0.13	62,62,62,62	0
56	MG	DA	3290	1/1	0.94	0.13	59,59,59,59	0
56	MG	DA	3295	1/1	0.94	0.11	31,31,31,31	0
56	MG	BA	3361	1/1	0.94	0.06	39,39,39,39	0
56	MG	DA	3597	1/1	0.94	0.12	66,66,66,66	0
56	MG	BA	3548	1/1	0.94	0.20	40,40,40,40	0
56	MG	B0	101	1/1	0.94	0.14	57,57,57,57	0
56	MG	B0	104	1/1	0.94	0.12	55,55,55,55	0
56	MG	BA	3002	1/1	0.94	0.15	38,38,38,38	0
56	MG	AA	3167	1/1	0.94	0.17	78,78,78,78	0
56	MG	DA	3316	1/1	0.94	0.22	47,47,47,47	0
56	MG	B1	3002	1/1	0.94	0.06	29,29,29,29	0
56	MG	DA	3320	1/1	0.94	0.18	50,50,50,50	0
56	MG	AA	3210	1/1	0.94	0.09	48,48,48,48	0
56	MG	DA	3094	1/1	0.94	0.16	26,26,26,26	0
56	MG	BA	3557	1/1	0.94	0.18	35,35,35,35	0
56	MG	DA	3328	1/1	0.94	0.20	33,33,33,33	0
56	MG	AA	3185	1/1	0.94	0.19	47,47,47,47	0
56	MG	AA	3213	1/1	0.94	0.09	74,74,74,74	0
56	MG	BA	3268	1/1	0.94	0.19	29,29,29,29	0
56	MG	DA	3338	1/1	0.94	0.14	58,58,58,58	0
56	MG	BA	3383	1/1	0.94	0.16	51,51,51,51	0
56	MG	BA	3384	1/1	0.94	0.18	47,47,47,47	0
56	MG	BA	3577	1/1	0.94	0.14	63,63,63,63	0
56	MG	CA	3131	1/1	0.94	0.08	48,48,48,48	0
56	MG	DA	3623	1/1	0.94	0.08	63,63,63,63	0
56	MG	DA	3104	1/1	0.94	0.12	46,46,46,46	0
56	MG	DA	3105	1/1	0.94	0.13	56,56,56,56	0
56	MG	CA	3006	1/1	0.94	0.08	72,72,72,72	0
56	MG	CA	3134	1/1	0.94	0.11	92,92,92,92	0
56	MG	BA	3011	1/1	0.94	0.12	39,39,39,39	0
56	MG	BA	3698	1/1	0.94	0.26	58,58,58,58	0
56	MG	DA	3369	1/1	0.94	0.10	53,53,53,53	0
56	MG	BA	3391	1/1	0.94	0.12	39,39,39,39	0
56	MG	AA	3062	1/1	0.94	0.09	30,30,30,30	0
56	MG	DA	3638	1/1	0.94	0.08	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3274	1/1	0.94	0.21	54,54,54,54	0
56	MG	DA	3640	1/1	0.94	0.12	53,53,53,53	0
56	MG	DA	3379	1/1	0.94	0.09	63,63,63,63	0
56	MG	DA	3114	1/1	0.94	0.09	47,47,47,47	0
56	MG	CA	3143	1/1	0.94	0.12	91,91,91,91	0
56	MG	DA	3647	1/1	0.94	0.14	45,45,45,45	0
56	MG	DA	3390	1/1	0.94	0.12	58,58,58,58	0
56	MG	BA	3193	1/1	0.94	0.16	53,53,53,53	0
56	MG	BA	3595	1/1	0.94	0.10	37,37,37,37	0
56	MG	BA	3404	1/1	0.94	0.05	42,42,42,42	0
56	MG	AA	3014	1/1	0.94	0.06	24,24,24,24	0
56	MG	DA	3399	1/1	0.94	0.23	39,39,39,39	0
56	MG	DA	3400	1/1	0.94	0.16	42,42,42,42	0
56	MG	CA	3148	1/1	0.94	0.12	65,65,65,65	0
56	MG	DB	3007	1/1	0.94	0.27	45,45,45,45	0
56	MG	DA	3406	1/1	0.94	0.09	48,48,48,48	0
56	MG	DA	3407	1/1	0.94	0.09	35,35,35,35	0
56	MG	AA	3170	1/1	0.94	0.16	83,83,83,83	0
56	MG	DA	3413	1/1	0.94	0.12	44,44,44,44	0
56	MG	BA	3281	1/1	0.94	0.08	45,45,45,45	0
56	MG	BA	3198	1/1	0.94	0.20	29,29,29,29	0
56	MG	DA	3127	1/1	0.94	0.07	44,44,44,44	0
56	MG	BA	3434	1/1	0.94	0.16	22,22,22,22	0
56	MG	BA	3605	1/1	0.94	0.09	35,35,35,35	0
56	MG	BA	3719	1/1	0.94	0.08	63,63,63,63	0
56	MG	AA	3190	1/1	0.94	0.26	61,61,61,61	0
56	MG	BA	3019	1/1	0.94	0.17	42,42,42,42	0
56	MG	DA	3434	1/1	0.94	0.10	51,51,51,51	0
56	MG	BA	3087	1/1	0.94	0.23	48,48,48,48	0
56	MG	DA	3140	1/1	0.94	0.27	55,55,55,55	0
56	MG	BA	3613	1/1	0.94	0.17	47,47,47,47	0
56	MG	DA	3145	1/1	0.94	0.11	52,52,52,52	0
56	MG	AA	3151	1/1	0.94	0.07	49,49,49,49	0
56	MG	DA	3148	1/1	0.94	0.10	41,41,41,41	0
56	MG	BA	3615	1/1	0.94	0.17	55,55,55,55	0
56	MG	DA	3446	1/1	0.94	0.14	46,46,46,46	0
56	MG	CA	3035	1/1	0.94	0.18	49,49,49,49	0
56	MG	BA	3089	1/1	0.94	0.14	50,50,50,50	0
56	MG	BA	3092	1/1	0.94	0.09	28,28,28,28	0
56	MG	CA	3165	1/1	0.94	0.15	47,47,47,47	0
58	ZN	D4	501	1/1	0.94	0.10	155,155,155,155	0
56	MG	CA	3167	1/1	0.94	0.06	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3147	1/1	0.94	0.12	42,42,42,42	0
56	MG	BA	3464	1/1	0.94	0.10	40,40,40,40	0
56	MG	CA	3040	1/1	0.94	0.21	47,47,47,47	0
56	MG	DA	3417	1/1	0.95	0.12	54,54,54,54	0
56	MG	BA	3225	1/1	0.95	0.23	42,42,42,42	0
56	MG	BA	3227	1/1	0.95	0.15	67,67,67,67	0
56	MG	DA	3422	1/1	0.95	0.19	45,45,45,45	0
56	MG	AA	3035	1/1	0.95	0.08	59,59,59,59	0
56	MG	CA	3128	1/1	0.95	0.14	55,55,55,55	0
56	MG	DA	3428	1/1	0.95	0.10	30,30,30,30	0
56	MG	BA	3307	1/1	0.95	0.08	35,35,35,35	0
56	MG	BA	3125	1/1	0.95	0.16	26,26,26,26	0
56	MG	DA	3433	1/1	0.95	0.20	39,39,39,39	0
56	MG	BA	3010	1/1	0.95	0.05	35,35,35,35	0
56	MG	DA	3130	1/1	0.95	0.07	34,34,34,34	0
56	MG	BU	207	1/1	0.95	0.14	38,38,38,38	0
56	MG	BA	3128	1/1	0.95	0.11	28,28,28,28	0
56	MG	DA	3438	1/1	0.95	0.20	50,50,50,50	0
56	MG	BU	209	1/1	0.95	0.40	36,36,36,36	0
56	MG	BA	3129	1/1	0.95	0.27	44,44,44,44	0
56	MG	DA	3137	1/1	0.95	0.28	62,62,62,62	0
56	MG	DA	3138	1/1	0.95	0.30	53,53,53,53	0
56	MG	DA	3139	1/1	0.95	0.12	47,47,47,47	0
56	MG	CA	3137	1/1	0.95	0.13	59,59,59,59	0
56	MG	BA	3237	1/1	0.95	0.16	43,43,43,43	0
56	MG	DA	3143	1/1	0.95	0.10	53,53,53,53	0
56	MG	DA	3144	1/1	0.95	0.21	37,37,37,37	0
56	MG	BA	3645	1/1	0.95	0.23	63,63,63,63	0
56	MG	BA	3646	1/1	0.95	0.12	39,39,39,39	0
56	MG	DA	3147	1/1	0.95	0.15	46,46,46,46	0
56	MG	BW	3003	1/1	0.95	0.14	39,39,39,39	0
56	MG	AA	3160	1/1	0.95	0.19	52,52,52,52	0
56	MG	DA	3459	1/1	0.95	0.09	43,43,43,43	0
