



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 05:38 am BST

PDB ID : 1VY7
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in the pre-attack state of peptide bond formation containing short substrate-mimic Cytidine-Cytidine-Puromycin in the A site and acylated tRNA in the P site.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

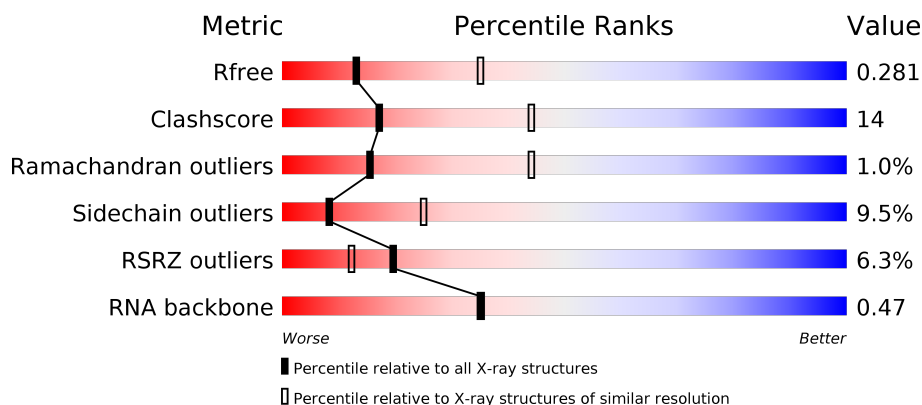
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	1521	<div> <div>2%</div> <div> <div></div> <div>38%</div> <div>43%</div> <div>16%</div> <div>..</div> </div> </div>
1	CA	1521	<div> <div>2%</div> <div> <div></div> <div>33%</div> <div>47%</div> <div>17%</div> <div>..</div> </div> </div>
2	AB	256	<div> <div>6%</div> <div> <div></div> <div>50%</div> <div>32%</div> <div>8%</div> <div>10%</div> </div> </div>
2	CB	256	<div> <div>43%</div> <div> <div></div> <div>49%</div> <div>32%</div> <div>8%</div> <div>10%</div> </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	



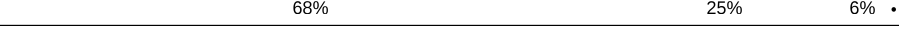
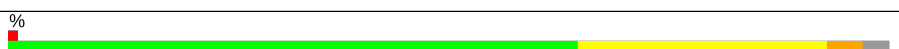



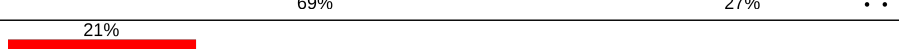


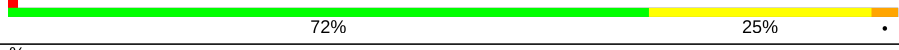





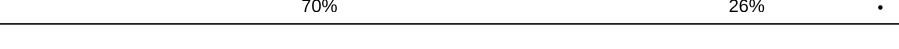
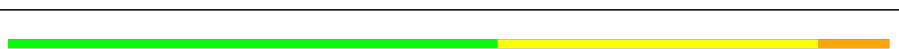






Continued on next page...

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	AW	3	
23	CW	3	
24	AX	77	
24	CX	77	
25	AY	76	
25	CY	76	
26	BA	2915	
26	DA	2915	
27	BB	121	
27	DB	121	




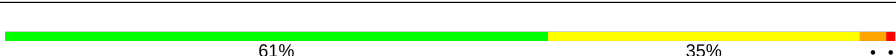
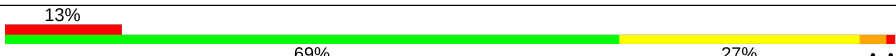
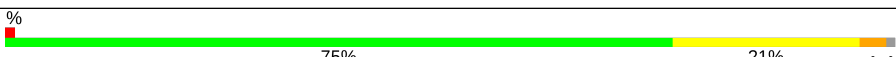
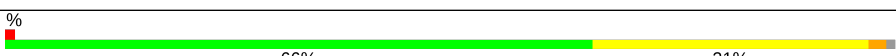
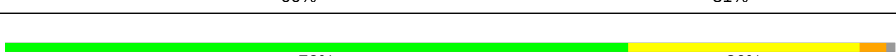
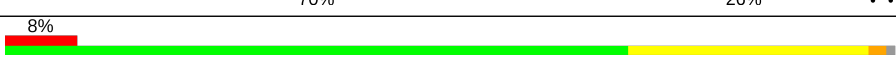

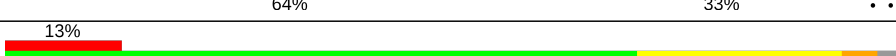



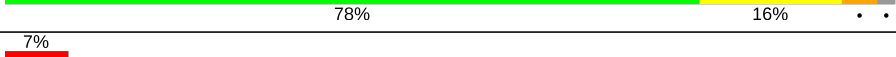




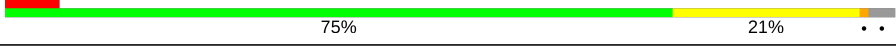

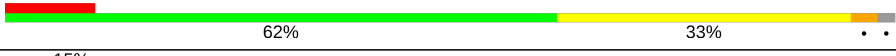
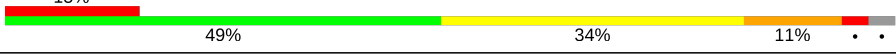


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	BD	276	% 
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	% 
30	DF	210	
31	BG	182	3% 
31	DG	182	27% 
32	BH	180	% 
32	DH	180	21% 
33	BI	148	9% 
33	DI	148	53% 
34	BN	140	% 
34	DN	140	% 
35	BO	122	
35	DO	122	
36	BP	150	% 
36	DP	150	4% 
37	BQ	141	
37	DQ	141	11% 
38	BR	118	
38	DR	118	
39	BS	112	% 
39	DS	112	10% 
40	BT	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	71	
51	D4	71	
52	B5	60	
52	D5	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	
56	B9	37	
56	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
57	MG	BF	309	-	-	-	X
57	MG	DA	3069	-	-	-	X
57	MG	DA	3553	-	-	-	X
57	MG	DV	202	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 290205 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
			32205	14333	5970	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 type Z.

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	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

- Molecule 23 is a RNA chain called Cytidine-Puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
23	CW	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 24 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0	0
			1633	730	296	529	76	2			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			

- Molecule 25 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	5	Total	C	N	O	P	0	0	0
			104	47	19	33	5			
25	CY	5	Total	C	N	O	P	0	0	0
			104	47	19	33	5			

- Molecule 26 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BA	2819	Total	C	N	O	P	0	0	0
			60729	27026	11370	19515	2818			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	DA	2800	Total	C	N	O	P	0	0	0
			60311	26840	11284	19388	2799			

- Molecule 27 is a RNA chain called 5S Ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			
51	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BA	720	Total	Mg	0	0
			720	720		
57	AK	1	Total	Mg	0	0
			1	1		
57	DQ	3	Total	Mg	0	0
			3	3		
57	D3	1	Total	Mg	0	0
			1	1		
57	DF	4	Total	Mg	0	0
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B8	1	Total 1	Mg 1	0	0
57	BE	7	Total 7	Mg 7	0	0
57	AW	1	Total 1	Mg 1	0	0
57	DU	4	Total 4	Mg 4	0	0
57	B1	1	Total 1	Mg 1	0	0
57	AN	2	Total 2	Mg 2	0	0
57	BP	4	Total 4	Mg 4	0	0
57	AX	11	Total 11	Mg 11	0	0
57	DN	1	Total 1	Mg 1	0	0
57	AS	1	Total 1	Mg 1	0	0
57	CA	160	Total 160	Mg 160	0	0
57	B5	2	Total 2	Mg 2	0	0
57	BB	20	Total 20	Mg 20	0	0
57	AJ	1	Total 1	Mg 1	0	0
57	D8	2	Total 2	Mg 2	0	0
57	AE	2	Total 2	Mg 2	0	0
57	DG	1	Total 1	Mg 1	0	0
57	B9	1	Total 1	Mg 1	0	0
57	BF	10	Total 10	Mg 10	0	0
57	AV	1	Total 1	Mg 1	0	0
57	BX	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

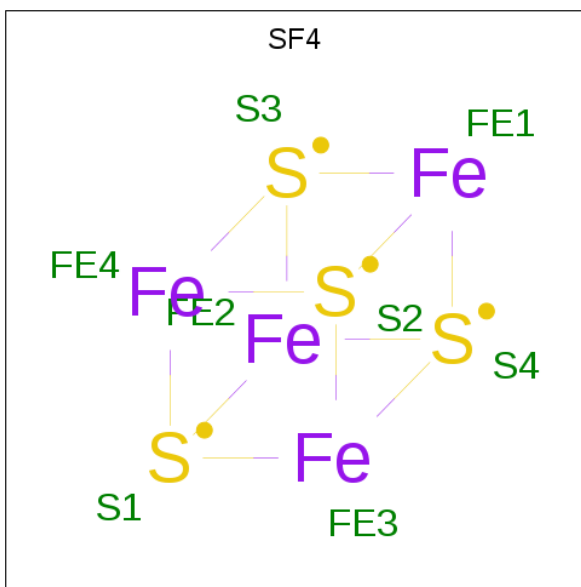
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B2	1	Total 1	Mg 1	0	0
57	AA	207	Total 207	Mg 207	0	0
57	BQ	5	Total 5	Mg 5	0	0
57	CX	2	Total 2	Mg 2	0	0
57	DV	2	Total 2	Mg 2	0	0
57	AM	1	Total 1	Mg 1	0	0
57	BU	8	Total 8	Mg 8	0	0
57	DR	2	Total 2	Mg 2	0	0
57	AD	2	Total 2	Mg 2	0	0
57	BN	6	Total 6	Mg 6	0	0
57	CT	1	Total 1	Mg 1	0	0
57	BG	2	Total 2	Mg 2	0	0
57	BY	1	Total 1	Mg 1	0	0
57	DE	4	Total 4	Mg 4	0	0
57	B3	2	Total 2	Mg 2	0	0
57	CJ	1	Total 1	Mg 1	0	0
57	BR	3	Total 3	Mg 3	0	0
57	DA	629	Total 629	Mg 629	0	0
57	DP	2	Total 2	Mg 2	0	0
57	DW	2	Total 2	Mg 2	0	0
57	B7	3	Total 3	Mg 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CF	1	Total 1	Mg 1	0	0
57	BV	4	Total 4	Mg 4	0	0
57	DO	1	Total 1	Mg 1	0	0
57	BO	1	Total 1	Mg 1	0	0
57	BZ	1	Total 1	Mg 1	0	0
57	DY	1	Total 1	Mg 1	0	0
57	CW	1	Total 1	Mg 1	0	0
57	D5	1	Total 1	Mg 1	0	0
57	BD	11	Total 11	Mg 11	0	0
57	B0	4	Total 4	Mg 4	0	0
57	CE	1	Total 1	Mg 1	0	0
57	BW	5	Total 5	Mg 5	0	0
57	DD	7	Total 7	Mg 7	0	0
57	CK	1	Total 1	Mg 1	0	0
57	AF	1	Total 1	Mg 1	0	0
57	DB	10	Total 10	Mg 10	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D9	1	Total 1	Zn 1	0	0
59	B6	1	Total 1	Zn 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AX	1	Total 1	K 1	0	0
60	CX	1	Total 1	K 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	170	Total 170	O 170	0	0
61	AL	2	Total 2	O 2	0	0
61	AO	1	Total 1	O 1	0	0
61	AU	1	Total 1	O 1	0	0
61	AV	2	Total 2	O 2	0	0
61	AW	3	Total 3	O 3	0	0
61	BA	1102	Total 1102	O 1102	0	0
61	BB	36	Total 36	O 36	0	0
61	BD	8	Total 8	O 8	0	0
61	BE	13	Total 13	O 13	0	0
61	BF	4	Total 4	O 4	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	BS	1	Total 1	O 1	0	0
61	BT	3	Total 3	O 3	0	0
61	BU	1	Total 1	O 1	0	0
61	BV	4	Total 4	O 4	0	0
61	BW	2	Total 2	O 2	0	0
61	BX	2	Total 2	O 2	0	0
61	B0	4	Total 4	O 4	0	0
61	B1	1	Total 1	O 1	0	0
61	B3	1	Total 1	O 1	0	0
61	B5	5	Total 5	O 5	0	0
61	B7	1	Total 1	O 1	0	0
61	B8	7	Total 7	O 7	0	0
61	CA	130	Total 130	O 130	0	0
61	CE	1	Total 1	O 1	0	0
61	CJ	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	CV	1	Total 1	O 1	0	0

Continued on next page...

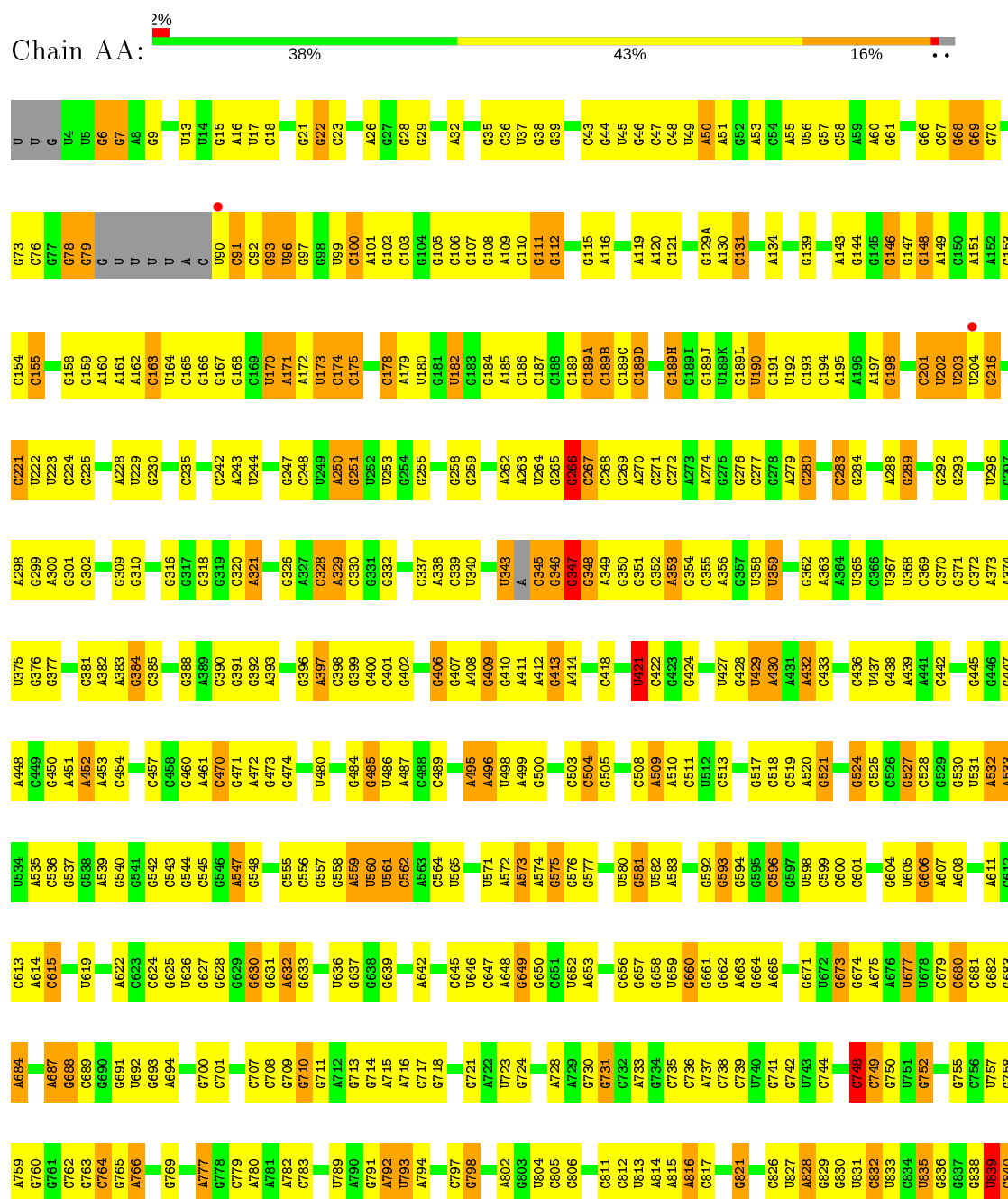
Continued from previous page...