56	MG	BA	3132	1/1	0.95	0.11	28,28,28,28	0
56	MG	BA	3484	1/1	0.95	0.08	40,40,40,40	0
56	MG	BA	3650	1/1	0.95	0.09	44,44,44,44	0
56	MG	AA	3060	1/1	0.95	0.29	52,52,52,52	0
56	MG	BA	3245	1/1	0.95	0.15	45,45,45,45	0
56	MG	B0	105	1/1	0.95	0.23	44,44,44,44	0
56	MG	DA	3466	1/1	0.95	0.07	43,43,43,43	0
56	MG	DA	3160	1/1	0.95	0.10	47,47,47,47	0
56	MG	DA	3469	1/1	0.95	0.14	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3498	1/1	0.95	0.07	81,81,81,81	0
56	MG	AA	3041	1/1	0.95	0.08	41,41,41,41	0
56	MG	BA	3501	1/1	0.95	0.10	35,35,35,35	0
56	MG	CA	3154	1/1	0.95	0.16	54,54,54,54	0
56	MG	BA	3016	1/1	0.95	0.13	50,50,50,50	0
56	MG	BA	3097	1/1	0.95	0.17	30,30,30,30	0
56	MG	BA	3249	1/1	0.95	0.13	46,46,46,46	0
56	MG	BA	3056	1/1	0.95	0.23	39,39,39,39	0
56	MG	BA	3506	1/1	0.95	0.11	33,33,33,33	0
56	MG	BA	3059	1/1	0.95	0.23	35,35,35,35	0
56	MG	B9	502	1/1	0.95	0.15	49,49,49,49	0
56	MG	CA	3002	1/1	0.95	0.06	74,74,74,74	0
56	MG	AA	3054	1/1	0.95	0.13	46,46,46,46	0
56	MG	DA	3176	1/1	0.95	0.11	52,52,52,52	0
56	MG	BA	3668	1/1	0.95	0.11	42,42,42,42	0
56	MG	CA	3005	1/1	0.95	0.24	37,37,37,37	0
56	MG	DA	3497	1/1	0.95	0.07	37,37,37,37	0
56	MG	CA	3166	1/1	0.95	0.09	71,71,71,71	0
56	MG	DA	3186	1/1	0.95	0.10	38,38,38,38	0
56	MG	AA	3205	1/1	0.95	0.13	66,66,66,66	0
56	MG	BA	3341	1/1	0.95	0.11	31,31,31,31	0
56	MG	BA	3513	1/1	0.95	0.21	51,51,51,51	0
56	MG	BA	3189	1/1	0.95	0.07	39,39,39,39	0
56	MG	BA	3516	1/1	0.95	0.09	64,64,64,64	0
56	MG	DA	3193	1/1	0.95	0.15	42,42,42,42	0
56	MG	CA	3012	1/1	0.95	0.05	50,50,50,50	0
56	MG	BA	3517	1/1	0.95	0.11	52,52,52,52	0
56	MG	AA	3221	1/1	0.95	0.22	52,52,52,52	0
56	MG	BA	3346	1/1	0.95	0.07	33,33,33,33	0
56	MG	BA	3678	1/1	0.95	0.13	47,47,47,47	0
56	MG	CX	102	1/1	0.95	0.07	60,60,60,60	0
56	MG	BA	3349	1/1	0.95	0.07	31,31,31,31	0
56	MG	DA	3202	1/1	0.95	0.09	39,39,39,39	0
56	MG	CX	104	1/1	0.95	0.08	52,52,52,52	0
56	MG	BA	3527	1/1	0.95	0.17	45,45,45,45	0
56	MG	BA	3529	1/1	0.95	0.10	22,22,22,22	0
56	MG	BA	3685	1/1	0.95	0.21	58,58,58,58	0
56	MG	DA	3210	1/1	0.95	0.14	46,46,46,46	0
56	MG	BA	3350	1/1	0.95	0.10	36,36,36,36	0
56	MG	DA	3006	1/1	0.95	0.11	41,41,41,41	0
56	MG	DA	3007	1/1	0.95	0.14	43,43,43,43	0
56	MG	BA	3532	1/1	0.95	0.15	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3011	1/1	0.95	0.07	42,42,42,42	0
56	MG	BA	3689	1/1	0.95	0.09	25,25,25,25	0
56	MG	DA	3013	1/1	0.95	0.17	38,38,38,38	0
56	MG	BA	3692	1/1	0.95	0.17	36,36,36,36	0
56	MG	AA	3179	1/1	0.95	0.15	34,34,34,34	0
56	MG	BA	3355	1/1	0.95	0.07	39,39,39,39	0
56	MG	BA	3067	1/1	0.95	0.29	55,55,55,55	0
56	MG	BA	3258	1/1	0.95	0.05	35,35,35,35	0
56	MG	DA	3228	1/1	0.95	0.20	49,49,49,49	0
56	MG	BA	3259	1/1	0.95	0.14	59,59,59,59	0
56	MG	DA	3021	1/1	0.95	0.19	43,43,43,43	0
56	MG	BA	3700	1/1	0.95	0.13	26,26,26,26	0
56	MG	DA	3233	1/1	0.95	0.10	58,58,58,58	0
56	MG	DA	3548	1/1	0.95	0.13	60,60,60,60	0
56	MG	BA	3543	1/1	0.95	0.11	24,24,24,24	0
56	MG	BA	3260	1/1	0.95	0.11	47,47,47,47	0
56	MG	DA	3027	1/1	0.95	0.20	49,49,49,49	0
56	MG	BA	3360	1/1	0.95	0.09	39,39,39,39	0
56	MG	BA	3194	1/1	0.95	0.25	43,43,43,43	0
56	MG	DA	3242	1/1	0.95	0.11	31,31,31,31	0
56	MG	BA	3367	1/1	0.95	0.11	29,29,29,29	0
56	MG	DA	3562	1/1	0.95	0.09	41,41,41,41	0
56	MG	BA	3146	1/1	0.95	0.24	56,56,56,56	0
56	MG	AX	109	1/1	0.95	0.13	56,56,56,56	0
56	MG	BA	3264	1/1	0.95	0.10	29,29,29,29	0
56	MG	BA	3713	1/1	0.95	0.07	49,49,49,49	0
56	MG	BA	3553	1/1	0.95	0.17	46,46,46,46	0
56	MG	BA	3715	1/1	0.95	0.14	44,44,44,44	0
56	MG	DA	3038	1/1	0.95	0.06	37,37,37,37	0
56	MG	BA	3554	1/1	0.95	0.16	25,25,25,25	0
56	MG	BA	3265	1/1	0.95	0.22	39,39,39,39	0
56	MG	BA	3558	1/1	0.95	0.13	47,47,47,47	0
56	MG	BA	3148	1/1	0.95	0.35	49,49,49,49	0
56	MG	DA	3262	1/1	0.95	0.19	60,60,60,60	0
56	MG	DA	3044	1/1	0.95	0.25	45,45,45,45	0
56	MG	DA	3267	1/1	0.95	0.11	40,40,40,40	0
56	MG	AX	110	1/1	0.95	0.11	45,45,45,45	0
56	MG	DA	3269	1/1	0.95	0.12	47,47,47,47	0
56	MG	DA	3590	1/1	0.95	0.08	39,39,39,39	0
56	MG	AA	3031	1/1	0.95	0.20	41,41,41,41	0
56	MG	DA	3592	1/1	0.95	0.10	49,49,49,49	0
56	MG	DA	3271	1/1	0.95	0.08	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3050	1/1	0.95	0.09	30,30,30,30	0
56	MG	BA	3723	1/1	0.95	0.09	25,25,25,25	0
56	MG	BA	3151	1/1	0.95	0.17	40,40,40,40	0
56	MG	DA	3279	1/1	0.95	0.13	32,32,32,32	0
56	MG	DA	3280	1/1	0.95	0.12	46,46,46,46	0
56	MG	DA	3599	1/1	0.95	0.17	69,69,69,69	0
56	MG	BA	3726	1/1	0.95	0.11	29,29,29,29	0
56	MG	BA	3729	1/1	0.95	0.08	54,54,54,54	0
56	MG	BA	3385	1/1	0.95	0.07	56,56,56,56	0
56	MG	BA	3733	1/1	0.95	0.16	40,40,40,40	0
56	MG	DA	3059	1/1	0.95	0.07	42,42,42,42	0
56	MG	BA	3387	1/1	0.95	0.10	49,49,49,49	0
56	MG	AA	3119	1/1	0.95	0.20	42,42,42,42	0
56	MG	BA	3073	1/1	0.95	0.05	43,43,43,43	0
56	MG	DA	3294	1/1	0.95	0.15	30,30,30,30	0
56	MG	BA	3205	1/1	0.95	0.19	38,38,38,38	0
56	MG	AA	3051	1/1	0.95	0.08	56,56,56,56	0
56	MG	DA	3298	1/1	0.95	0.21	45,45,45,45	0
56	MG	DA	3614	1/1	0.95	0.12	46,46,46,46	0
56	MG	BA	3031	1/1	0.95	0.15	44,44,44,44	0
56	MG	BA	3594	1/1	0.95	0.17	55,55,55,55	0
56	MG	DA	3305	1/1	0.95	0.11	33,33,33,33	0
56	MG	BA	3400	1/1	0.95	0.06	29,29,29,29	0
56	MG	BA	3282	1/1	0.95	0.11	34,34,34,34	0
56	MG	DA	3312	1/1	0.95	0.11	24,24,24,24	0
56	MG	DA	3313	1/1	0.95	0.11	30,30,30,30	0
56	MG	BA	3033	1/1	0.95	0.25	54,54,54,54	0
56	MG	BA	3406	1/1	0.95	0.19	54,54,54,54	0
56	MG	DA	3317	1/1	0.95	0.13	34,34,34,34	0
56	MG	DA	3626	1/1	0.95	0.10	63,63,63,63	0
56	MG	BA	3408	1/1	0.95	0.08	28,28,28,28	0
56	MG	BA	3423	1/1	0.95	0.15	45,45,45,45	0
56	MG	BA	3602	1/1	0.95	0.08	44,44,44,44	0
56	MG	BA	3210	1/1	0.95	0.20	39,39,39,39	0
56	MG	BA	3428	1/1	0.95	0.18	36,36,36,36	0
56	MG	DA	3635	1/1	0.95	0.07	39,39,39,39	0
56	MG	CA	3080	1/1	0.95	0.13	51,51,51,51	0
56	MG	DA	3329	1/1	0.95	0.08	40,40,40,40	0
56	MG	DA	3080	1/1	0.95	0.16	43,43,43,43	0
56	MG	BA	3606	1/1	0.95	0.06	44,44,44,44	0
56	MG	BA	3285	1/1	0.95	0.14	44,44,44,44	0
56	MG	CA	3085	1/1	0.95	0.18	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3644	1/1	0.95	0.19	50,50,50,50	0
56	MG	DA	3339	1/1	0.95	0.15	35,35,35,35	0
56	MG	BD	301	1/1	0.95	0.15	35,35,35,35	0
56	MG	BD	302	1/1	0.95	0.38	44,44,44,44	0
56	MG	DA	3347	1/1	0.95	0.09	39,39,39,39	0
56	MG	BA	3609	1/1	0.95	0.16	29,29,29,29	0
56	MG	DA	3652	1/1	0.95	0.16	26,26,26,26	0
56	MG	DA	3654	1/1	0.95	0.08	50,50,50,50	0
56	MG	CA	3089	1/1	0.95	0.12	54,54,54,54	0
56	MG	BA	3430	1/1	0.95	0.11	47,47,47,47	0
56	MG	DA	3355	1/1	0.95	0.19	39,39,39,39	0
56	MG	BA	3005	1/1	0.95	0.11	43,43,43,43	0
56	MG	DA	3358	1/1	0.95	0.08	38,38,38,38	0
56	MG	BD	306	1/1	0.95	0.07	47,47,47,47	0
56	MG	CA	3093	1/1	0.95	0.11	65,65,65,65	0
56	MG	CA	3095	1/1	0.95	0.12	35,35,35,35	0
56	MG	DA	3365	1/1	0.95	0.07	52,52,52,52	0
56	MG	AA	3058	1/1	0.95	0.25	59,59,59,59	0
56	MG	BD	310	1/1	0.95	0.12	48,48,48,48	0
56	MG	DD	302	1/1	0.95	0.28	48,48,48,48	0
56	MG	AA	3105	1/1	0.95	0.25	54,54,54,54	0
56	MG	DD	304	1/1	0.95	0.22	40,40,40,40	0
56	MG	DD	305	1/1	0.95	0.13	73,73,73,73	0
56	MG	DE	301	1/1	0.95	0.20	51,51,51,51	0
56	MG	BA	3436	1/1	0.95	0.12	35,35,35,35	0
56	MG	DA	3377	1/1	0.95	0.14	32,32,32,32	0
56	MG	BA	3438	1/1	0.95	0.13	30,30,30,30	0
56	MG	BA	3443	1/1	0.95	0.16	34,34,34,34	0
56	MG	DF	301	1/1	0.95	0.17	40,40,40,40	0
56	MG	BF	302	1/1	0.95	0.18	49,49,49,49	0
56	MG	BA	3120	1/1	0.95	0.20	56,56,56,56	0
56	MG	DA	3385	1/1	0.95	0.22	58,58,58,58	0
56	MG	DA	3387	1/1	0.95	0.10	50,50,50,50	0
56	MG	BF	304	1/1	0.95	0.21	30,30,30,30	0
56	MG	DQ	3001	1/1	0.95	0.16	40,40,40,40	0
56	MG	DA	3107	1/1	0.95	0.12	50,50,50,50	0
56	MG	BA	3215	1/1	0.95	0.08	32,32,32,32	0
56	MG	BA	3451	1/1	0.95	0.09	31,31,31,31	0
56	MG	DR	5001	1/1	0.95	0.13	39,39,39,39	0
56	MG	DA	3394	1/1	0.95	0.07	46,46,46,46	0
56	MG	DU	3002	1/1	0.95	0.23	52,52,52,52	0
56	MG	BA	3165	1/1	0.95	0.28	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3121	1/1	0.95	0.14	50,50,50,50	0
56	MG	BA	3086	1/1	0.95	0.06	50,50,50,50	0
56	MG	DA	3402	1/1	0.95	0.14	33,33,33,33	0
56	MG	BA	3459	1/1	0.95	0.08	51,51,51,51	0
56	MG	D5	102	1/1	0.95	0.25	44,44,44,44	0
56	MG	BA	3222	1/1	0.95	0.25	56,56,56,56	0
56	MG	BA	3169	1/1	0.95	0.11	39,39,39,39	0
56	MG	DA	3408	1/1	0.95	0.09	35,35,35,35	0
56	MG	BA	3298	1/1	0.95	0.26	45,45,45,45	0
56	MG	BP	202	1/1	0.95	0.24	47,47,47,47	0
56	MG	BA	3170	1/1	0.95	0.23	34,34,34,34	0
56	MG	BP	204	1/1	0.95	0.08	53,53,53,53	0
56	MG	AK	3001	1/1	0.96	0.10	48,48,48,48	0
56	MG	DA	3046	1/1	0.96	0.11	48,48,48,48	0
56	MG	DA	3047	1/1	0.96	0.10	36,36,36,36	0
56	MG	BD	308	1/1	0.96	0.17	21,21,21,21	0
56	MG	DA	3479	1/1	0.96	0.11	35,35,35,35	0
56	MG	DA	3480	1/1	0.96	0.09	42,42,42,42	0
56	MG	BA	3490	1/1	0.96	0.07	40,40,40,40	0
56	MG	DA	3226	1/1	0.96	0.22	47,47,47,47	0
56	MG	BA	3493	1/1	0.96	0.08	51,51,51,51	0
56	MG	DA	3051	1/1	0.96	0.08	39,39,39,39	0
56	MG	CA	3076	1/1	0.96	0.14	48,48,48,48	0
56	MG	CA	3077	1/1	0.96	0.24	51,51,51,51	0
56	MG	BA	3496	1/1	0.96	0.20	21,21,21,21	0
56	MG	DA	3488	1/1	0.96	0.08	48,48,48,48	0
56	MG	DA	3232	1/1	0.96	0.05	39,39,39,39	0
56	MG	AL	3001	1/1	0.96	0.11	50,50,50,50	0
56	MG	DA	3494	1/1	0.96	0.07	50,50,50,50	0
56	MG	BE	302	1/1	0.96	0.12	29,29,29,29	0
56	MG	BE	305	1/1	0.96	0.23	44,44,44,44	0
56	MG	AA	3008	1/1	0.96	0.12	61,61,61,61	0
56	MG	DA	3239	1/1	0.96	0.13	54,54,54,54	0
56	MG	BA	3278	1/1	0.96	0.19	53,53,53,53	0
56	MG	BE	308	1/1	0.96	0.16	27,27,27,27	0
56	MG	DA	3501	1/1	0.96	0.15	67,67,67,67	0
56	MG	BF	301	1/1	0.96	0.10	46,46,46,46	0
56	MG	BA	3034	1/1	0.96	0.06	37,37,37,37	0
56	MG	BA	3218	1/1	0.96	0.09	58,58,58,58	0
56	MG	DA	3245	1/1	0.96	0.19	43,43,43,43	0
56	MG	BA	3076	1/1	0.96	0.13	40,40,40,40	0
56	MG	BA	3642	1/1	0.96	0.09	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3036	1/1	0.96	0.13	25,25,25,25	0
56	MG	AA	3138	1/1	0.96	0.21	38,38,38,38	0