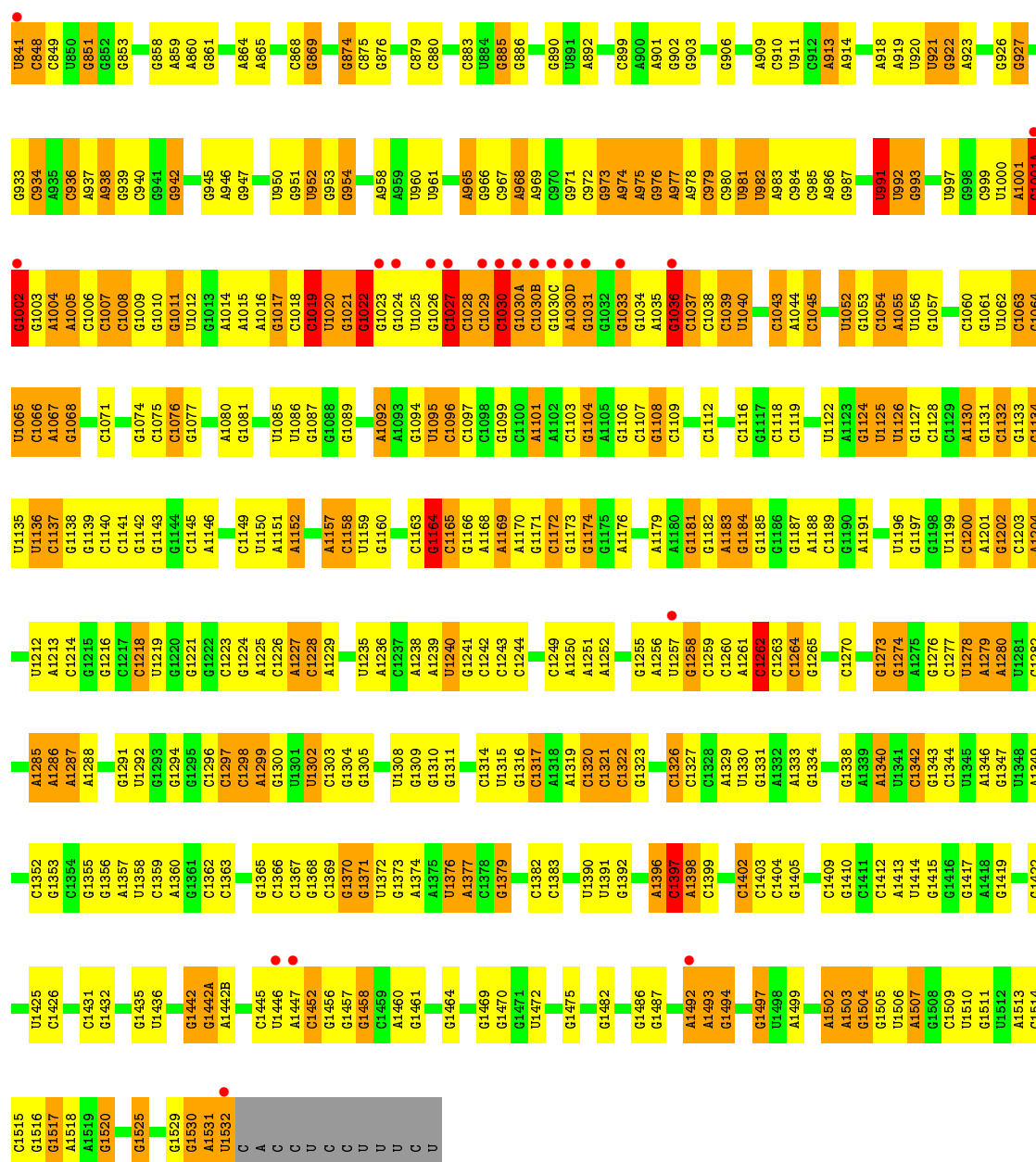
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CW	1	Total	O	0	0
			1	1		
61	CX	1	Total	O	0	0
			1	1		
61	DA	767	Total	O	0	0
			767	767		
61	DB	9	Total	O	0	0
			9	9		
61	DD	9	Total	O	0	0
			9	9		
61	DE	5	Total	O	0	0
			5	5		
61	DF	6	Total	O	0	0
			6	6		
61	DN	2	Total	O	0	0
			2	2		
61	DP	12	Total	O	0	0
			12	12		
61	DR	2	Total	O	0	0
			2	2		
61	DT	1	Total	O	0	0
			1	1		
61	DU	2	Total	O	0	0
			2	2		
61	DV	1	Total	O	0	0
			1	1		
61	DX	2	Total	O	0	0
			2	2		
61	DY	1	Total	O	0	0
			1	1		
61	D0	5	Total	O	0	0
			5	5		
61	D1	1	Total	O	0	0
			1	1		
61	D3	2	Total	O	0	0
			2	2		
61	D7	1	Total	O	0	0
			1	1		
61	D8	4	Total	O	0	0
			4	4		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

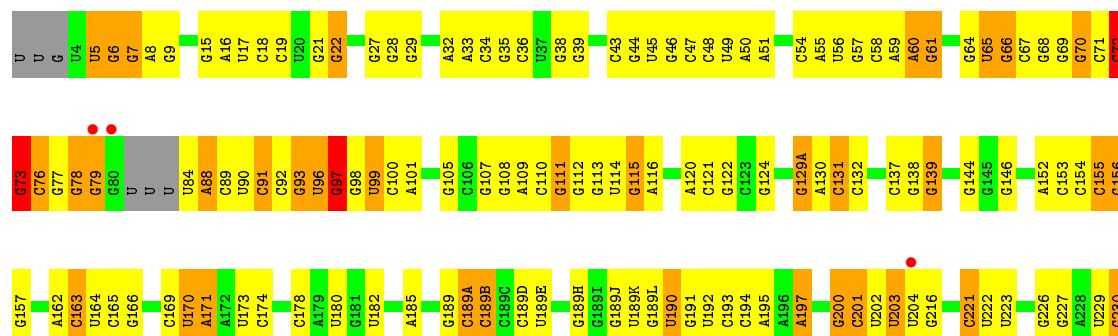
• Molecule 1: 16S Ribosomal RNA



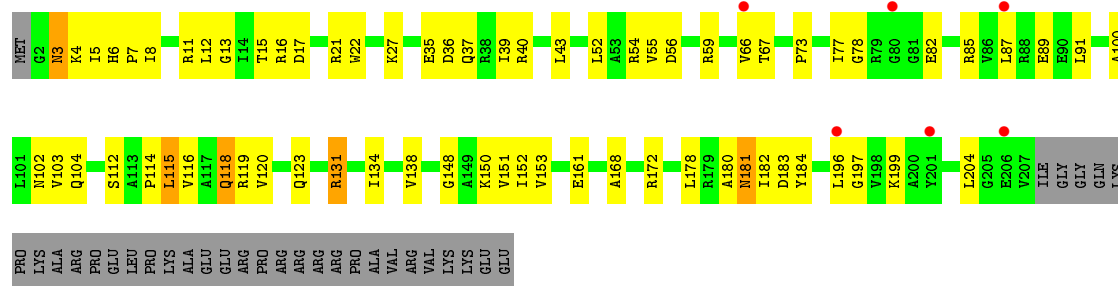


• Molecule 1: 16S Ribosomal RNA

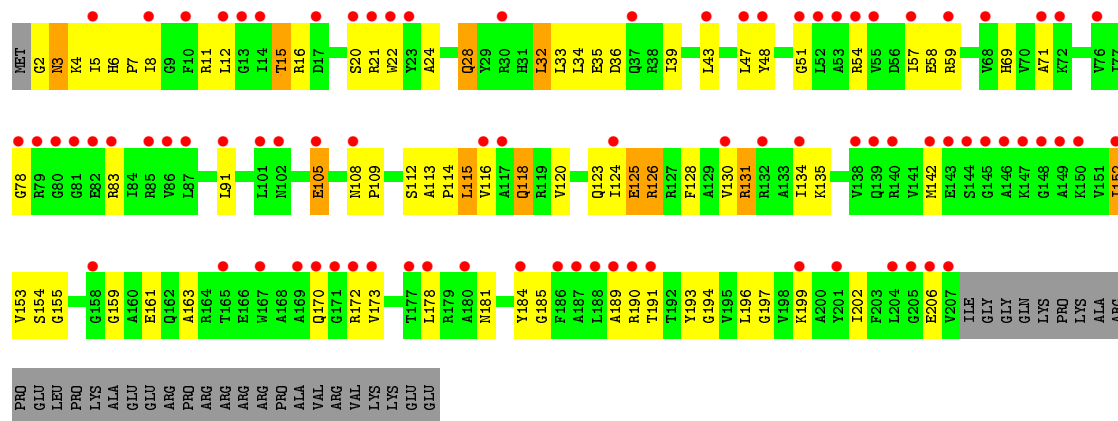
Chain CA: 29% 33% 47% 17%



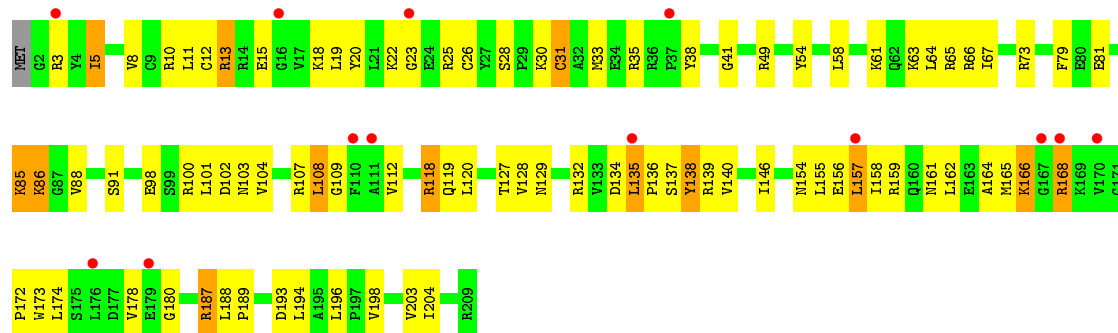
C1226	G1160	C1100	G979	G839	U751	C615	G544	U887	A315	C235
A1227	G1161	A1101	C980	G830	G752	G616	C545	A461	G316	
C1228	C1162	A1102	U981	U831	A753	G617	G546	C390	G317	A243
A1229	C1163	C1103	U982	C832	G754	C618	A547	G391	G318	U244
G1230	G1165	A1104	A983	U833	G755	U619	G548	G392	G319	
G1231	G1166	C1105	C984	C834	G756	C620	G549	A393	C320	
	A1106	U985	C985	U835	U757	C621	G550		A821	G247
U1235	C1107	A986	A986	G836	G758	A622	U551	A397	C248	
A1236	C1108	U987	U987	G837	A759	C623	U552	C398	U249	
C1237	C1109	G988	C988	U838	G760	G624		G399	A250	
A1238	A1110	C989	A919	U839	G761	C625		C400	G251	
U1239	A1111	C990	U920	C840	G762	U626	G485	C401		
U1240	G1174	U991	U921	U841	G763	G627	U486		C328	
	C1112	U992	G922	C846	C764	G628	A487		A329	
C1243	A1176	A923	A923	C849	G765	G629	U561	U405		
C1244	G1177	U994	U994	U850	A766	G630	U562	G406	G332	
A1245	C1114	C995	C995	U851	G767	G631		G407	G333	
	G1116	A996	A996	G852	A768	C701	G485	A408	C334	
C1249	C1117	U997	U997	G853	G769	A702	U494	G409	G335	A262
A1250	A1118	U998	G998	C857	G775		A495	G410	C336	A263
A1251	G1181	C999	C999	U857	G776	G634	U496	A411	C337	
A1252	A1182	U1000	A935	G858	G777	C635	U498	A412	A338	
	G1184	A1001	C936	A859	A777	U636	A499	G413	C339	G265
	G1185	C1059	U1001	A860	G778	A572	G500	U340	G266	
G1255	G1186	C1060	A937	U860	G779	G638	C501	C417	C341	
A1256	G1187	G1061	A938	G861	C779	G639	G502	C418	C267	
U1257	C1062	U1062	G939	A864	A780		C503	U419	C268	
C1258	C1063	C1063	C942	A865	G786	A642	C504	G420	U343	
G1259	A1005	A1005	G942	A866	G787		G505	U421	C344	A274
A1260	C1064	C1006	U943	C866	A715	C645	U422	G347	G346	
C1261	U1065	C1007	G944	G867	A716	U646	C508	U423	G347	
C1262	C1066	C1008	U945	C868	G717	C647	A509	G424	G348	
C1263	A1067	C1009	A946	C869	G718	U582	A510		A349	
U1264	G1068	G947	U947	U870	G719	A583	C511	U427	A279	
G1265	C1072	C948	C948	U871	G720	G584	U512	G351	C280	
G1266	G1073	U949	U949	A872	A794	A653	C513	U428	C352	
	C1074	U950	U950	A873	A722		G514	U429	G353	
A1269	G1075	G951	G951	G874	U723	C656	G515	A430	A354	
C1270	C1076	U952	U952		G724	G657	U516	A431	C355	
G1271	G1077	G953	G953	C877	G798	G592	G517	A432	A356	
A1272	U1078	G954	G954	U878	G800	G593	C518	C433	A288	
U1273	C1079	C1018	C1018	C879	U801	G660	C519	U434	G289	
G1274	A1080	C1019	A958	C880	A802	C596	A520	U435	U359	
A1275	G1081	U1020	A959	G881	G803	G662	G521	C436	G293	
C1276	C1082	G1021	U960	G885	U804	A663	C522	U437		
C1277	U1084	G1022	U961	G886	C805	G664	A523	G438	U296	
	C1085	G1023	A965	G887	C806	A665	G524	A439	G297	
U1278	U1086	G1024	G966	G888	G811	G666	C601	A441	A298	
A1279	C1087	U1025	C967	G889	C812	G667	A602	C442	U367	
C1281	G1088	G1026	A968	G890	U813	G671	G603	C443	G301	
U1281	U1089	C1027	A969	U891	A814	U672	G604	C444	G302	
C1282	C1090	C1028	A969	A892	A815	G673	U605	G445	A373	
G1283	U1091	U1029	C970	C893	G816	G674	G606	G446	U374	
A1284	A1092	C1030	G971	G894	A816	A532	C607	G447	U375	
C1285	C1093	G1030A	C972	C895	C817	A608	A533	A448	G306	
A1286	G1094	C1030B	G973	C899	G821	U677	A609		C307	
U1287	U1095	A1030C	A974	A900		G678	G610	A452	G377	
A1288	C1096	A1030D	A975	A901	G747	C679	A611		A382	
C1289	C1097	G1031	G976	A902	C748	C680	G540	C456	A383	
G1290	U1098	G1032	A977	G902	C749		G541		G384	
U1291	G1099	G1033	A978	G903	A828	G683	A614	C458	C314	