56	MG	BA	3372	1/1	0.96	0.08	42,42,42,42	0
56	MG	BA	3508	1/1	0.96	0.09	46,46,46,46	0
56	MG	BA	3124	1/1	0.96	0.11	46,46,46,46	0
56	MG	AA	3024	1/1	0.96	0.12	49,49,49,49	0
56	MG	BA	3511	1/1	0.96	0.17	40,40,40,40	0
56	MG	DA	3076	1/1	0.96	0.24	38,38,38,38	0
56	MG	DA	3261	1/1	0.96	0.13	44,44,44,44	0
56	MG	BA	3009	1/1	0.96	0.12	36,36,36,36	0
56	MG	DA	3522	1/1	0.96	0.08	46,46,46,46	0
56	MG	BO	201	1/1	0.96	0.07	63,63,63,63	0
56	MG	DA	3264	1/1	0.96	0.07	38,38,38,38	0
56	MG	BA	3226	1/1	0.96	0.25	31,31,31,31	0
56	MG	BA	3652	1/1	0.96	0.18	54,54,54,54	0
56	MG	BA	3653	1/1	0.96	0.20	46,46,46,46	0
56	MG	DA	3083	1/1	0.96	0.05	44,44,44,44	0
56	MG	BA	3085	1/1	0.96	0.20	35,35,35,35	0
56	MG	DA	3272	1/1	0.96	0.13	36,36,36,36	0
56	MG	BA	3290	1/1	0.96	0.08	35,35,35,35	0
56	MG	DA	3533	1/1	0.96	0.12	59,59,59,59	0
56	MG	BA	3386	1/1	0.96	0.07	29,29,29,29	0
56	MG	DA	3277	1/1	0.96	0.05	46,46,46,46	0
56	MG	BA	3175	1/1	0.96	0.18	40,40,40,40	0
56	MG	BA	3659	1/1	0.96	0.06	42,42,42,42	0
56	MG	DA	3538	1/1	0.96	0.13	37,37,37,37	0
56	MG	CA	3115	1/1	0.96	0.06	81,81,81,81	0
56	MG	BU	201	1/1	0.96	0.34	33,33,33,33	0
56	MG	BA	3388	1/1	0.96	0.07	30,30,30,30	0
56	MG	DA	3283	1/1	0.96	0.06	47,47,47,47	0
56	MG	CA	3118	1/1	0.96	0.09	39,39,39,39	0
56	MG	DA	3546	1/1	0.96	0.14	38,38,38,38	0
56	MG	BU	204	1/1	0.96	0.13	49,49,49,49	0
56	MG	BA	3521	1/1	0.96	0.10	38,38,38,38	0
56	MG	BA	3040	1/1	0.96	0.10	40,40,40,40	0
56	MG	BA	3526	1/1	0.96	0.12	49,49,49,49	0
56	MG	BA	3130	1/1	0.96	0.37	51,51,51,51	0
56	MG	DA	3291	1/1	0.96	0.12	42,42,42,42	0
56	MG	BA	3232	1/1	0.96	0.15	32,32,32,32	0
56	MG	AA	3183	1/1	0.96	0.12	56,56,56,56	0
56	MG	AA	3212	1/1	0.96	0.10	36,36,36,36	0
56	MG	DA	3561	1/1	0.96	0.12	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3396	1/1	0.96	0.13	41,41,41,41	0
56	MG	AA	3034	1/1	0.96	0.14	46,46,46,46	0
56	MG	BA	3401	1/1	0.96	0.11	49,49,49,49	0
56	MG	BA	3402	1/1	0.96	0.13	23,23,23,23	0
56	MG	BA	3090	1/1	0.96	0.08	42,42,42,42	0
56	MG	DA	3309	1/1	0.96	0.09	25,25,25,25	0
56	MG	AA	3199	1/1	0.96	0.08	62,62,62,62	0
56	MG	B0	103	1/1	0.96	0.07	46,46,46,46	0
56	MG	BA	3241	1/1	0.96	0.23	41,41,41,41	0
56	MG	BA	3136	1/1	0.96	0.10	47,47,47,47	0
56	MG	DA	3576	1/1	0.96	0.09	57,57,57,57	0
56	MG	CA	3138	1/1	0.96	0.15	59,59,59,59	0
56	MG	DA	3581	1/1	0.96	0.10	41,41,41,41	0
56	MG	BA	3412	1/1	0.96	0.16	29,29,29,29	0
56	MG	DA	3583	1/1	0.96	0.12	35,35,35,35	0
56	MG	CA	3140	1/1	0.96	0.14	75,75,75,75	0
56	MG	BA	3419	1/1	0.96	0.31	36,36,36,36	0
56	MG	BA	3302	1/1	0.96	0.08	48,48,48,48	0
56	MG	DA	3118	1/1	0.96	0.07	44,44,44,44	0
56	MG	BA	3424	1/1	0.96	0.10	44,44,44,44	0
56	MG	DA	3120	1/1	0.96	0.41	50,50,50,50	0
56	MG	BA	3683	1/1	0.96	0.20	37,37,37,37	0
56	MG	DA	3330	1/1	0.96	0.07	30,30,30,30	0
56	MG	BA	3551	1/1	0.96	0.13	31,31,31,31	0
56	MG	BA	3243	1/1	0.96	0.10	43,43,43,43	0
56	MG	DA	3334	1/1	0.96	0.11	37,37,37,37	0
56	MG	BA	3426	1/1	0.96	0.09	34,34,34,34	0
56	MG	DA	3125	1/1	0.96	0.09	55,55,55,55	0
56	MG	BA	3688	1/1	0.96	0.08	58,58,58,58	0
56	MG	BA	3244	1/1	0.96	0.22	46,46,46,46	0
56	MG	BA	3690	1/1	0.96	0.16	55,55,55,55	0
56	MG	BA	3556	1/1	0.96	0.07	25,25,25,25	0
56	MG	BA	3308	1/1	0.96	0.13	33,33,33,33	0
56	MG	AA	3103	1/1	0.96	0.14	43,43,43,43	0
56	MG	BA	3695	1/1	0.96	0.23	34,34,34,34	0
56	MG	BA	3559	1/1	0.96	0.17	29,29,29,29	0
56	MG	BA	3048	1/1	0.96	0.21	33,33,33,33	0
56	MG	BA	3095	1/1	0.96	0.21	55,55,55,55	0
56	MG	BA	3140	1/1	0.96	0.18	50,50,50,50	0
56	MG	DA	3610	1/1	0.96	0.06	49,49,49,49	0
56	MG	CA	3011	1/1	0.96	0.19	27,27,27,27	0
56	MG	BA	3096	1/1	0.96	0.23	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3013	1/1	0.96	0.05	46,46,46,46	0
56	MG	DA	3366	1/1	0.96	0.06	43,43,43,43	0
56	MG	DA	3142	1/1	0.96	0.20	33,33,33,33	0
56	MG	AA	3186	1/1	0.96	0.11	51,51,51,51	0
56	MG	BA	3703	1/1	0.96	0.10	44,44,44,44	0
56	MG	DA	3371	1/1	0.96	0.07	37,37,37,37	0
56	MG	BA	3576	1/1	0.96	0.06	45,45,45,45	0
56	MG	DA	3374	1/1	0.96	0.11	40,40,40,40	0
56	MG	CA	3017	1/1	0.96	0.18	54,54,54,54	0
56	MG	BA	3052	1/1	0.96	0.15	29,29,29,29	0
56	MG	BA	3581	1/1	0.96	0.18	54,54,54,54	0
56	MG	BA	3053	1/1	0.96	0.12	52,52,52,52	0
56	MG	DA	3150	1/1	0.96	0.05	57,57,57,57	0
56	MG	DA	3151	1/1	0.96	0.31	48,48,48,48	0
56	MG	BA	3446	1/1	0.96	0.11	25,25,25,25	0
56	MG	CA	3170	1/1	0.96	0.14	44,44,44,44	0
56	MG	BA	3587	1/1	0.96	0.13	23,23,23,23	0
56	MG	DA	3632	1/1	0.96	0.16	60,60,60,60	0
56	MG	BA	3712	1/1	0.96	0.11	47,47,47,47	0
56	MG	BA	3055	1/1	0.96	0.23	44,44,44,44	0
56	MG	BA	3449	1/1	0.96	0.11	59,59,59,59	0
56	MG	DA	3158	1/1	0.96	0.28	47,47,47,47	0
56	MG	DA	3398	1/1	0.96	0.07	50,50,50,50	0
56	MG	BA	3450	1/1	0.96	0.08	40,40,40,40	0
56	MG	BA	3325	1/1	0.96	0.11	39,39,39,39	0
56	MG	BA	3452	1/1	0.96	0.07	16,16,16,16	0
56	MG	DA	3404	1/1	0.96	0.09	57,57,57,57	0
56	MG	AA	3104	1/1	0.96	0.10	35,35,35,35	0
56	MG	BA	3197	1/1	0.96	0.21	39,39,39,39	0
56	MG	DA	3165	1/1	0.96	0.30	48,48,48,48	0