• Molecule 3: 30S ribosomal protein S3

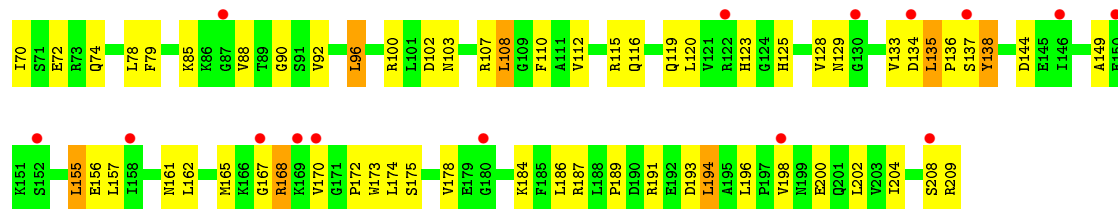


• Molecule 4: 30S ribosomal protein S4

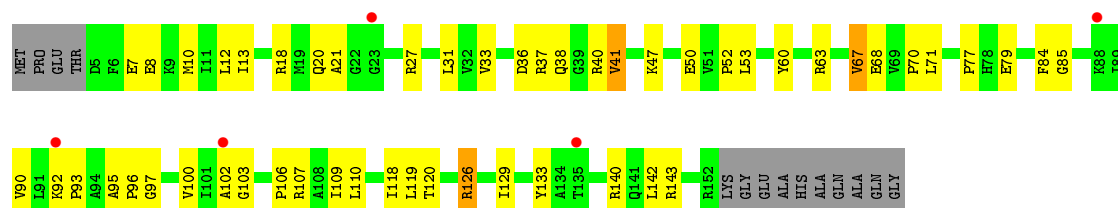


• Molecule 4: 30S ribosomal protein S4

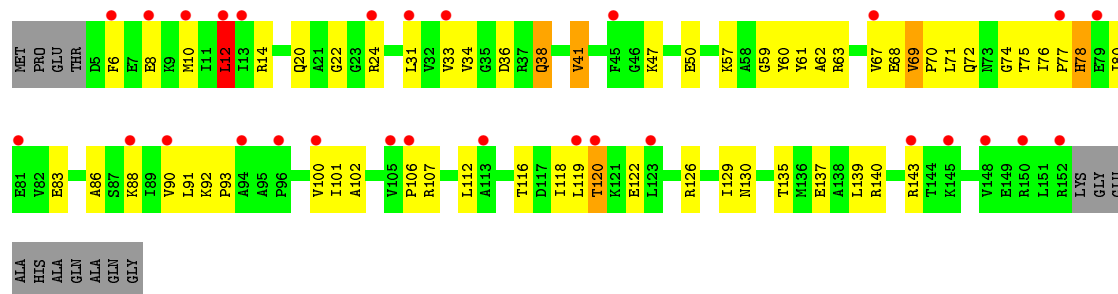




• Molecule 5: 30S ribosomal protein S5



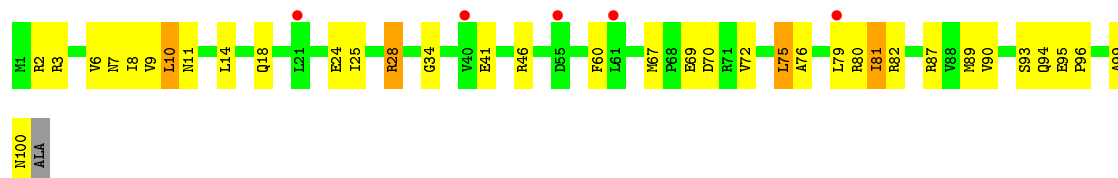
• Molecule 5: 30S ribosomal protein S5



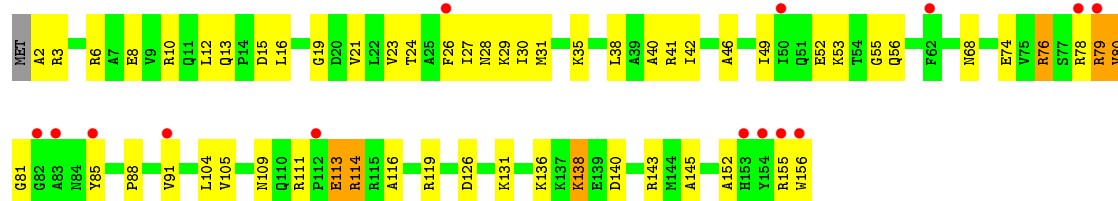
• Molecule 6: 30S ribosomal protein S6



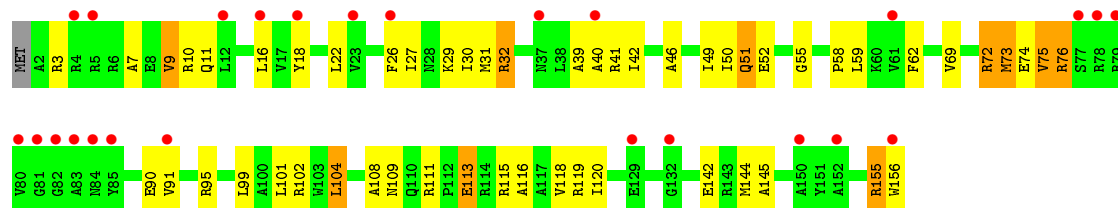
• Molecule 6: 30S ribosomal protein S6



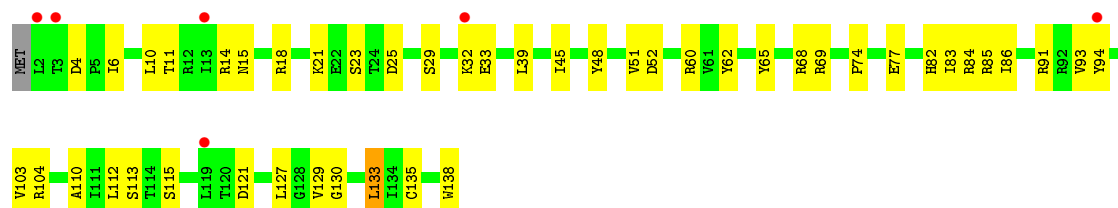
• Molecule 7: 30S ribosomal protein S7



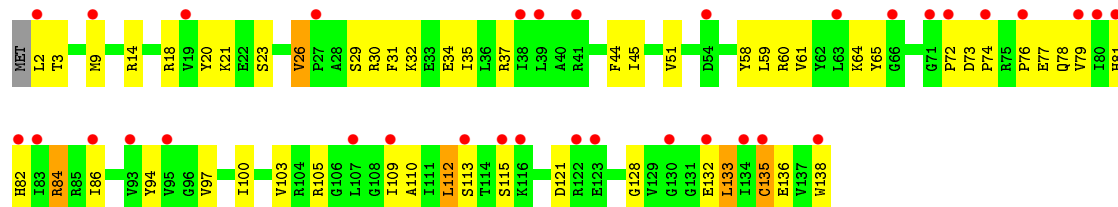
• Molecule 7: 30S ribosomal protein S7



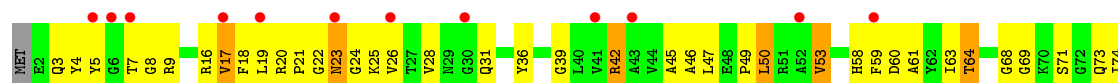
• Molecule 8: 30S ribosomal protein S8

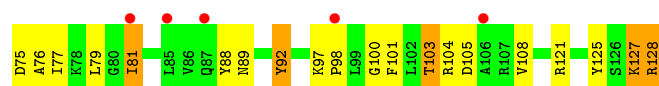


• Molecule 8: 30S ribosomal protein S8

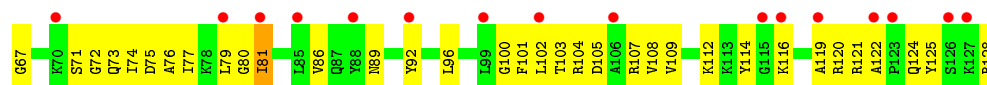
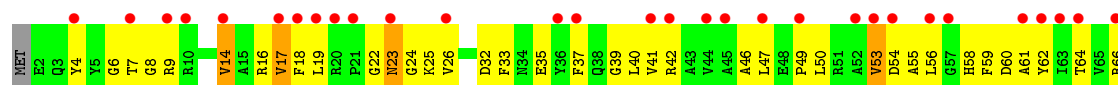
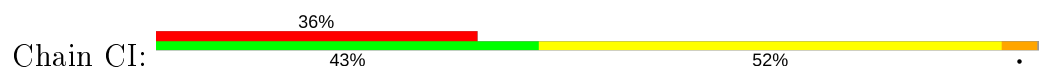


• Molecule 9: 30S ribosomal protein S9

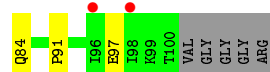




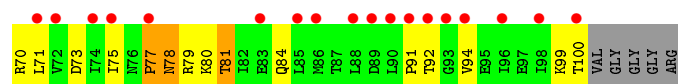
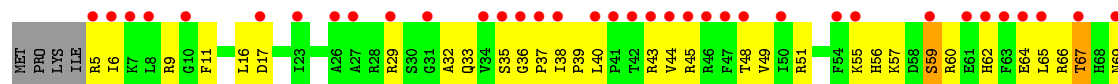
• Molecule 9: 30S ribosomal protein S9



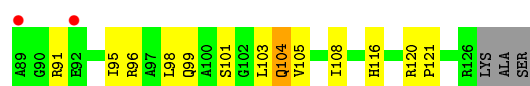
• Molecule 10: 30S ribosomal protein S10



• Molecule 10: 30S ribosomal protein S10

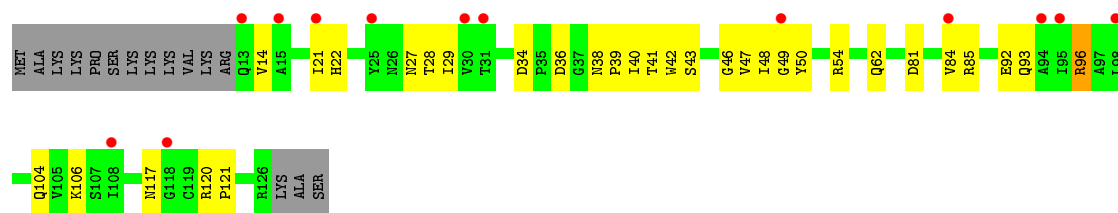


• Molecule 11: 30S ribosomal protein S11

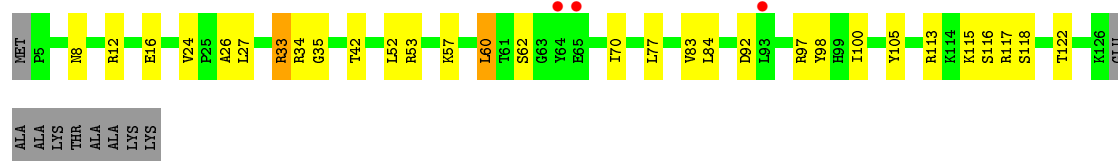
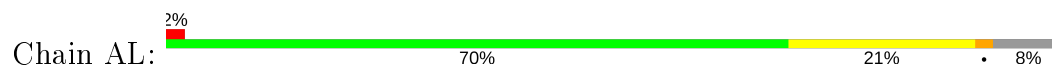


• Molecule 11: 30S ribosomal protein S11

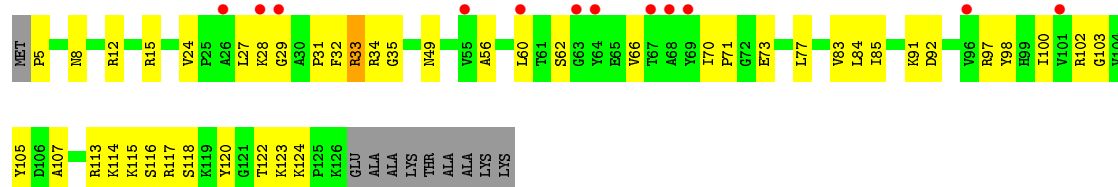




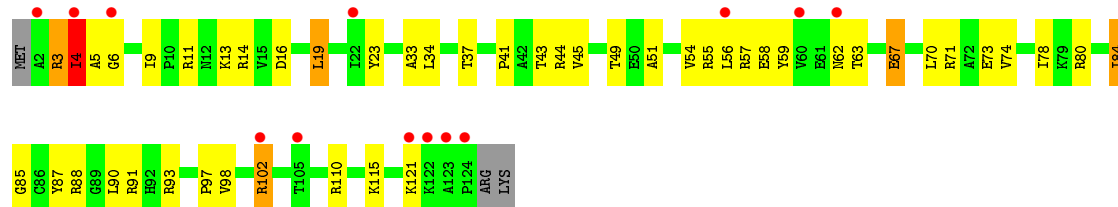
• Molecule 12: 30S ribosomal protein S12



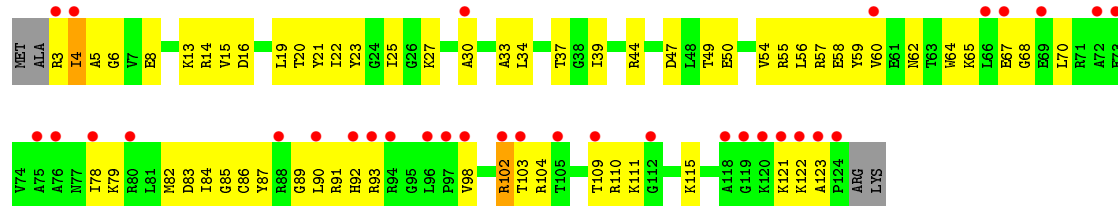
• Molecule 12: 30S ribosomal protein S12



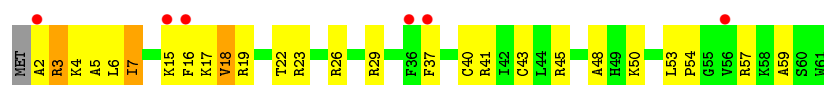
• Molecule 13: 30S ribosomal protein S13



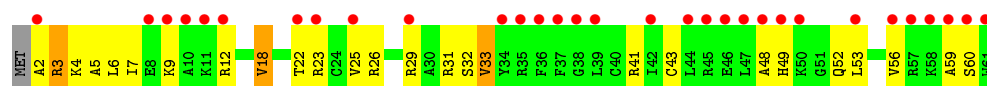
• Molecule 13: 30S ribosomal protein S13



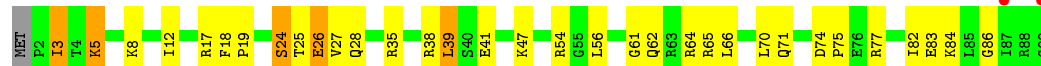
• Molecule 14: 30S ribosomal protein S14 type Z



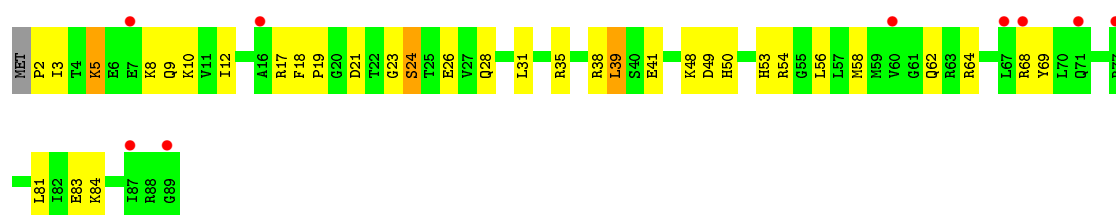
- Molecule 14: 30S ribosomal protein S14 type Z



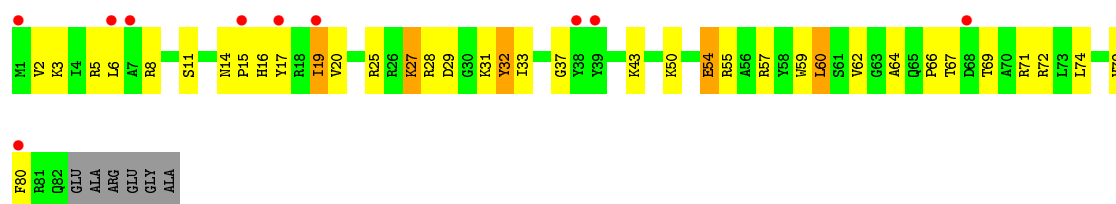
- Molecule 15: 30S ribosomal protein S15



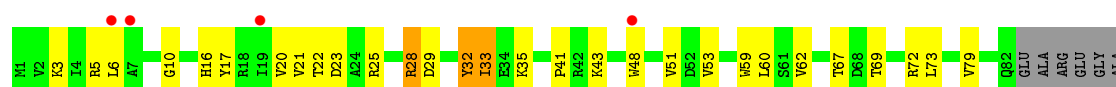
- Molecule 15: 30S ribosomal protein S15



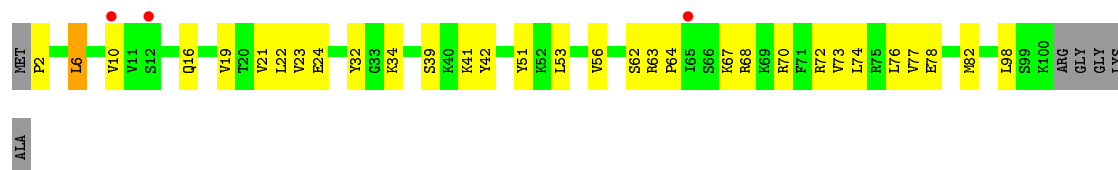
- Molecule 16: 30S ribosomal protein S16



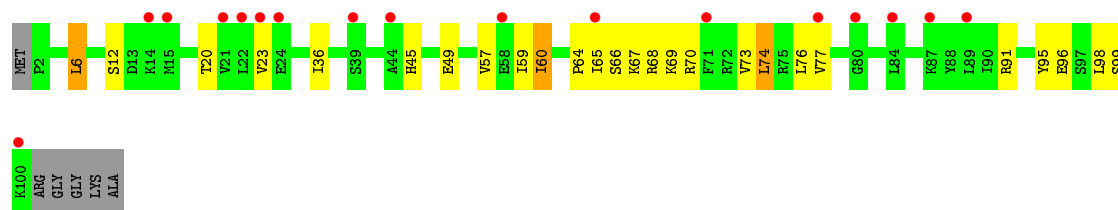
- Molecule 16: 30S ribosomal protein S16



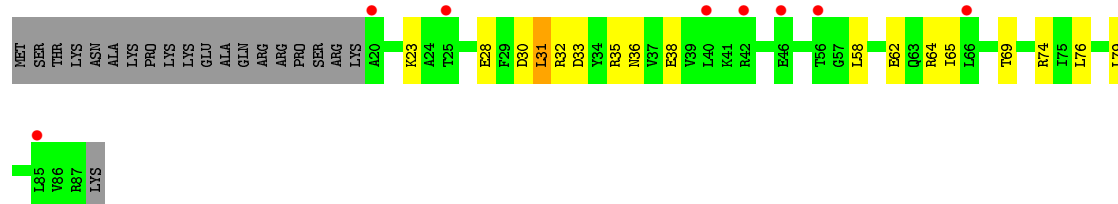
- Molecule 17: 30S ribosomal protein S17



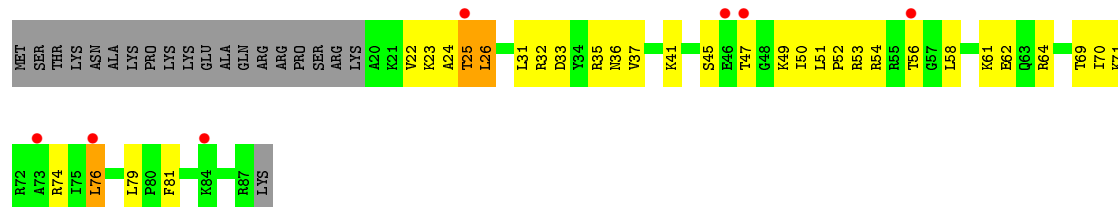
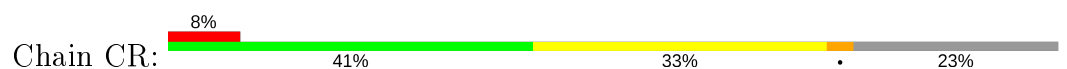
- Molecule 17: 30S ribosomal protein S17



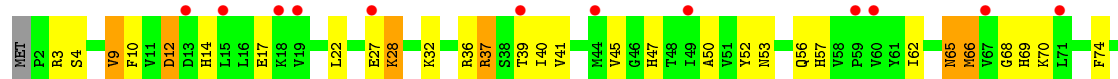
- Molecule 18: 30S ribosomal protein S18

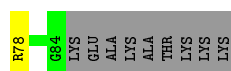


- Molecule 18: 30S ribosomal protein S18

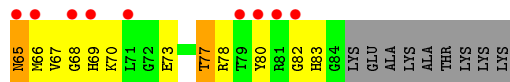
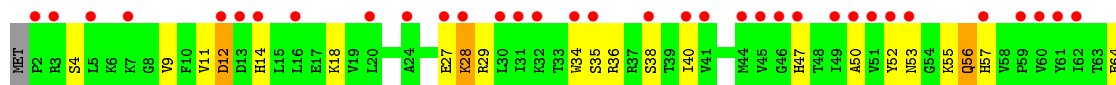


- Molecule 19: 30S ribosomal protein S19

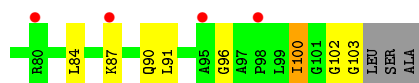
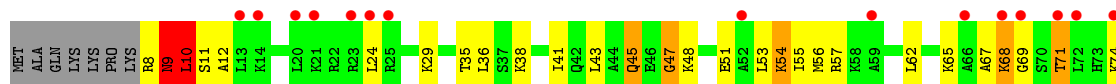




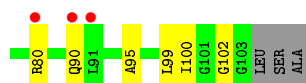
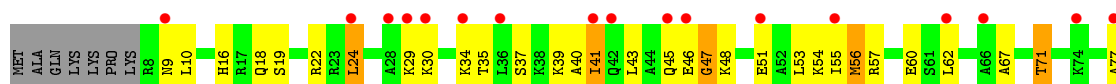
- Molecule 19: 30S ribosomal protein S19



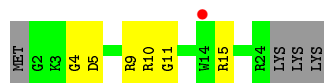
- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



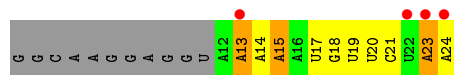
- Molecule 21: 30S ribosomal protein Thx



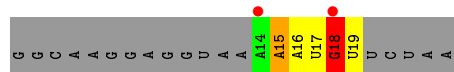
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: mRNA



- Molecule 22: mRNA



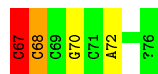
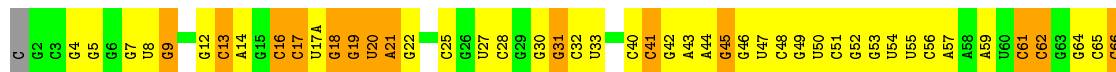
- Molecule 23: Cytidine-Puromycin



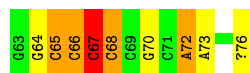
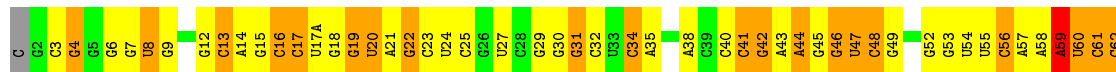
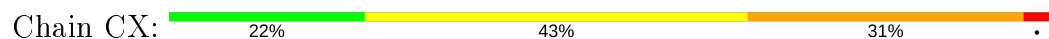
- Molecule 23: Cytidine-Puromycin



- Molecule 24: P-site tRNA

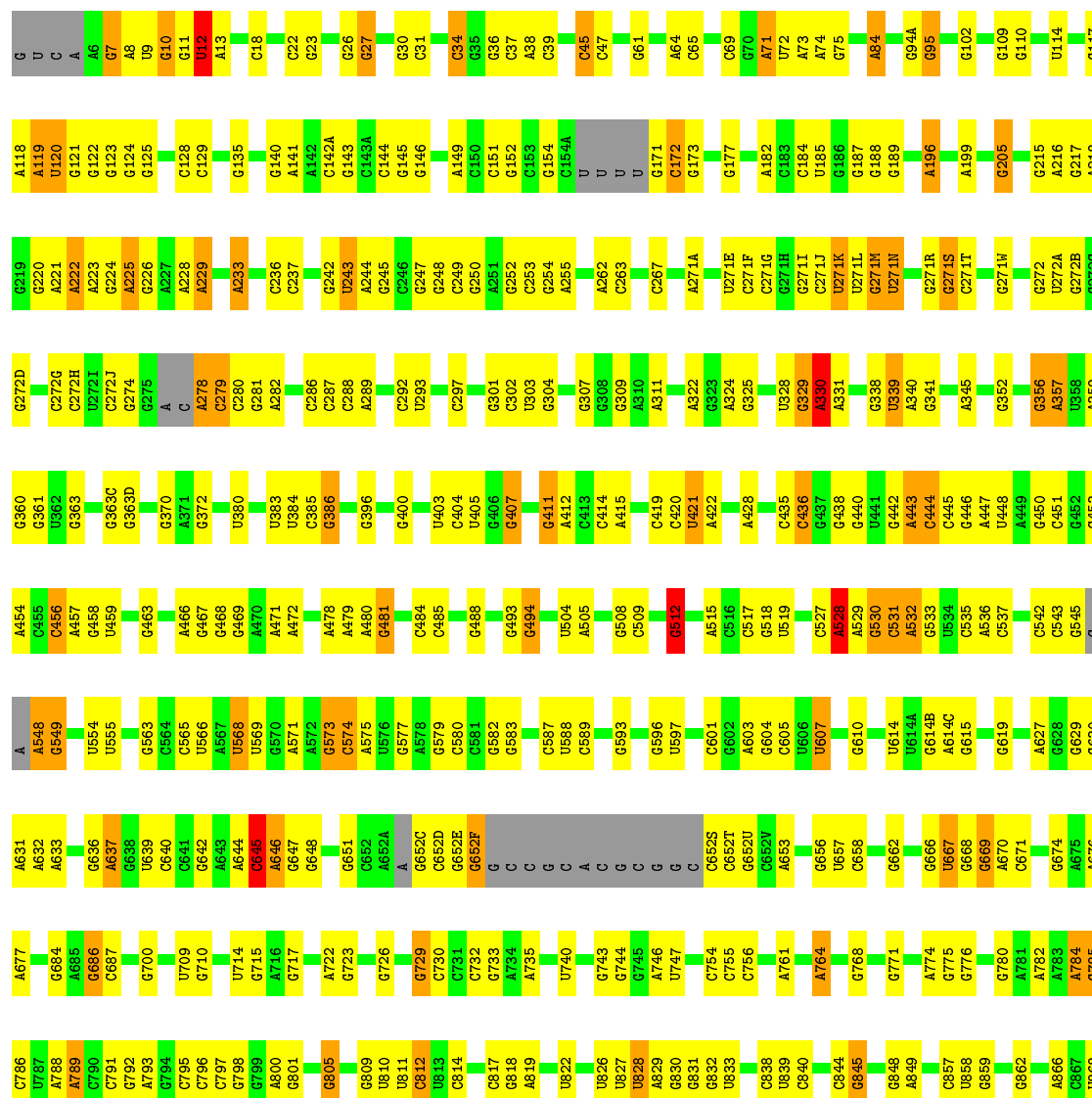
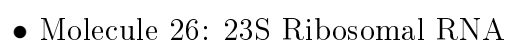
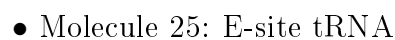


- Molecule 24: P-site tRNA

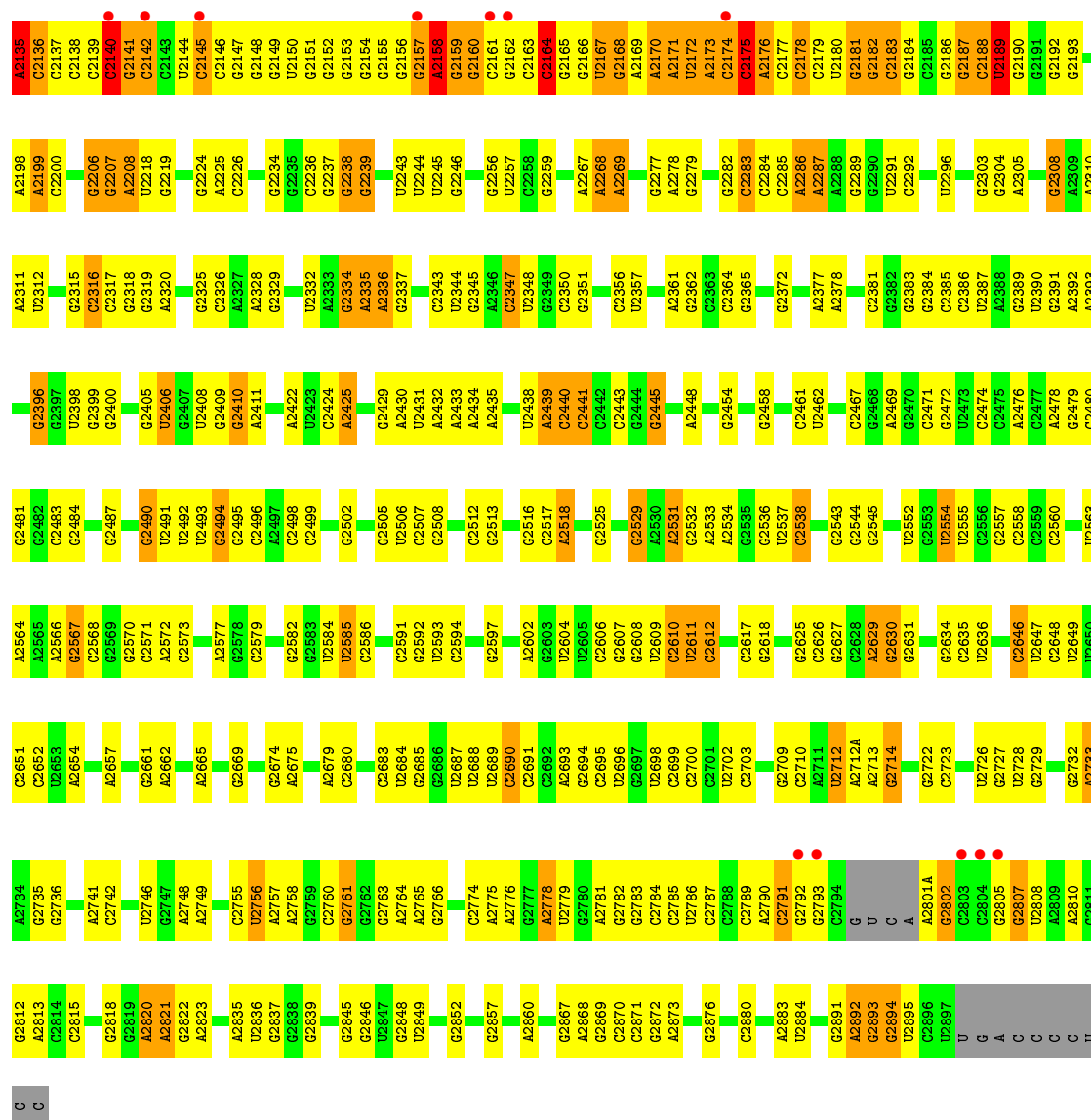


- Molecule 25: E-site tRNA

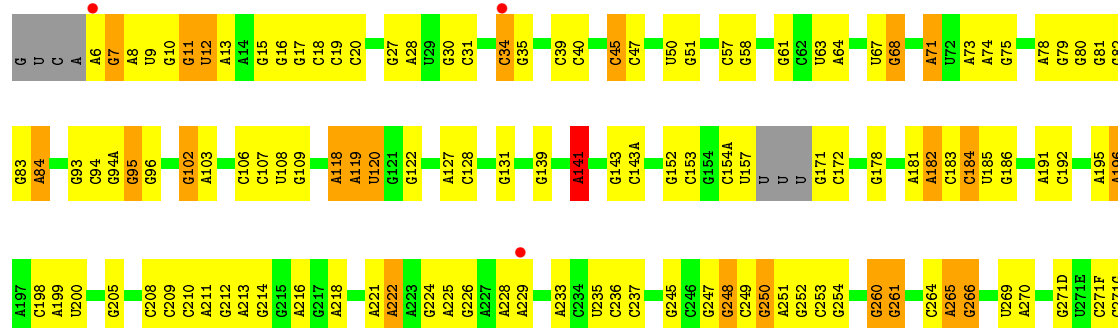
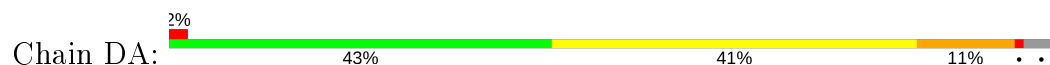