56	MG	BA	3720	1/1	0.96	0.07	51,51,51,51	0
56	MG	DA	3649	1/1	0.96	0.06	39,39,39,39	0
56	MG	BA	3598	1/1	0.96	0.09	32,32,32,32	0
56	MG	BA	3058	1/1	0.96	0.20	41,41,41,41	0
56	MG	BA	3332	1/1	0.96	0.13	52,52,52,52	0
56	MG	DA	3004	1/1	0.96	0.06	24,24,24,24	0
56	MG	DA	3657	1/1	0.96	0.08	55,55,55,55	0
56	MG	DA	3658	1/1	0.96	0.27	50,50,50,50	0
56	MG	BA	3334	1/1	0.96	0.08	41,41,41,41	0
56	MG	BA	3461	1/1	0.96	0.07	33,33,33,33	0
56	MG	BA	3462	1/1	0.96	0.13	30,30,30,30	0
56	MG	DA	3174	1/1	0.96	0.22	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3423	1/1	0.96	0.07	29,29,29,29	0
56	MG	BA	3731	1/1	0.96	0.11	52,52,52,52	0
56	MG	DA	3009	1/1	0.96	0.04	33,33,33,33	0
56	MG	DA	3010	1/1	0.96	0.08	42,42,42,42	0
56	MG	AA	3010	1/1	0.96	0.05	71,71,71,71	0
56	MG	DA	3181	1/1	0.96	0.31	55,55,55,55	0
56	MG	DA	3182	1/1	0.96	0.15	29,29,29,29	0
56	MG	DA	3183	1/1	0.96	0.11	42,42,42,42	0
56	MG	BA	3020	1/1	0.96	0.31	43,43,43,43	0
56	MG	BA	3337	1/1	0.96	0.13	48,48,48,48	0
56	MG	BA	3608	1/1	0.96	0.13	51,51,51,51	0
56	MG	AA	3161	1/1	0.96	0.07	61,61,61,61	0
56	MG	DA	3439	1/1	0.96	0.13	45,45,45,45	0
56	MG	DA	3440	1/1	0.96	0.05	48,48,48,48	0
56	MG	BA	3738	1/1	0.96	0.17	58,58,58,58	0
56	MG	BA	3106	1/1	0.96	0.23	52,52,52,52	0
56	MG	DF	302	1/1	0.96	0.09	47,47,47,47	0
56	MG	DF	303	1/1	0.96	0.11	42,42,42,42	0
56	MG	DA	3443	1/1	0.96	0.13	30,30,30,30	0
56	MG	DF	305	1/1	0.96	0.22	55,55,55,55	0
56	MG	BA	3611	1/1	0.96	0.07	61,61,61,61	0
56	MG	AA	3066	1/1	0.96	0.19	41,41,41,41	0
56	MG	BA	3025	1/1	0.96	0.09	48,48,48,48	0
56	MG	BA	3472	1/1	0.96	0.07	53,53,53,53	0
56	MG	AA	3091	1/1	0.96	0.12	75,75,75,75	0
56	MG	BA	3474	1/1	0.96	0.11	43,43,43,43	0
56	MG	CA	3055	1/1	0.96	0.27	61,61,61,61	0
56	MG	DA	3453	1/1	0.96	0.09	44,44,44,44	0
56	MG	AA	3050	1/1	0.96	0.08	50,50,50,50	0
56	MG	BB	3008	1/1	0.96	0.15	49,49,49,49	0
56	MG	BA	3069	1/1	0.96	0.12	33,33,33,33	0
56	MG	DV	201	1/1	0.96	0.07	56,56,56,56	0
56	MG	BA	3003	1/1	0.96	0.08	24,24,24,24	0
56	MG	BA	3029	1/1	0.96	0.29	53,53,53,53	0
56	MG	DW	201	1/1	0.96	0.08	45,45,45,45	0
56	MG	BA	3269	1/1	0.96	0.15	32,32,32,32	0
56	MG	BA	3623	1/1	0.96	0.12	43,43,43,43	0
56	MG	BA	3354	1/1	0.96	0.06	45,45,45,45	0
56	MG	D5	101	1/1	0.96	0.15	44,44,44,44	0
56	MG	DA	3211	1/1	0.96	0.22	46,46,46,46	0
56	MG	BA	3270	1/1	0.96	0.13	29,29,29,29	0
56	MG	BA	3626	1/1	0.96	0.06	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3162	1/1	0.96	0.09	43,43,43,43	0
56	MG	BA	3628	1/1	0.96	0.09	39,39,39,39	0
56	MG	DA	3217	1/1	0.96	0.18	33,33,33,33	0
56	MG	BA	3486	1/1	0.96	0.12	55,55,55,55	0
56	MG	BA	3630	1/1	0.96	0.11	48,48,48,48	0
56	MG	BA	3445	1/1	0.97	0.10	16,16,16,16	0
56	MG	BA	3603	1/1	0.97	0.12	40,40,40,40	0
56	MG	DA	3342	1/1	0.97	0.09	31,31,31,31	0
56	MG	DA	3185	1/1	0.97	0.16	42,42,42,42	0
56	MG	DA	3345	1/1	0.97	0.06	16,16,16,16	0
56	MG	BA	3054	1/1	0.97	0.07	39,39,39,39	0
56	MG	BA	3321	1/1	0.97	0.14	47,47,47,47	0
56	MG	DA	3348	1/1	0.97	0.05	39,39,39,39	0
56	MG	DA	3350	1/1	0.97	0.12	21,21,21,21	0
56	MG	BA	3013	1/1	0.97	0.16	36,36,36,36	0
56	MG	BE	304	1/1	0.97	0.15	45,45,45,45	0
56	MG	DA	3539	1/1	0.97	0.10	35,35,35,35	0
56	MG	AA	3214	1/1	0.97	0.17	42,42,42,42	0
56	MG	DA	3191	1/1	0.97	0.07	31,31,31,31	0
56	MG	DA	3072	1/1	0.97	0.14	40,40,40,40	0
56	MG	DA	3357	1/1	0.97	0.06	50,50,50,50	0
56	MG	BA	3377	1/1	0.97	0.04	27,27,27,27	0
56	MG	DA	3545	1/1	0.97	0.14	35,35,35,35	0
56	MG	BA	3380	1/1	0.97	0.11	32,32,32,32	0
56	MG	BA	3382	1/1	0.97	0.13	21,21,21,21	0
56	MG	BA	3220	1/1	0.97	0.19	27,27,27,27	0
56	MG	BA	3522	1/1	0.97	0.13	42,42,42,42	0
56	MG	DA	3550	1/1	0.97	0.09	54,54,54,54	0
56	MG	BA	3456	1/1	0.97	0.08	24,24,24,24	0
56	MG	DA	3553	1/1	0.97	0.12	58,58,58,58	0
56	MG	DA	3199	1/1	0.97	0.16	46,46,46,46	0
56	MG	BA	3525	1/1	0.97	0.09	31,31,31,31	0
56	MG	DA	3556	1/1	0.97	0.07	35,35,35,35	0
56	MG	BF	305	1/1	0.97	0.15	38,38,38,38	0
56	MG	BA	3457	1/1	0.97	0.06	25,25,25,25	0
56	MG	BA	3078	1/1	0.97	0.11	44,44,44,44	0
56	MG	DA	3204	1/1	0.97	0.24	44,44,44,44	0
56	MG	DA	3375	1/1	0.97	0.07	40,40,40,40	0
56	MG	DA	3376	1/1	0.97	0.09	42,42,42,42	0
56	MG	BA	3617	1/1	0.97	0.15	30,30,30,30	0
56	MG	DA	3085	1/1	0.97	0.07	35,35,35,35	0
56	MG	DA	3207	1/1	0.97	0.13	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3329	1/1	0.97	0.07	49,49,49,49	0
56	MG	BA	3330	1/1	0.97	0.07	35,35,35,35	0
56	MG	DA	3383	1/1	0.97	0.08	27,27,27,27	0
56	MG	DA	3088	1/1	0.97	0.06	47,47,47,47	0
56	MG	DA	3386	1/1	0.97	0.06	18,18,18,18	0
56	MG	BA	3531	1/1	0.97	0.11	28,28,28,28	0
56	MG	DA	3577	1/1	0.97	0.10	44,44,44,44	0
56	MG	DA	3213	1/1	0.97	0.15	48,48,48,48	0
56	MG	DA	3579	1/1	0.97	0.11	38,38,38,38	0
56	MG	DA	3580	1/1	0.97	0.08	35,35,35,35	0
56	MG	BA	3699	1/1	0.97	0.08	23,23,23,23	0
56	MG	AA	3177	1/1	0.97	0.05	58,58,58,58	0
56	MG	BA	3168	1/1	0.97	0.29	52,52,52,52	0
56	MG	DA	3584	1/1	0.97	0.09	47,47,47,47	0