G2056	G1967	U1864	G1555	G1477	U1300	A1111	C961	G869
G2060	G1968	G1865	C1596	G1478	A1301	G1112	G962	A870
G2061	A1969	A1877	C1557	U1394	A1302	G1113	U963	U871
A2062	G1878	G1878	A1558	G1482	G1303	G1114	U969	G874
G2065	G1883	G1782	A1566	U1489	A1308	G1120	C970	G875
C2066	A1783	U1673	A1567	A1490	G1309	C1121	A	C876
G2069	A1784	G1674	G1568	G1491	G1310	G1122	A	
G2069	A1785	C1675	A1569	G1492	G1311	C1123	G	G879
G1983	A1786	A1570	U1405	U1406	U1312	G1209	U	G880
G1985	A1787	A1494	C1407	C1407	U1313	G1209	U	G880
A1986	G1788	A1495	C1408	C1408	U1314	G1125	U	G881
U2074	A1789	G1682	U1578	A1496	C1315	A1126	G	
U2075	C1790	U1688	A1579	A1412	U1316	A1127	G	C884
G2080	A1791	A1689	A1580	G1413	U1317	A1128	C	C885
U2086	G1792	A1690	G1581	G1414	C1318	A1129	U	C886
G2087	C1907	C1691	C1582	U1415	A1319	U1130	U	A887
G2093	C1908	U1692	A1583	U1416	G1320	G1131	A	C888
G2094	A1912	U1693	C1584	C1417	A1321	C1135	A	C889
C2095	A1913	C1694	A1586	G1418	G1324	G1136	A	A890
G2096	C1914	C1695	A1587	A1419	U1329	U1141	A	C892
G2097	U1915	G1696	C1588	U1420	G1328	G1139	G	U895
A2001	G1799	G1697	C1589	G1421	G1421	G1231	C	A896
G2002	C1800	A1698	A1509B	G1422	U1329	G1232	A	C897
U2099	G1801	G1699	G1510	G1423	C1333	U1142	C	C898
G2100	A1802	A1700	G1511	G1424	U1334	A1142A	C	
G2101	C1804	G1701	C1512	G1425	U1335	A1143	A	C904
C2103	U1805	G1703	C1513	A1427	G1338	G1144	U	U905
A2013	A1812	U1709	U1518	U1428	U1341	C1145	C	G906
A2014	G1813	C1710	G1519	G1429	A1342	U1146	U	U907
A2015	G1814	A1610	G1525	U1430	U1342	C1147	U	A910
A2019	A1815	A1614	G1526	U1431	A1343	G1148	U	A911
G2110	G1816	A1614	G1527	C1432	U1352	C1153	A	C914
C2111	G1817	A1632	A1528	A1434	A1353	G1154	A	
G2112	U1720	A1632	A1528A	C1437	G1355	A1155	G	A918
U2113	G1721	C1636	G1529	U1437	U1356	U1165	A	G919
A2114	A1722	A1637	C1530	A1445	U1357	C1166	G	G931
G2115	U1739	C1638	C1531	C1445A	G1358	U1167	U	G932
G2116	A1741	U1639	C1532	C1446	A1359	A1027	C	A933
A2117	G1746	A1641	U	G1447	U1364	G1169	G	
U2118	G1747	G1642	C	U1448	A1365	U1170	U	A941
A2119	G1747A	G1643	G1537	A1449	U1366	G1171	A	
G2120	A1749	C1644	G1538	G1450	A1365	U1033	A	G944
G2123	G1756	G1647	U1540	U1453	G1369	G1034	U	A945
G2124	U1757	C1648	G1541	U1459	C1270	U1035	A	G946
G2125	A1842	G1649	A1542	A1460	G1370	G1036	G	G947
G2126	A1847	A1762	C1653	A1544	G1371	G1176	A	G948
C2127	A1853	G1763	A1654	U1545	U1372	C1177	C	
C2128	A1854	G1764	C1546	C1547	C1376	C1178	U	
C2129	C1957	A1854	C1547	C1547	G1379	A1182	C	G952
A2042	C1958	G1769	C1551	C1551	A1380	G1183	C	A953
C2043	U1963	A1773	A1664	A1554	G1386	G1184	C	G954
A2051	G1964	A1773	A1664	A1554	U1188	C1185	U	G955
C2055			A1665			G1186	G	A956
						G1187	A	A957
						G1188	C	U958
						G1189	C	A959
						G1190	C	A960

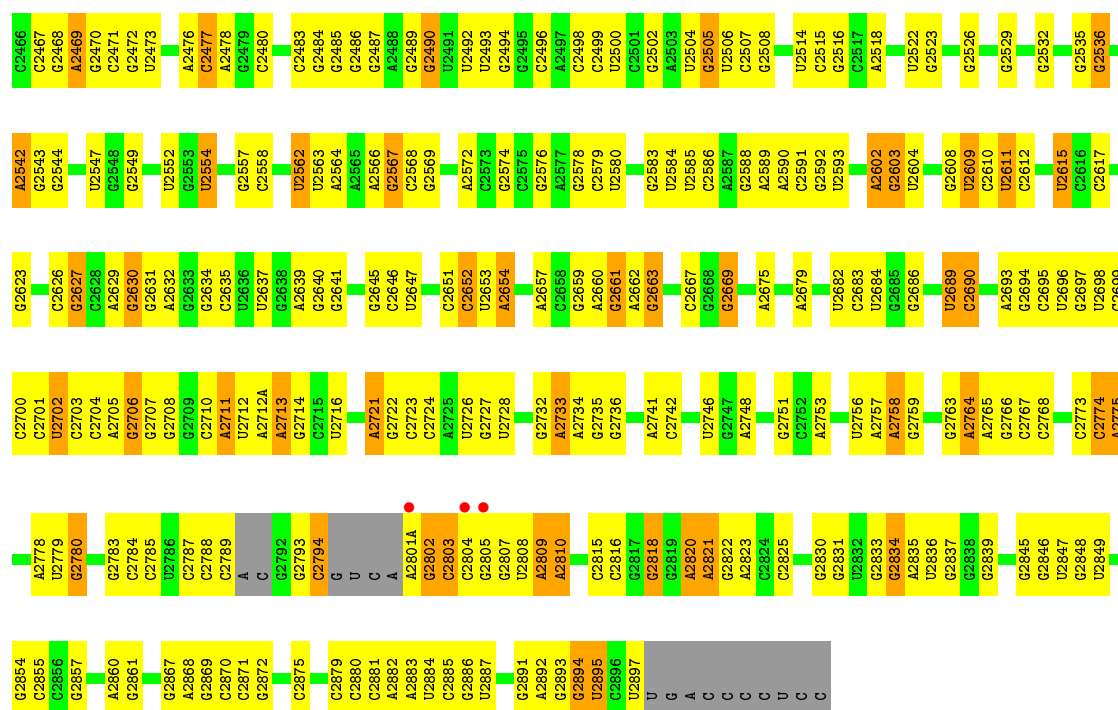


• Molecule 26: 23S Ribosomal RNA



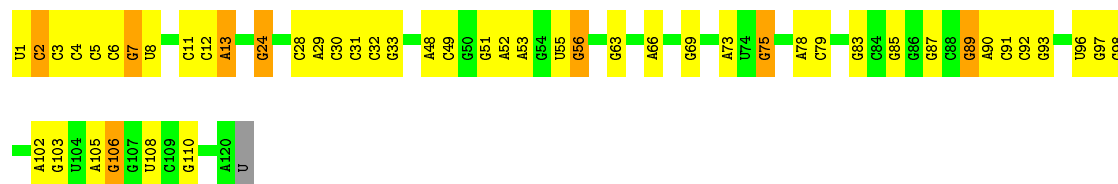
G1235	U1159	A	U1026	A957	G878	A802	G717	A652B	A586	G508	A422	U339	G271H
G1236	G1160	G	A1027	G958	G879	G905	A718	G652C	C587	C509	A423	A340	G271I
G1239	G1163	U	A1028	A960	G881	G809	C720	G652D	U588	G512	A428	G341	G271J
A1241	G1164	C	G1031	C961	G883	C912	U724	G	G593	A514	C433	A345	U271K
A1242	U1165	G	A1032	G966	G884	C915	G725	G	U594	A515	C433	A346	G271L
G1243	C1166	U	U1033	C967	C885	C916	G726	C	C595	G516	G442	A347	U271M
G1244	G1167	A	G1034	G968	C886	C917	C729	C	G598	C517	A443	G348	U271N
G1248	U1169	U	U1035	U969	C887	C918	C730	A	G599	U519	G445	C271P	G271Q
U1249	G1170	A	G1036	C971	C888	G818	C731	C	G600	G522	G446	G352	G271R
G1250	G1171	G	U1037	G972	A890	A819	G734	C	C601	C523	G447	G355	G271S
G1250	G1171	C	G1038	A973	G892	A820	A734	C	G602	G523	U448	G356	G271T
A1253	A	U	G1042	G974	C893	A821	A735	G	A603	A528	G452	A357	U272A
G1256	U	C	A1043	C975	C894	U822	A735	G	G604	G529	G452	U358	U272B
G1256	A	C	G	G975A	U895	G823	U740	C	C605	G530	A454	G360	C272G
U1263	C1178	U	A	G979	C897	A824	G741	C	U607	C531	C455	G361	
G1264	C1179	U	A	A980	C898	U827	A746	G652T	A608	A532	C456	G363	G274
A1265	C1180	G	G	A980	A899	U828	U747	G652V	A609	G533	A457	G363A	G275
G1265	A1182	U	A	A983	A900	A829	G759	A653	G610	U534	G458	G363B	A276
G1269	G1183	C	C	A983	A901	G830	A752	A654	G610	C535	U459	G363C	C277
G1270	G1184	A	G	G987	C904	G832	C754	G656	G614B	A536	A460	G363D	A278
G1271	C1185	G	C	A990	G916	U833	C755	U657	A614C	C537	A466	U363E	C279
A1272	G1186	U	C	C991	A910	U839	G765	C658	G615	G538	G467	A363F	C280
U1273	U1187	A	A	C992	A911	U839	G771	G659	G616	C540	G468	C366	C285
A1276	G1188	U	G	G993	C912	C940	A773	G669	G618	G545	G469	A371	G286
G1277	A1189	G	A	C994	C912	G760	A774	A670	G619	C	A470	G372	C287
G1278	G1190	U	G	C995	C915	A761	G775	A676	G620	A	A471		
G1279	G1191	C	G	A996	G916	C946	G776	A677	G623	A	A472	C375	C292
G1280	G1192	U	U	G997	A917	U847	G765	A678	C624	G549	G473	C376	G298
A1287	C1201	U	U	C997	A918	G848	G771	U667	G625	G549	G474	C376	G299
U1288	G1202	U	G	A1000	G919	U851	G772	U668	U626	G549	U475	A300	A300
A1204	G1203	C	C	A1001	G920	G852	U773	G669	A627	G556	G476	U383	G301
U1295	A1204	G	G	G1002	G921	G853	A774	A670	G628	U557	A477	U384	G301
G1293	U1205	U	U	G1003	U922	G854	G775	A670	G629	G558	A478	C302	C302
G1296	G1206	U	U	C1004	C923	G855	G776	A676	G630	G563	A479	G386	G307
C1297	C1207	A	A	C1005	C924	C956	G780	A677	A631	C564	A480	U387	G308
U1300	A1210	G	G	C1006	C925	C957	A781	C978	A632	C565	A482	G391	A310
A1301	U1211	U	A	C1007	A926	U858	A782	C683	A633	U566	A483	G391	A310
A1302	G1212	C	C	C1008	G927	G859	A783	C683	C634	A567		G396	A311
G1303	A1220	U	C	A1009	G928	U860	A784	G686	G635	U568	C487	G317	G317
G1304	C1221	A	G	G1011	G932	A861	G785	G686	G636	U569	U403	C404	
G1304	C1221A	G	A	U1012	G933	A863	C786	G695	G638	G570	C404	U405	A320
A1308	G1222	C	C	C1013	G934	G864	U787	G698	U639	A571	G493	G406	G321
G1308	G1223	A	A	U1014	G938	C965	A788	C698	C640	A572	G494	G407	A322
U1313	C1224	U	U	G1015	G939	A866	A789	C698	G640	G573	G495	G408	G323
G1314	G1227	C	C	G1016	G940	G869	C790	G701	A644	C574	G496	A502	A324
G1315	U1018	U	U	G1017	A941	A870	C791	C708	G645	A575	U499	G411	G327
U1316	U1019	U	C	C1018	A945	U871	G792	U709	A646	U576	A503	A412	U328
A1317	A1020	U	U	U1019	G946	A872	C796	G710	G648	U577	A504	C413	G329
G1320	C1231	A	A	G1021	G947	G873	C797	G711	G649	A578	A504	C414	A330
A1321	G1232	U	U	G1022	A953	G874	G798	G712	C850	C581	U504	A415	A330
G1322	U1023	A	A	U1023	G956	G875	G799	G715	G851	G582	A505	C416	C336
U1234	U1025	G	G	G1025	G956	C976	A800	A716	G852	G583	A507	U421	

U2390	G2318	U2243	G2166	G2024	G1930	G1839	A1652	A1571	G1493	C1411	U1323
C2394	G2319	U2244	U2167	U2022	U1931	G1840	G1653	A1578	A1494	A1412	G1324
C2395	A2320	U2245	G2168	G2023	A1932	U1841	A1654	A1579	A1495		C1327
G2396	G2321	G2246	A2169	G2024	G1933	G1842		G1577	A1496	G1416	
G2397	A2247	G2247	A2170	C2025	G1934	A1847	G1660	G1580	U1497	G1417	
U2398	C2248	C2248	A2171	A2030	G1935	A1848	G1661	G1581	G1498	G1418	C1333
G2399	U2249	U2249	U2172	A2031	A1936	G1849	A1665	G1582	G1499	A1419	G1334
G2400	G2250	G2250	A2173	G2032	A1937	G1850	A1666	C1583	G1500	U1420	U1335
U2401	G2253	G2253	C2174	A2033	A1938	U1851	C1670	C1584		G1421	
C2402	G2254	G2254	C2175	U2034	U1940	U1852	C1671	C1585	U1503	U1341	U1342
	G2255	G2255	A2176	U2035	U1941	U1853	C1672	C1586	G1505	G1422	
G2405	G2259	G2259	C2177	G2036	U1951	A1853	C1673	C1587	G1506	G1423	
U2406	U2262	U2262	C2178	C2037	U1952	G1857	A1674	C1588	C1506	G1424	C1351
G2407	C2263	C2263	C2179	U2038	A1953	G1858	A1675	C1589	A1507	G1425	U1352
U2408	C2264	C2264	U2180	C2040	A1954	A1859	A1676	C1592	A1508	U1426	U1353
G2409	G2265	G2265	G2181	U2041	G1954	G1860	A1677	C1593	A1509	A1427	A1354
C2410	A2268	A2268	G2182	A2042	U1955	G1861	C1684	G1594	G1594	G1428	G1355
	A2269	A2269	C2183	C2043	G1956	U1785	C1685	G1595	A1509A	G1429	G1356
			G2184	G2044	G1957	U1786		G1596	A1509B	C1430	
C2416	G2341	A2273	C2185	A2051	G1959	U1787	U1688	A1597			U1357
C2417	C2342	A2274	G2186	G2052	A1960	U1788	U1689	C1598	U1512	A1434	G1358
A2418	G2343	G2274	G2187	C2055	U1963	A1876	U1693	C1599	C1513	A1360	A1359
U2419	U2344	C2275	C2188	G2056	G1964	A1877	C1694	C1600	U1514	U1437	
G2420	G2345	G2276	U2189	G2057	G1965	G1878	G1695	G1601	G1515	C1438	
G2421	C2347	G2277	G2190	A2060	A1966	G1879	G1696	U1602	G1516	G1439	C1363
A2422	U2348	A2278	G2191	C2061	C1967	C1882	G1697	A1603	G1517	G1440	A1364
	G2349	G2279	G2192	A2062	G1968			A1604			A1365
A2425	C2352	G2282	G2193	G2063	G1969	A1885	U1698	C1607	G1520	A1445	
A2426	G2353	C2283	G2194	C2064	G1970	A1886	U1699	U1700	U1523	C1445A	
G2428	G2354	C2284	A2198	C2065	A1971	A1889	A1701	A1608	G1524	G1446	C1370
C2429	G2357	G2285	C2199	G2066	A1972	A1890	G1702	U1609	G1525	G1447	G1371
A2430	U2357	A2286	C2200	G2069	A1973	A1891	G1703	A1610	G1526	G1448	U1372
A2435	G2358	A2287	U2203	G2070	C1974	C1894	U1709	G1613	A1528A	G1449	A1373
G2436	A2360	A2288	C2205	A2071	A1978	G1895	C1710	A1614	G1529	G1450	G1374
	A2361		G2206	U2074	C1979	G1897	C1711	G1619	C1531	C1450A	C1375
A2439	G2362	C2292	G2207	U2075	G1984	U1898	G1717	G1622	G1532	U1452	G1376
C2440	C2363	C2293	A2208	C2078	G1987	A1900	G1721	G1626	U	G1459	A1377
C2441	G2364	G2294	U2218	U2079	C1988	G1903	A1722	G1631	A1536		G1380
C2442	G2365	U2296	G2219	G2080	C1989	G1906	U1739	A1631	G1537	C1467	G1381
C2443	A2366	C2297	G2220	C2081	U1991	G1907	A1741	A1631A	G1538	C1468	A1384
G2444	G2367	A2298	G2221	A2082	U1992	C1908	G1742	A1632	G1539	A1469	G1385
			G2222	G2083	U1993	C1909	C1743	G1636	U1540	G1470	C1386
G2445	G2370	C2301	G2223	G2086	G1997	G1910	C1744	A1542	G1541	A1471	
G2446	G2371	G2302	G2224	G2087	G1997	U1911	C1745	A1637	A1545	A1472	A1392
A2447	G2372	G2303	A2225	G2088	G2000	A1912	G1745A	G1638	U1546	G1473	A1393
U2449	G2373	G2304	G2226	G2094	A2001	A1913	G1746	U1639	C1547	C1474	U1394
U2450	A2376	A2305	A2227		G2002	G1914		C1640	G1548	G1475	A1395
A2451			G2230		C2097	U1915	G1750	A1641	G1549		U1396
C2452	A2377	G2308	G2231	C2098	G2012	A1918	C1751	G1642	G1482	G1482	
G2453	G2378	A2309	U2232	U2099	A2013	U1919	G1752	G1484	G1485	C1399	
G2454	U2379	A2310	G2233	G2100	A2014	A1919	G1753	G1645	A1557	U1405	
			G2234	G2101	A2015	C1920	C1754	C1646	A1558	U1406	
U2457	G2383	C2312	C2161	U2102	U2016	U1834	A1755	G1657	G1487	G1407	
G2458	G2384	C2313	G2162	U2103	U2017	G1835	U1756	G1648	G1488	G1408	
A2459	C2385	C2314	C2163	G2104	U2017	C1836	U1757	G1649	U1489	C1409	
U2460			C2164	G2105	A2020	C1837			A1569		
	A2388	C2316	G2239			C1838			A1570	G1410	
C2465	G2389	C2317	G2242								