56	MG	BN	3006	1/1	0.97	0.04	33,33,33,33	0
56	MG	BA	3389	1/1	0.97	0.15	52,52,52,52	0
56	MG	DA	3397	1/1	0.97	0.11	40,40,40,40	0
56	MG	BP	201	1/1	0.97	0.24	37,37,37,37	0
56	MG	BA	3041	1/1	0.97	0.26	45,45,45,45	0
56	MG	AV	101	1/1	0.97	0.16	51,51,51,51	0
56	MG	AA	3049	1/1	0.97	0.18	46,46,46,46	0
56	MG	DA	3403	1/1	0.97	0.06	42,42,42,42	0
56	MG	BA	3706	1/1	0.97	0.12	38,38,38,38	0
56	MG	BA	3707	1/1	0.97	0.06	57,57,57,57	0
56	MG	DA	3101	1/1	0.97	0.13	59,59,59,59	0
56	MG	CA	3059	1/1	0.97	0.19	51,51,51,51	0
56	MG	BQ	3003	1/1	0.97	0.07	15,15,15,15	0
56	MG	BA	3542	1/1	0.97	0.11	37,37,37,37	0
56	MG	DA	3410	1/1	0.97	0.06	40,40,40,40	0
56	MG	AA	3057	1/1	0.97	0.05	45,45,45,45	0
56	MG	BA	3200	1/1	0.97	0.09	32,32,32,32	0
56	MG	BA	3065	1/1	0.97	0.15	31,31,31,31	0
56	MG	BA	3471	1/1	0.97	0.05	28,28,28,28	0
56	MG	CA	3066	1/1	0.97	0.06	47,47,47,47	0
56	MG	BA	3045	1/1	0.97	0.08	27,27,27,27	0
56	MG	DA	3421	1/1	0.97	0.12	43,43,43,43	0
56	MG	DA	3237	1/1	0.97	0.15	37,37,37,37	0
56	MG	BU	206	1/1	0.97	0.15	41,41,41,41	0
56	MG	AA	3158	1/1	0.97	0.13	47,47,47,47	0
56	MG	BA	3233	1/1	0.97	0.12	49,49,49,49	0
56	MG	DA	3426	1/1	0.97	0.10	41,41,41,41	0
56	MG	BA	3403	1/1	0.97	0.07	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3108	1/1	0.97	0.08	32,32,32,32	0
56	MG	BA	3344	1/1	0.97	0.07	65,65,65,65	0
56	MG	BV	3003	1/1	0.97	0.14	27,27,27,27	0
56	MG	AA	3149	1/1	0.97	0.05	49,49,49,49	0
56	MG	BA	3407	1/1	0.97	0.18	35,35,35,35	0
56	MG	DA	3247	1/1	0.97	0.17	34,34,34,34	0
56	MG	BA	3347	1/1	0.97	0.10	44,44,44,44	0
56	MG	BA	3266	1/1	0.97	0.21	47,47,47,47	0
56	MG	BA	3413	1/1	0.97	0.05	19,19,19,19	0
56	MG	BA	3560	1/1	0.97	0.15	24,24,24,24	0
56	MG	BA	3153	1/1	0.97	0.09	47,47,47,47	0
56	MG	BA	3727	1/1	0.97	0.10	27,27,27,27	0
56	MG	B0	102	1/1	0.97	0.07	50,50,50,50	0
56	MG	BA	3728	1/1	0.97	0.11	56,56,56,56	0
56	MG	DA	3629	1/1	0.97	0.09	30,30,30,30	0
56	MG	DA	3258	1/1	0.97	0.14	39,39,39,39	0
56	MG	BA	3562	1/1	0.97	0.11	42,42,42,42	0
56	MG	BA	3730	1/1	0.97	0.06	43,43,43,43	0
56	MG	BA	3110	1/1	0.97	0.11	43,43,43,43	0
56	MG	DA	3016	1/1	0.97	0.11	33,33,33,33	0
56	MG	DA	3451	1/1	0.97	0.04	68,68,68,68	0
56	MG	BA	3489	1/1	0.97	0.06	50,50,50,50	0
56	MG	DA	3265	1/1	0.97	0.12	44,44,44,44	0
56	MG	DA	3133	1/1	0.97	0.11	31,31,31,31	0
56	MG	BA	3566	1/1	0.97	0.12	43,43,43,43	0
56	MG	DA	3641	1/1	0.97	0.12	47,47,47,47	0
56	MG	BA	3303	1/1	0.97	0.11	11,11,11,11	0
56	MG	B3	3401	1/1	0.97	0.10	24,24,24,24	0
56	MG	B3	3402	1/1	0.97	0.07	49,49,49,49	0
56	MG	CA	3097	1/1	0.97	0.09	60,60,60,60	0
56	MG	BA	3568	1/1	0.97	0.07	68,68,68,68	0
56	MG	DA	3274	1/1	0.97	0.23	49,49,49,49	0
56	MG	DA	3275	1/1	0.97	0.12	34,34,34,34	0
56	MG	BA	3736	1/1	0.97	0.09	40,40,40,40	0
56	MG	DA	3025	1/1	0.97	0.20	38,38,38,38	0
56	MG	DA	3653	1/1	0.97	0.07	52,52,52,52	0
56	MG	CA	3101	1/1	0.97	0.08	58,58,58,58	0
56	MG	DA	3028	1/1	0.97	0.06	34,34,34,34	0
56	MG	DA	3656	1/1	0.97	0.08	62,62,62,62	0
56	MG	DA	3467	1/1	0.97	0.13	48,48,48,48	0
56	MG	BA	3569	1/1	0.97	0.09	55,55,55,55	0
56	MG	BA	3492	1/1	0.97	0.12	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3470	1/1	0.97	0.16	45,45,45,45	0
56	MG	DA	3471	1/1	0.97	0.09	32,32,32,32	0
56	MG	BA	3572	1/1	0.97	0.10	23,23,23,23	0
56	MG	DB	3005	1/1	0.97	0.15	41,41,41,41	0
56	MG	B8	5002	1/1	0.97	0.10	48,48,48,48	0
56	MG	BA	3655	1/1	0.97	0.11	44,44,44,44	0
56	MG	DB	3008	1/1	0.97	0.10	36,36,36,36	0
56	MG	BA	3239	1/1	0.97	0.06	33,33,33,33	0
56	MG	DA	3286	1/1	0.97	0.05	26,26,26,26	0
56	MG	BA	3494	1/1	0.97	0.09	28,28,28,28	0
56	MG	BA	3580	1/1	0.97	0.11	58,58,58,58	0
56	MG	DD	301	1/1	0.97	0.09	23,23,23,23	0
56	MG	BA	3495	1/1	0.97	0.15	27,27,27,27	0
56	MG	AA	3165	1/1	0.97	0.09	24,24,24,24	0
56	MG	BA	3427	1/1	0.97	0.07	20,20,20,20	0
56	MG	DA	3292	1/1	0.97	0.06	34,34,34,34	0
56	MG	BB	3007	1/1	0.97	0.04	49,49,49,49	0
56	MG	BA	3662	1/1	0.97	0.08	46,46,46,46	0
56	MG	DA	3042	1/1	0.97	0.15	38,38,38,38	0
56	MG	DA	3297	1/1	0.97	0.09	36,36,36,36	0
56	MG	DA	3489	1/1	0.97	0.05	36,36,36,36	0
56	MG	DA	3159	1/1	0.97	0.06	50,50,50,50	0
56	MG	DA	3492	1/1	0.97	0.05	44,44,44,44	0
56	MG	BA	3050	1/1	0.97	0.12	33,33,33,33	0
56	MG	DA	3300	1/1	0.97	0.07	47,47,47,47	0
56	MG	DA	3301	1/1	0.97	0.12	30,30,30,30	0
56	MG	BA	3588	1/1	0.97	0.07	41,41,41,41	0
56	MG	BA	3500	1/1	0.97	0.07	43,43,43,43	0
56	MG	BA	3035	1/1	0.97	0.06	32,32,32,32	0
56	MG	CA	3120	1/1	0.97	0.12	59,59,59,59	0
56	MG	BA	3023	1/1	0.97	0.18	34,34,34,34	0
56	MG	DA	3311	1/1	0.97	0.07	33,33,33,33	0
56	MG	BA	3275	1/1	0.97	0.21	28,28,28,28	0
56	MG	BA	3312	1/1	0.97	0.06	43,43,43,43	0
56	MG	DA	3052	1/1	0.97	0.05	20,20,20,20	0
56	MG	DA	3315	1/1	0.97	0.10	39,39,39,39	0
56	MG	BA	3670	1/1	0.97	0.09	55,55,55,55	0
56	MG	BA	3364	1/1	0.97	0.09	30,30,30,30	0
56	MG	BA	3160	1/1	0.97	0.15	24,24,24,24	0
56	MG	CA	3020	1/1	0.97	0.13	45,45,45,45	0
56	MG	DA	3322	1/1	0.97	0.10	41,41,41,41	0