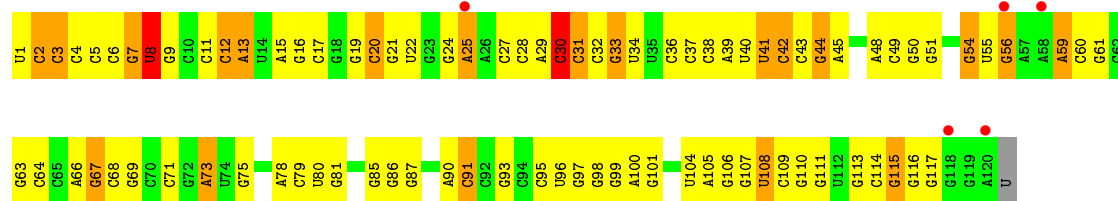
• Molecule 27: 5S Ribosomal RNA

Chain BB: 59% 34% 7%



• Molecule 27: 5S Ribosomal RNA

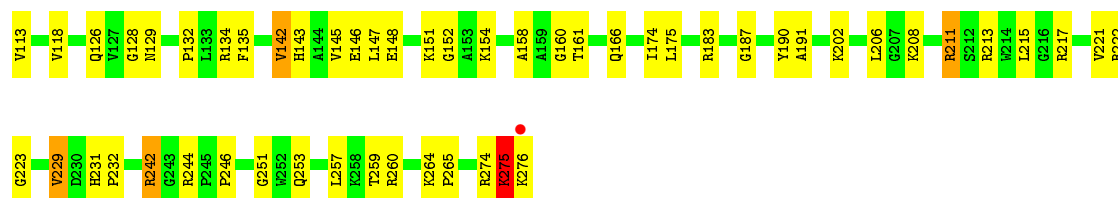
Chain DB: 4% 26% 55% 17%



• Molecule 28: 50S ribosomal protein L2

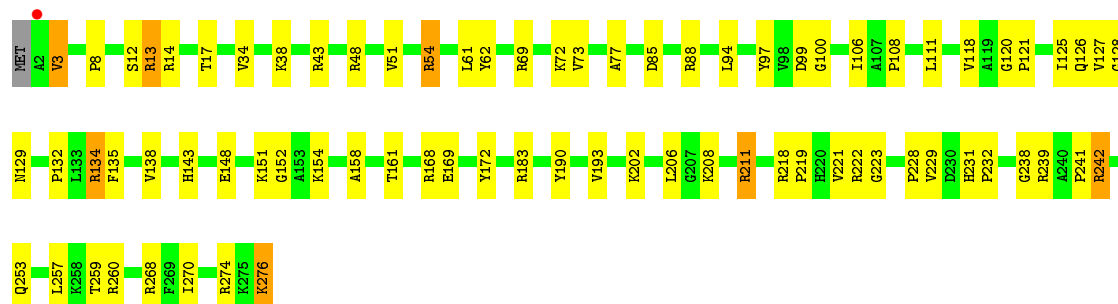
Chain BD: 69% 29%





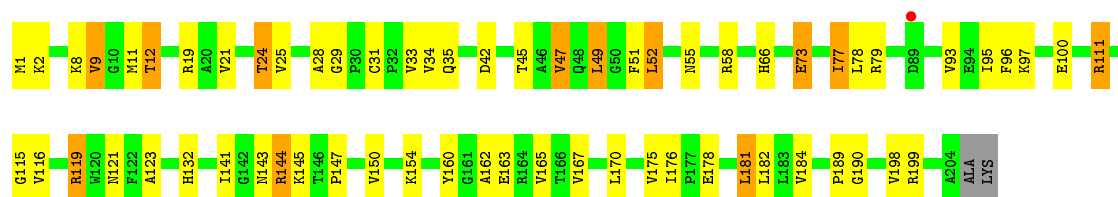
• Molecule 28: 50S ribosomal protein L2

Chain DD: 72% 25%



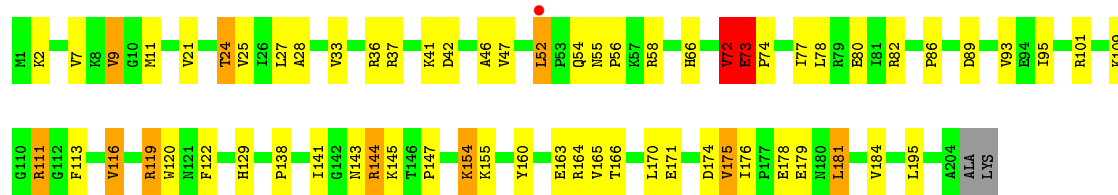
• Molecule 29: 50S ribosomal protein L3

Chain BE: 68% 25% 6%



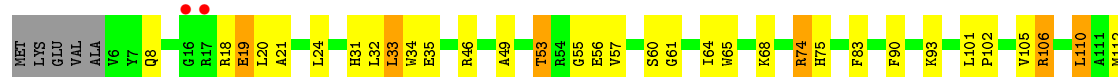
• Molecule 29: 50S ribosomal protein L3

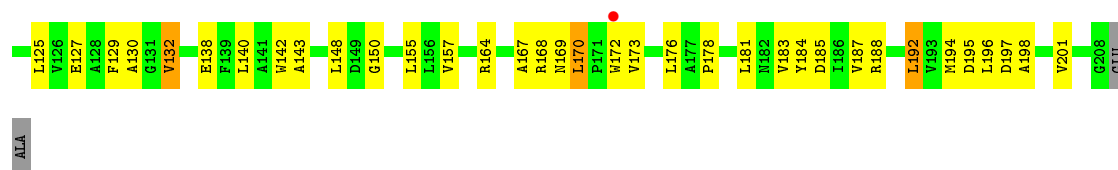
Chain DE: 67% 26% 5%



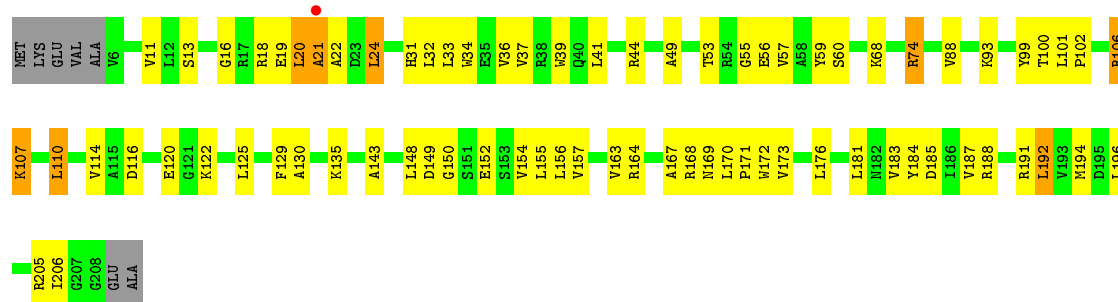
• Molecule 30: 50S ribosomal protein L4

Chain BF: 64% 28%

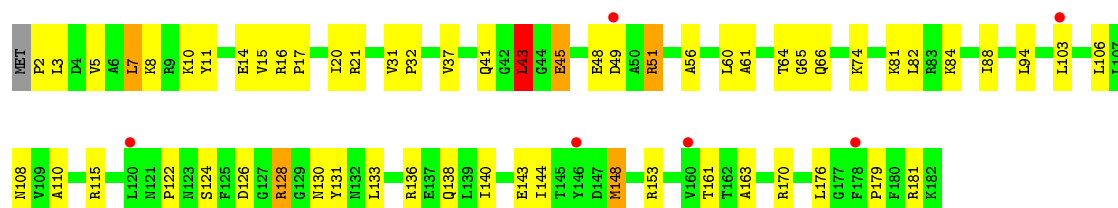




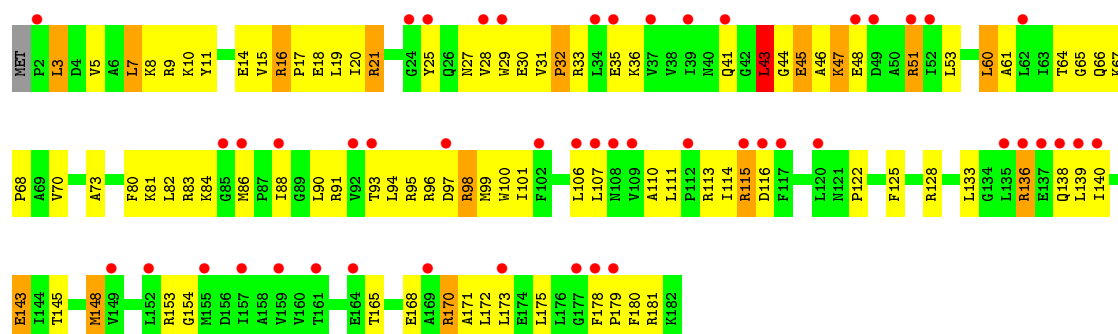
- Molecule 30: 50S ribosomal protein L4



- Molecule 31: 50S ribosomal protein L5

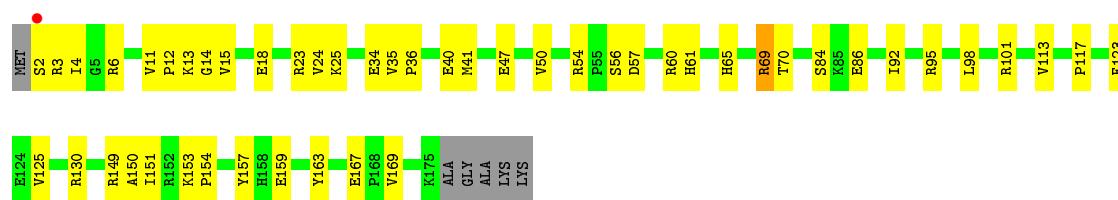


- Molecule 31: 50S ribosomal protein L5

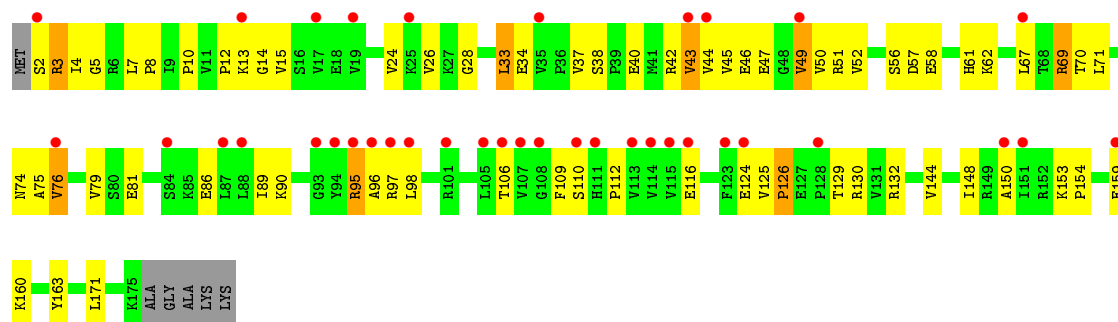


- Molecule 32: 50S ribosomal protein L6

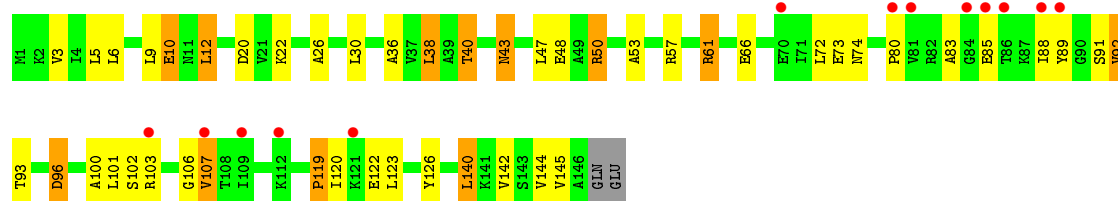




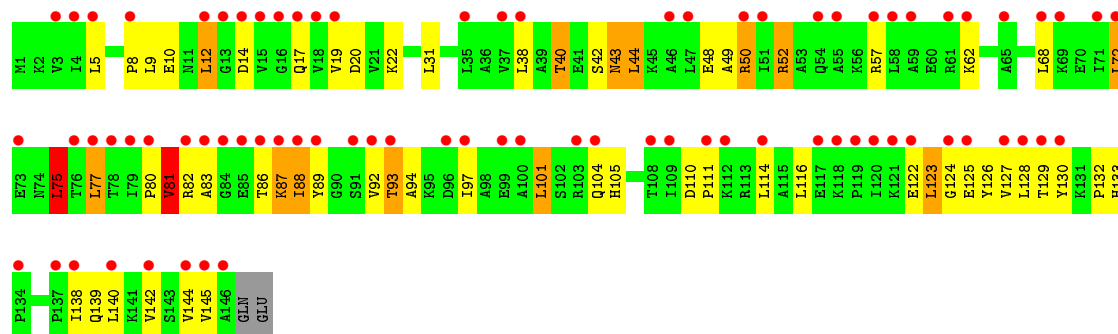
• Molecule 32: 50S ribosomal protein L6



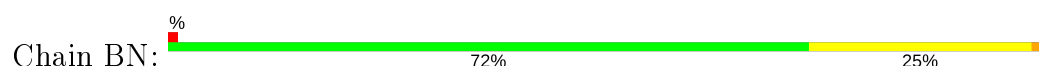
• Molecule 33: 50S ribosomal protein L9

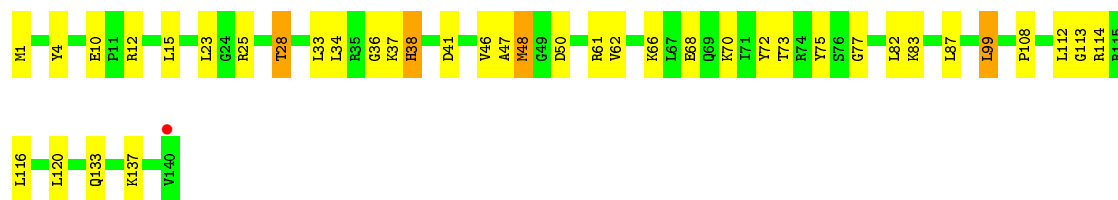


• Molecule 33: 50S ribosomal protein L9

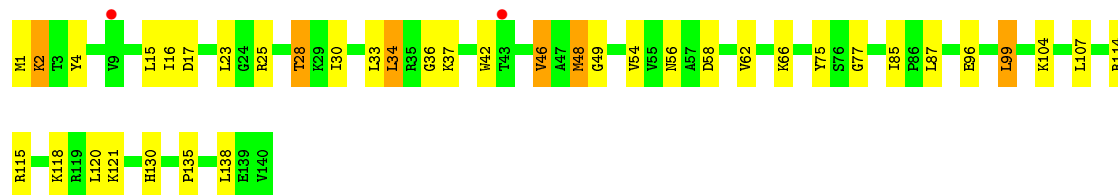
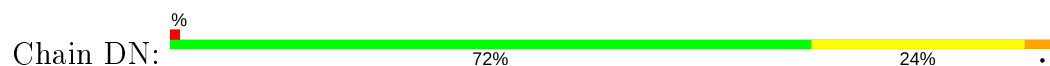


• Molecule 34: 50S ribosomal protein L13

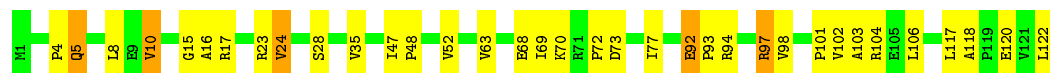




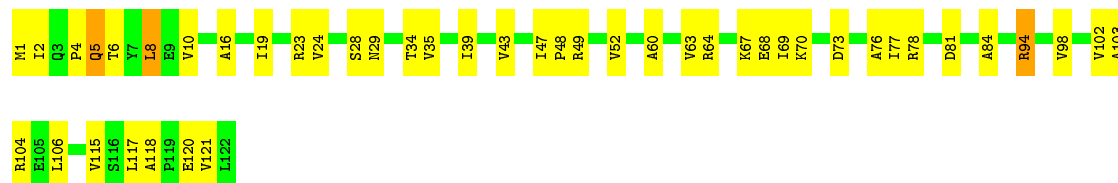
- Molecule 34: 50S ribosomal protein L13



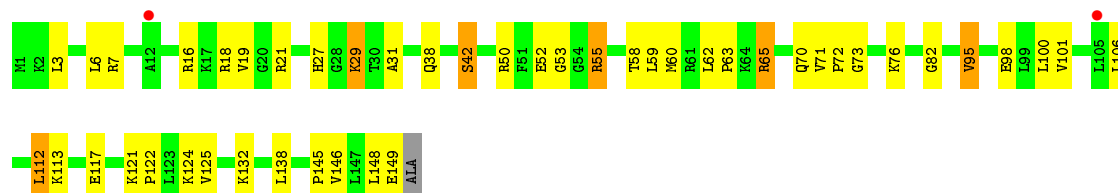
- Molecule 35: 50S ribosomal protein L14



- Molecule 35: 50S ribosomal protein L14

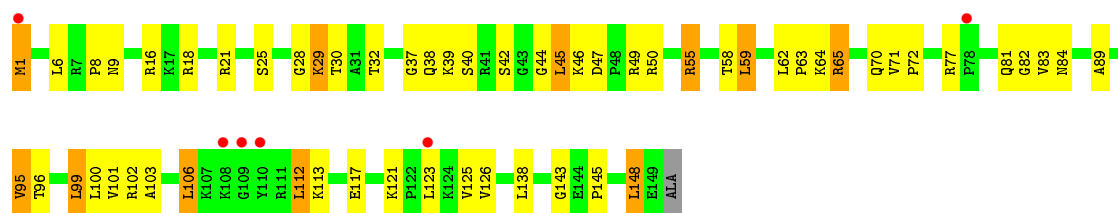


- Molecule 36: 50S ribosomal protein L15

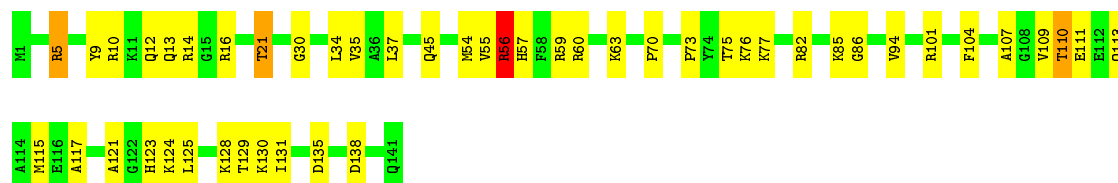


- Molecule 36: 50S ribosomal protein L15

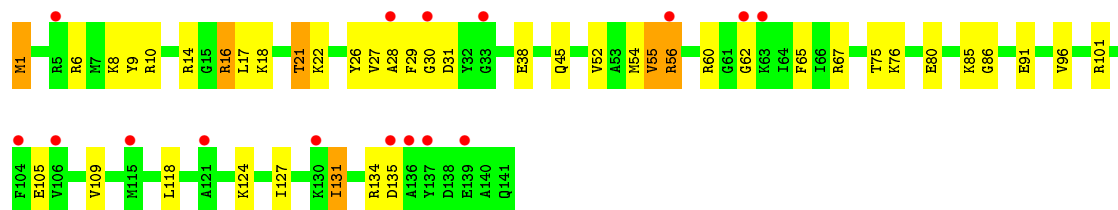
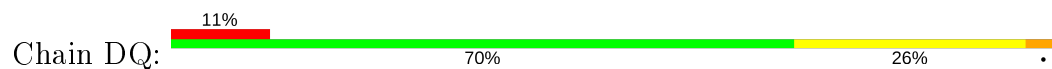




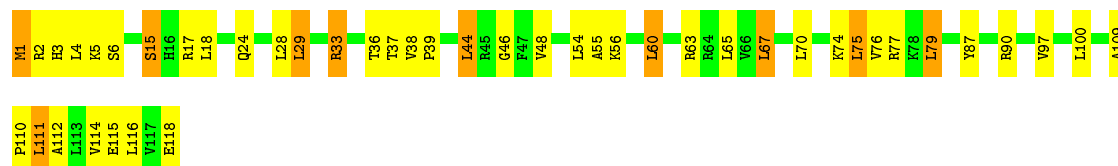
- Molecule 37: 50S ribosomal protein L16



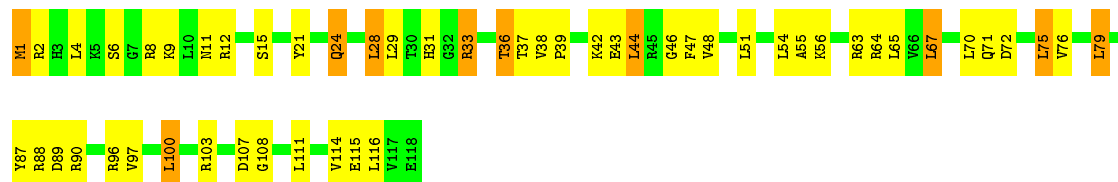
- Molecule 37: 50S ribosomal protein L16



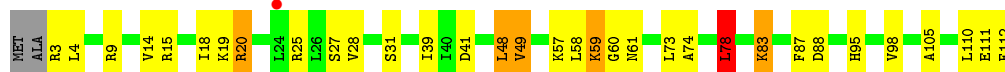
- Molecule 38: 50S ribosomal protein L17



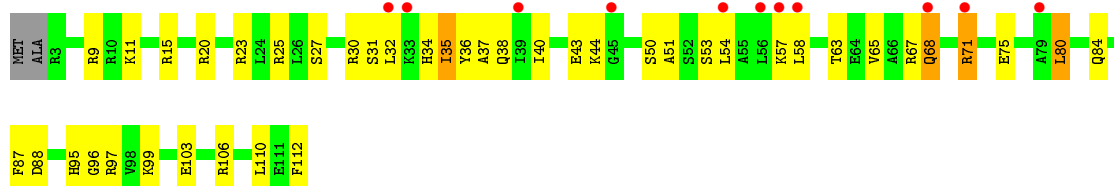
- Molecule 38: 50S ribosomal protein L17



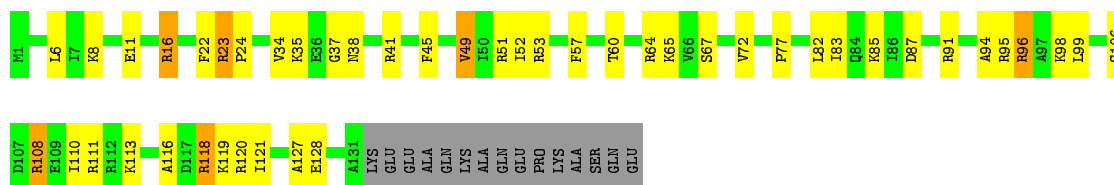
- Molecule 39: 50S ribosomal protein L18



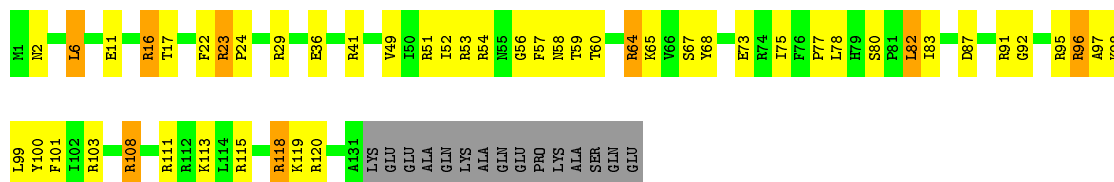
- Molecule 39: 50S ribosomal protein L18



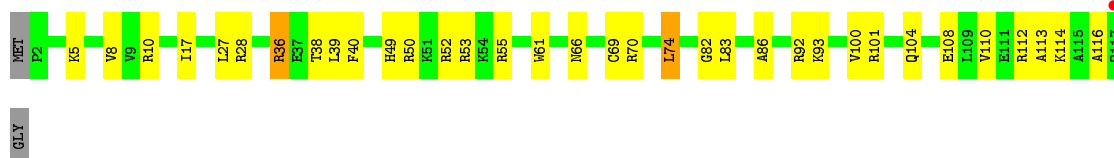
- Molecule 40: 50S ribosomal protein L19



- Molecule 40: 50S ribosomal protein L19

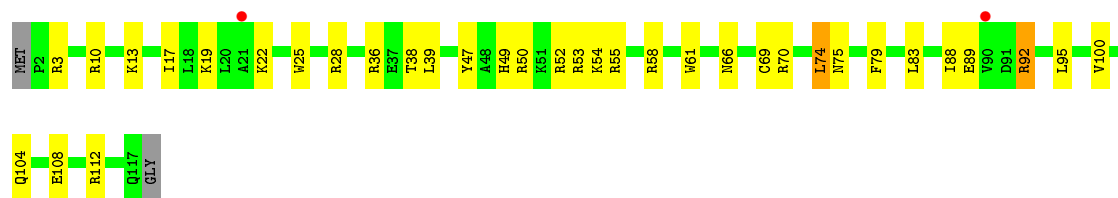


- Molecule 41: 50S ribosomal protein L20



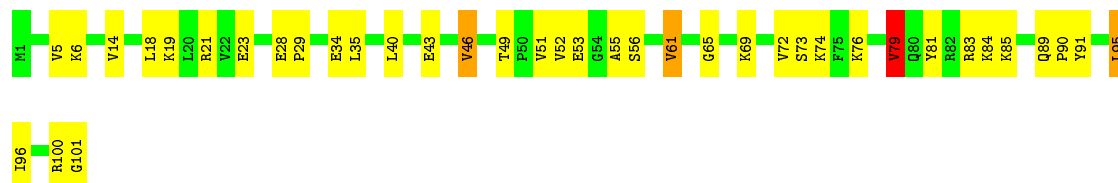
- Molecule 41: 50S ribosomal protein L20





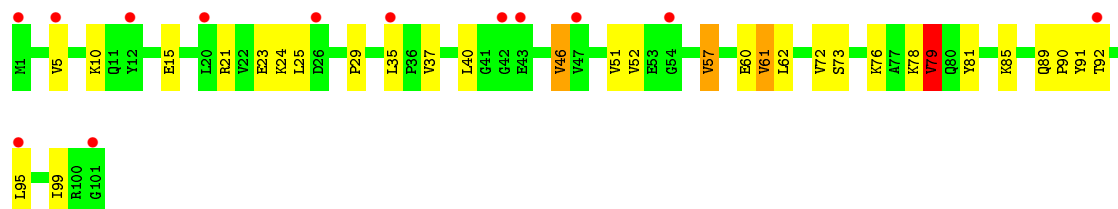
- Molecule 42: 50S ribosomal protein L21

Chain BV: 61% 35% ..