56	MG	BA	3115	1/1	0.97	0.14	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3439	1/1	0.97	0.05	35,35,35,35	0
56	MG	CA	3023	1/1	0.97	0.15	37,37,37,37	0
56	MG	DA	3327	1/1	0.97	0.06	45,45,45,45	0
56	MG	BA	3024	1/1	0.97	0.06	31,31,31,31	0
56	MG	DA	3177	1/1	0.97	0.13	30,30,30,30	0
56	MG	DA	3178	1/1	0.97	0.08	43,43,43,43	0
56	MG	BA	3216	1/1	0.97	0.09	46,46,46,46	0
56	MG	CA	3133	1/1	0.97	0.05	45,45,45,45	0
56	MG	DA	3063	1/1	0.97	0.08	55,55,55,55	0
56	MG	DA	3335	1/1	0.97	0.10	36,36,36,36	0
56	MG	CA	3026	1/1	0.97	0.04	52,52,52,52	0
56	MG	BA	3437	1/1	0.98	0.06	37,37,37,37	0
56	MG	BE	309	1/1	0.98	0.07	37,37,37,37	0
56	MG	BA	3271	1/1	0.98	0.18	40,40,40,40	0
56	MG	DA	3208	1/1	0.98	0.17	46,46,46,46	0
56	MG	BA	3320	1/1	0.98	0.07	41,41,41,41	0
56	MG	BA	3497	1/1	0.98	0.21	28,28,28,28	0
56	MG	BA	3440	1/1	0.98	0.05	40,40,40,40	0
56	MG	BA	3442	1/1	0.98	0.12	33,33,33,33	0
56	MG	DA	3319	1/1	0.98	0.05	31,31,31,31	0
56	MG	DA	3450	1/1	0.98	0.06	47,47,47,47	0
56	MG	AA	3144	1/1	0.98	0.08	56,56,56,56	0
56	MG	DA	3026	1/1	0.98	0.08	36,36,36,36	0
56	MG	BG	3001	1/1	0.98	0.07	65,65,65,65	0
56	MG	DA	3324	1/1	0.98	0.09	24,24,24,24	0
56	MG	BA	3351	1/1	0.98	0.10	21,21,21,21	0
56	MG	BA	3564	1/1	0.98	0.10	26,26,26,26	0
56	MG	BA	3322	1/1	0.98	0.06	46,46,46,46	0
56	MG	DA	3219	1/1	0.98	0.21	49,49,49,49	0
56	MG	BA	3353	1/1	0.98	0.11	31,31,31,31	0
56	MG	BA	3323	1/1	0.98	0.06	25,25,25,25	0
56	MG	BA	3639	1/1	0.98	0.06	35,35,35,35	0
56	MG	DA	3332	1/1	0.98	0.06	29,29,29,29	0
56	MG	BA	3062	1/1	0.98	0.28	46,46,46,46	0
56	MG	BA	3063	1/1	0.98	0.08	34,34,34,34	0
56	MG	BA	3236	1/1	0.98	0.13	37,37,37,37	0
56	MG	BA	3276	1/1	0.98	0.14	9,9,9,9	0
56	MG	DA	3337	1/1	0.98	0.09	50,50,50,50	0
56	MG	DA	3605	1/1	0.98	0.04	58,58,58,58	0
56	MG	BA	3573	1/1	0.98	0.07	53,53,53,53	0
56	MG	BA	3574	1/1	0.98	0.05	52,52,52,52	0
56	MG	DA	3340	1/1	0.98	0.05	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3341	1/1	0.98	0.04	40,40,40,40	0
56	MG	BA	3575	1/1	0.98	0.06	26,26,26,26	0
56	MG	DA	3343	1/1	0.98	0.07	37,37,37,37	0
56	MG	BA	3397	1/1	0.98	0.04	44,44,44,44	0
56	MG	DA	3476	1/1	0.98	0.05	35,35,35,35	0
56	MG	BA	3398	1/1	0.98	0.07	36,36,36,36	0
56	MG	DA	3136	1/1	0.98	0.05	39,39,39,39	0
56	MG	BA	3578	1/1	0.98	0.09	47,47,47,47	0
56	MG	BA	3579	1/1	0.98	0.12	21,21,21,21	0
56	MG	DA	3045	1/1	0.98	0.14	49,49,49,49	0
56	MG	BA	3399	1/1	0.98	0.10	22,22,22,22	0
56	MG	DA	3352	1/1	0.98	0.08	24,24,24,24	0
56	MG	BA	3724	1/1	0.98	0.11	22,22,22,22	0
56	MG	BR	202	1/1	0.98	0.09	25,25,25,25	0
56	MG	AA	3157	1/1	0.98	0.04	26,26,26,26	0
56	MG	BA	3127	1/1	0.98	0.12	42,42,42,42	0
56	MG	BA	3032	1/1	0.98	0.15	36,36,36,36	0
56	MG	BU	203	1/1	0.98	0.10	26,26,26,26	0
56	MG	DA	3490	1/1	0.98	0.04	46,46,46,46	0
56	MG	BA	3584	1/1	0.98	0.07	43,43,43,43	0
56	MG	DA	3362	1/1	0.98	0.20	42,42,42,42	0
56	MG	BU	205	1/1	0.98	0.10	39,39,39,39	0
56	MG	BA	3585	1/1	0.98	0.10	25,25,25,25	0
56	MG	BA	3515	1/1	0.98	0.12	46,46,46,46	0
56	MG	BA	3363	1/1	0.98	0.06	29,29,29,29	0
56	MG	BA	3589	1/1	0.98	0.12	34,34,34,34	0
56	MG	DA	3368	1/1	0.98	0.06	34,34,34,34	0
56	MG	AA	3040	1/1	0.98	0.06	46,46,46,46	0
56	MG	BA	3365	1/1	0.98	0.05	63,63,63,63	0
56	MG	BA	3519	1/1	0.98	0.04	57,57,57,57	0
56	MG	DA	3253	1/1	0.98	0.05	35,35,35,35	0
56	MG	BA	3188	1/1	0.98	0.06	49,49,49,49	0
56	MG	BA	3206	1/1	0.98	0.10	32,32,32,32	0
56	MG	BA	3077	1/1	0.98	0.04	20,20,20,20	0
56	MG	BA	3409	1/1	0.98	0.07	40,40,40,40	0
56	MG	BA	3370	1/1	0.98	0.03	39,39,39,39	0
56	MG	DA	3510	1/1	0.98	0.05	67,67,67,67	0
56	MG	DA	3260	1/1	0.98	0.03	32,32,32,32	0
56	MG	DA	3512	1/1	0.98	0.09	37,37,37,37	0
56	MG	BA	3091	1/1	0.98	0.16	55,55,55,55	0
56	MG	BA	3416	1/1	0.98	0.08	25,25,25,25	0
56	MG	DA	3382	1/1	0.98	0.07	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3528	1/1	0.98	0.09	44,44,44,44	0
56	MG	DA	3384	1/1	0.98	0.05	24,24,24,24	0
56	MG	BA	3418	1/1	0.98	0.14	20,20,20,20	0
56	MG	AA	3172	1/1	0.98	0.04	36,36,36,36	0
56	MG	DA	3266	1/1	0.98	0.08	32,32,32,32	0
56	MG	DA	3388	1/1	0.98	0.07	25,25,25,25	0
56	MG	DA	3389	1/1	0.98	0.09	32,32,32,32	0
56	MG	BA	3421	1/1	0.98	0.07	28,28,28,28	0
56	MG	BA	3422	1/1	0.98	0.08	23,23,23,23	0
56	MG	BA	3475	1/1	0.98	0.05	42,42,42,42	0
56	MG	DA	3526	1/1	0.98	0.05	49,49,49,49	0
56	MG	BA	3534	1/1	0.98	0.11	36,36,36,36	0
56	MG	BB	3010	1/1	0.98	0.10	44,44,44,44	0
56	MG	BA	3176	1/1	0.98	0.10	50,50,50,50	0
56	MG	BB	3012	1/1	0.98	0.09	42,42,42,42	0
56	MG	BA	3536	1/1	0.98	0.07	37,37,37,37	0
56	MG	BA	3679	1/1	0.98	0.06	39,39,39,39	0
56	MG	B5	502	1/1	0.98	0.05	56,56,56,56	0
56	MG	DA	3082	1/1	0.98	0.04	7,7,7,7	0
56	MG	BA	3374	1/1	0.98	0.12	26,26,26,26	0
56	MG	B7	102	1/1	0.98	0.06	29,29,29,29	0
56	MG	BA	3287	1/1	0.98	0.07	11,11,11,11	0
56	MG	CA	3082	1/1	0.98	0.05	46,46,46,46	0
56	MG	BA	3228	1/1	0.98	0.06	23,23,23,23	0
56	MG	BA	3541	1/1	0.98	0.07	37,37,37,37	0
56	MG	BA	3684	1/1	0.98	0.13	44,44,44,44	0
56	MG	DE	306	1/1	0.98	0.07	44,44,44,44	0
56	MG	BA	3079	1/1	0.98	0.09	50,50,50,50	0
56	MG	DA	3411	1/1	0.98	0.10	33,33,33,33	0
56	MG	DA	3412	1/1	0.98	0.13	34,34,34,34	0
56	MG	CA	3001	1/1	0.98	0.06	48,48,48,48	0
56	MG	BA	3378	1/1	0.98	0.09	24,24,24,24	0
56	MG	DA	3415	1/1	0.98	0.04	22,22,22,22	0
56	MG	BA	3483	1/1	0.98	0.09	18,18,18,18	0
56	MG	DO	5001	1/1	0.98	0.05	33,33,33,33	0
56	MG	BA	3379	1/1	0.98	0.07	43,43,43,43	0
56	MG	BD	307	1/1	0.98	0.06	36,36,36,36	0
56	MG	BA	3049	1/1	0.98	0.15	17,17,17,17	0
56	MG	DA	3420	1/1	0.98	0.04	43,43,43,43	0
56	MG	CA	3094	1/1	0.98	0.19	37,37,37,37	0
56	MG	BA	3431	1/1	0.98	0.18	54,54,54,54	0
56	MG	CA	3096	1/1	0.98	0.06	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3691	1/1	0.98	0.10	40,40,40,40	0
56	MG	CA	3098	1/1	0.98	0.12	37,37,37,37	0
56	MG	BA	3432	1/1	0.98	0.05	27,27,27,27	0
56	MG	DA	3560	1/1	0.98	0.05	57,57,57,57	0
56	MG	DA	3427	1/1	0.98	0.04	29,29,29,29	0
56	MG	BA	3381	1/1	0.98	0.04	25,25,25,25	0
56	MG	DA	3429	1/1	0.98	0.05	30,30,30,30	0
56	MG	BE	301	1/1	0.98	0.14	28,28,28,28	0
56	MG	CA	3102	1/1	0.98	0.04	55,55,55,55	0
56	MG	AA	3137	1/1	0.98	0.14	40,40,40,40	0
56	MG	DA	3303	1/1	0.98	0.06	37,37,37,37	0
56	MG	BA	3491	1/1	0.98	0.08	38,38,38,38	0
57	SF4	CD	501	8/8	0.98	0.03	63,76,87,96	0
56	MG	BA	3345	1/1	0.98	0.03	37,37,37,37	0
58	ZN	CN	501	1/1	0.98	0.04	104,104,104,104	0
58	ZN	DY	501	1/1	0.98	0.04	90,90,90,90	0
56	MG	DA	3307	1/1	0.98	0.08	40,40,40,40	0
56	MG	DA	3574	1/1	0.98	0.11	22,22,22,22	0
56	MG	DA	3308	1/1	0.98	0.05	32,32,32,32	0
56	MG	AA	3220	1/1	0.98	0.06	42,42,42,42	0
56	MG	BA	3555	1/1	0.98	0.18	31,31,31,31	0
56	MG	AA	3192	1/1	0.99	0.08	73,73,73,73	0
56	MG	DA	3304	1/1	0.99	0.04	44,44,44,44	0
56	MG	BA	3314	1/1	0.99	0.06	22,22,22,22	0
56	MG	BA	3410	1/1	0.99	0.05	21,21,21,21	0
56	MG	DA	3349	1/1	0.99	0.04	27,27,27,27	0
56	MG	DA	3396	1/1	0.99	0.06	37,37,37,37	0
56	MG	BA	3586	1/1	0.99	0.08	26,26,26,26	0
56	MG	BA	3411	1/1	0.99	0.08	21,21,21,21	0
56	MG	BA	3463	1/1	0.99	0.06	32,32,32,32	0
56	MG	BA	3523	1/1	0.99	0.09	32,32,32,32	0
56	MG	DA	3552	1/1	0.99	0.05	42,42,42,42	0
56	MG	DA	3401	1/1	0.99	0.11	41,41,41,41	0
56	MG	BA	3192	1/1	0.99	0.04	48,48,48,48	0
56	MG	BA	3393	1/1	0.99	0.07	27,27,27,27	0
56	MG	BA	3592	1/1	0.99	0.08	43,43,43,43	0
56	MG	BA	3414	1/1	0.99	0.12	51,51,51,51	0
56	MG	DA	3505	1/1	0.99	0.07	24,24,24,24	0
56	MG	BA	3415	1/1	0.99	0.06	28,28,28,28	0
56	MG	DA	3616	1/1	0.99	0.04	41,41,41,41	0
56	MG	DA	3359	1/1	0.99	0.07	21,21,21,21	0
56	MG	DA	3508	1/1	0.99	0.05	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3360	1/1	0.99	0.02	36,36,36,36	0
56	MG	AA	3152	1/1	0.99	0.07	29,29,29,29	0
56	MG	DA	3564	1/1	0.99	0.03	29,29,29,29	0
56	MG	BA	3441	1/1	0.99	0.10	29,29,29,29	0
56	MG	BE	303	1/1	0.99	0.04	39,39,39,39	0
56	MG	BA	3417	1/1	0.99	0.07	21,21,21,21	0
56	MG	AA	3145	1/1	0.99	0.10	63,63,63,63	0
56	MG	DA	3321	1/1	0.99	0.04	31,31,31,31	0
56	MG	BA	3306	1/1	0.99	0.06	19,19,19,19	0
56	MG	BA	3420	1/1	0.99	0.10	13,13,13,13	0
56	MG	DA	3572	1/1	0.99	0.05	39,39,39,39	0
56	MG	DA	3573	1/1	0.99	0.10	32,32,32,32	0
56	MG	BA	3362	1/1	0.99	0.06	23,23,23,23	0
56	MG	BA	3333	1/1	0.99	0.09	27,27,27,27	0
56	MG	DA	3633	1/1	0.99	0.09	25,25,25,25	0
56	MG	BA	3448	1/1	0.99	0.10	23,23,23,23	0
56	MG	DA	3372	1/1	0.99	0.03	37,37,37,37	0
56	MG	CA	3083	1/1	0.99	0.05	30,30,30,30	0
56	MG	BA	3537	1/1	0.99	0.06	45,45,45,45	0
56	MG	BA	3570	1/1	0.99	0.10	33,33,33,33	0
56	MG	BA	3348	1/1	0.99	0.06	29,29,29,29	0
56	MG	DA	3474	1/1	0.99	0.05	49,49,49,49	0
56	MG	BA	3319	1/1	0.99	0.10	34,34,34,34	0
56	MG	BA	3366	1/1	0.99	0.06	30,30,30,30	0
56	MG	DA	3643	1/1	0.99	0.13	18,18,18,18	0
56	MG	BA	3057	1/1	0.99	0.17	36,36,36,36	0
56	MG	BA	3159	1/1	0.99	0.10	47,47,47,47	0
56	MG	DA	3293	1/1	0.99	0.04	34,34,34,34	0
56	MG	DA	3430	1/1	0.99	0.11	75,75,75,75	0
56	MG	BA	3454	1/1	0.99	0.08	20,20,20,20	0
57	SF4	AD	501	8/8	0.99	0.04	62,75,82,88	0
56	MG	BA	3015	1/1	0.99	0.13	30,30,30,30	0
58	ZN	AN	102	1/1	0.99	0.02	88,88,88,88	0
58	ZN	BY	501	1/1	0.99	0.03	67,67,67,67	0
56	MG	DA	3650	1/1	0.99	0.04	35,35,35,35	0
58	ZN	B5	501	1/1	0.99	0.02	49,49,49,49	0
56	MG	BB	3013	1/1	0.99	0.07	31,31,31,31	0
56	MG	DA	3257	1/1	0.99	0.09	25,25,25,25	0
56	MG	BA	3080	1/1	0.99	0.03	12,12,12,12	0
58	ZN	D5	103	1/1	0.99	0.02	61,61,61,61	0
58	ZN	D6	501	1/1	0.99	0.03	65,65,65,65	0
58	ZN	D9	501	1/1	0.99	0.04	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3156	1/1	0.99	0.07	31,31,31,31	0
56	MG	BA	3547	1/1	0.99	0.10	30,30,30,30	0
56	MG	AA	3163	1/1	0.99	0.10	23,23,23,23	0
56	MG	BA	3488	1/1	0.99	0.14	43,43,43,43	0
56	MG	BA	3327	1/1	1.00	0.05	21,21,21,21	0
56	MG	BA	3480	1/1	1.00	0.03	22,22,22,22	0
56	MG	BX	101	1/1	1.00	0.04	38,38,38,38	0
58	ZN	B6	501	1/1	1.00	0.03	51,51,51,51	0
58	ZN	B9	501	1/1	1.00	0.02	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.