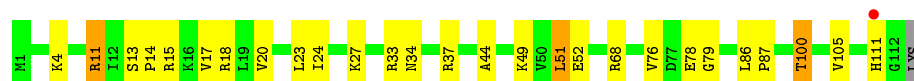
- Molecule 42: 50S ribosomal protein L21

Chain DV: 13% 69% 27% ..



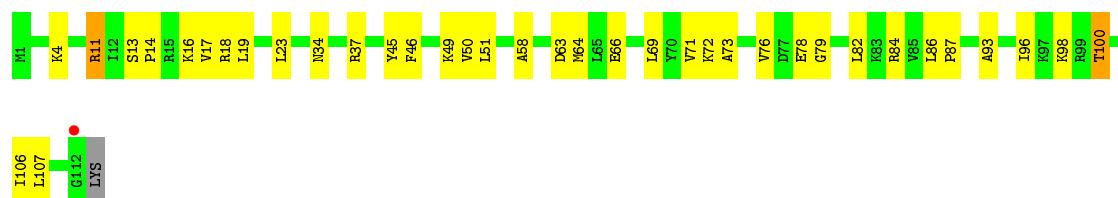
- Molecule 43: 50S ribosomal protein L22

Chain BW: % 75% 21% ..



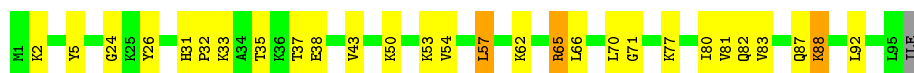
- Molecule 43: 50S ribosomal protein L22

Chain DW: % 66% 31% ..

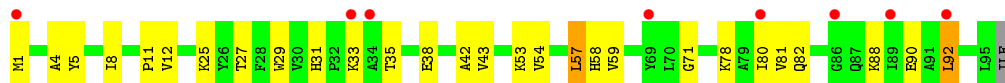
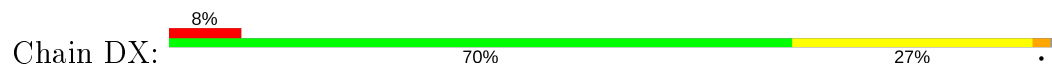


- Molecule 44: 50S ribosomal protein L23

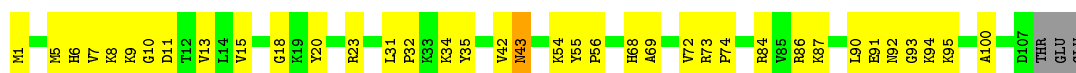
Chain BX: 70% 26% ..



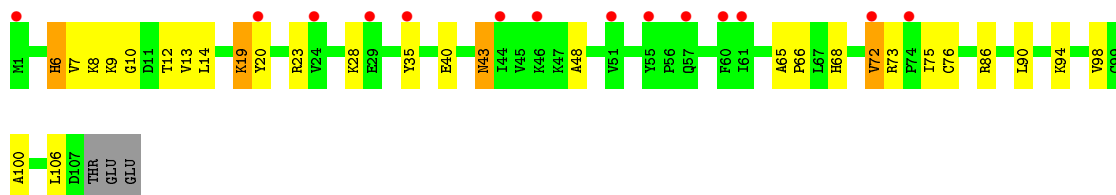
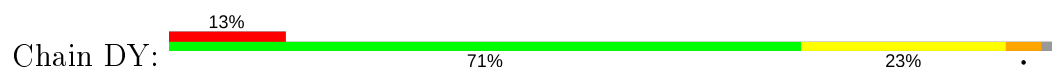
- Molecule 44: 50S ribosomal protein L23



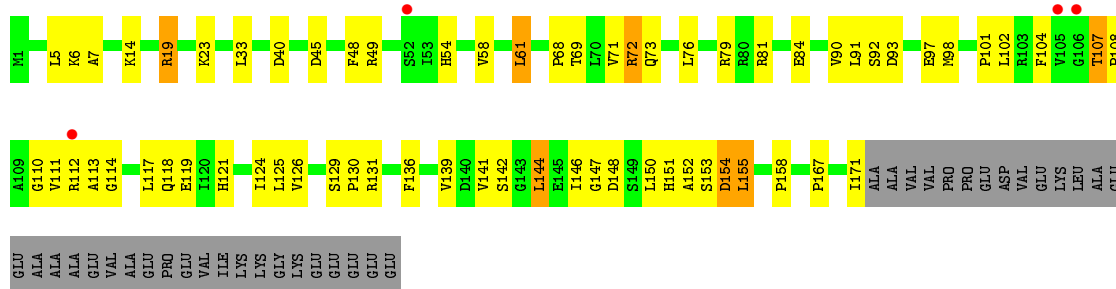
- Molecule 45: 50S ribosomal protein L24



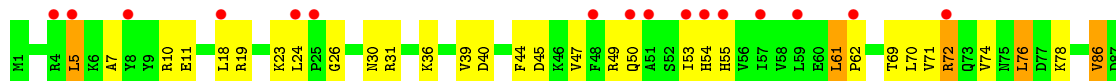
- Molecule 45: 50S ribosomal protein L24

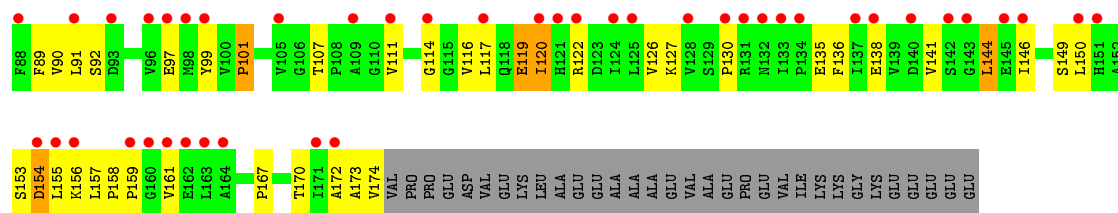


- Molecule 46: 50S ribosomal protein L25



- Molecule 46: 50S ribosomal protein L25





- Molecule 47: 50S ribosomal protein L27

Chain B0: 78% 16% . .



- Molecule 47: 50S ribosomal protein L27

Chain D0: 7% 72% 24% . .



- Molecule 48: 50S ribosomal protein L28

Chain B1: 70% 23% 5% .



- Molecule 48: 50S ribosomal protein L28

Chain D1: 3% 70% 23% 5% .



- Molecule 49: 50S ribosomal protein L29

Chain B2: 71% 22% . .



- Molecule 49: 50S ribosomal protein L29

Chain D2: 6% 75% 21% . .



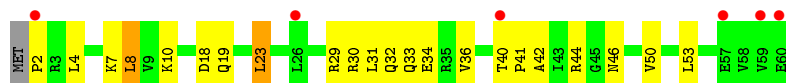
- Molecule 50: 50S ribosomal protein L30

Chain B3:  65% 27% 7% .



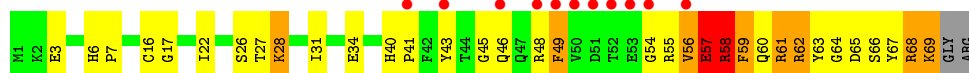
- Molecule 50: 50S ribosomal protein L30

Chain D3:  10% 62% 33% ..



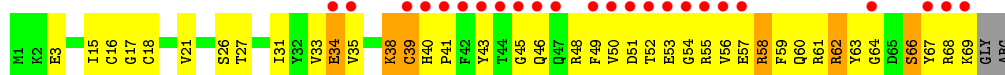
- Molecule 51: 50S ribosomal protein L31

Chain B4:  15% 49% 34% 11% . .




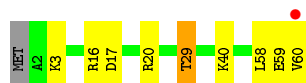
- Molecule 51: 50S ribosomal protein L31

Chain D4:  34% 41% 48% 8% .




- Molecule 52: 50S ribosomal protein L32

Chain B5:  2% 83% 13% . .



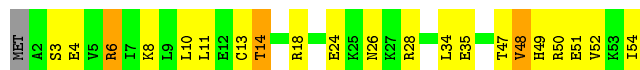
- Molecule 52: 50S ribosomal protein L32

Chain D5:  78% 18% . .

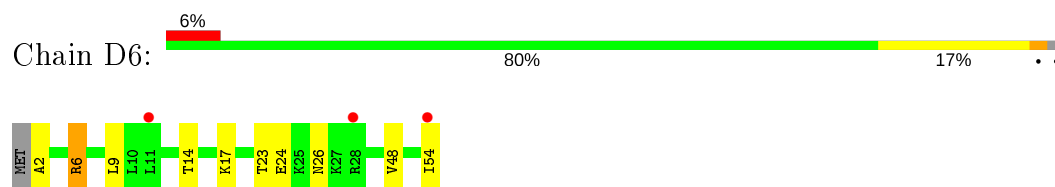


- Molecule 53: 50S ribosomal protein L33

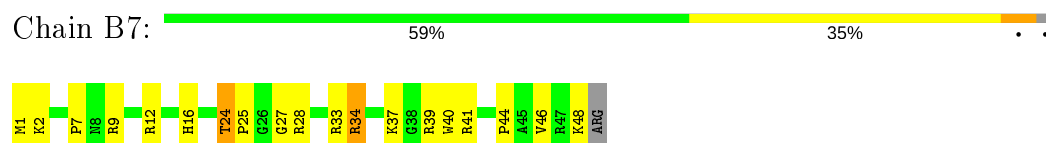
Chain B6:  59% 33% 6% .



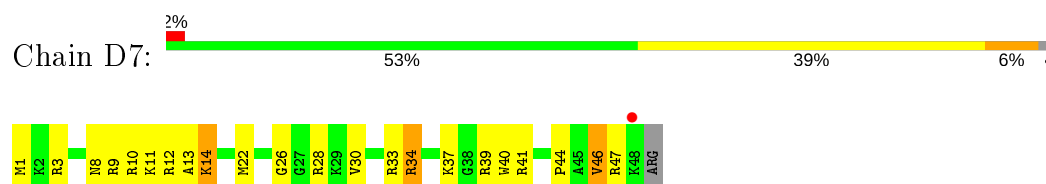
• Molecule 53: 50S ribosomal protein L33



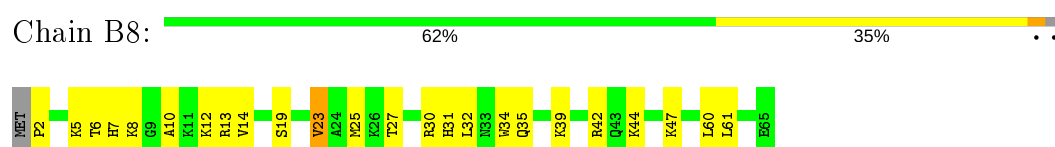
• Molecule 54: 50S ribosomal protein L34



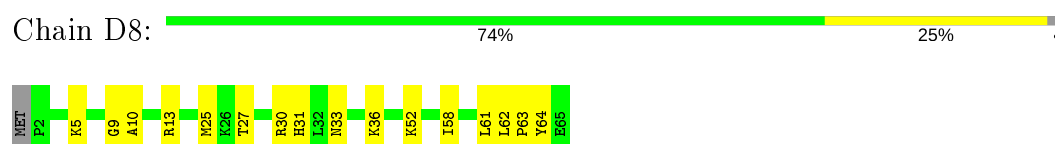
• Molecule 54: 50S ribosomal protein L34



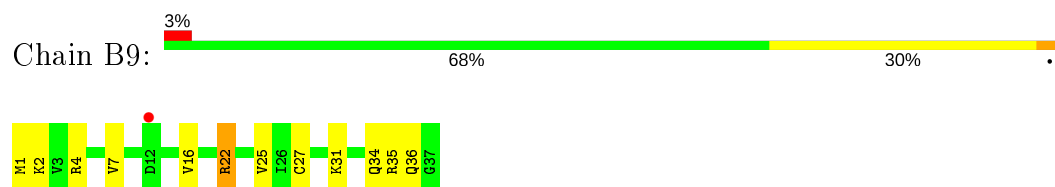
• Molecule 55: 50S ribosomal protein L35



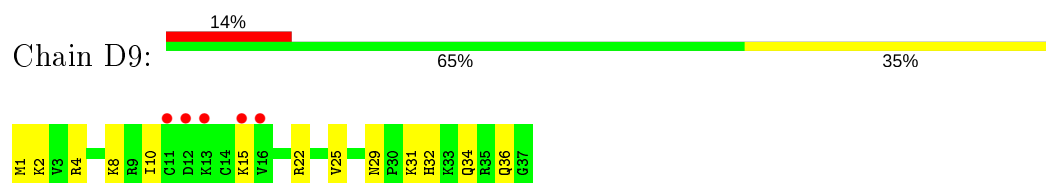
• Molecule 55: 50S ribosomal protein L35



• Molecule 56: 50S ribosomal protein L36



• Molecule 56: 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	207.56Å 444.23Å 613.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	150.38 – 2.80 150.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (150.38-2.80) 98.0 (150.38-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.234 , 0.280 0.234 , 0.281	Depositor DCC
R_{free} test set	67651 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	290205	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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: 5MU, MG, PPU, K, ZN, 31H, 5MC, 4SU, SF4, PSU

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	0.41	4/36049 (0.0%)	0.98	71/56261 (0.1%)
1	CA	0.42	7/36170 (0.0%)	1.05	147/56452 (0.3%)
2	AB	0.29	0/1881	0.59	0/2542
2	CB	0.33	0/1860	0.68	3/2518 (0.1%)
3	AC	0.28	0/1576	0.52	0/2130
3	CC	0.30	0/1566	0.58	0/2119
4	AD	0.28	0/1689	0.55	0/2267
4	CD	0.30	0/1704	0.56	0/2284
5	AE	0.29	0/1145	0.52	0/1543
5	CE	0.30	0/1149	0.58	1/1548 (0.1%)
6	AF	0.29	0/819	0.50	0/1111
6	CF	0.30	0/829	0.49	0/1123
7	AG	0.27	0/1250	0.51	0/1679
7	CG	0.29	0/1254	0.53	0/1683
8	AH	0.27	0/1108	0.51	0/1494
8	CH	0.27	0/1108	0.55	0/1494
9	AI	0.28	0/1002	0.54	0/1346
9	CI	0.30	0/997	0.56	0/1343
10	AJ	0.27	0/722	0.60	0/982
10	CJ	0.30	0/727	0.57	0/988
11	AK	0.29	0/844	0.50	0/1145
11	CK	0.27	0/848	0.50	0/1149
12	AL	0.29	0/946	0.51	0/1274
12	CL	0.29	0/946	0.56	0/1274
13	AM	0.28	0/969	0.58	0/1302
13	CM	0.29	0/961	0.57	0/1291
14	AN	0.30	0/501	0.55	0/664
14	CN	0.32	0/501	0.55	0/664
15	AO	0.27	0/739	0.53	0/985
15	CO	0.30	0/739	0.54	0/985
16	AP	0.29	0/697	0.53	0/939
16	CP	0.28	0/693	0.54	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.29	0/836	0.55	0/1117
17	CQ	0.29	0/836	0.53	0/1117
18	AR	0.27	0/560	0.48	0/746
18	CR	0.28	0/560	0.52	0/746
19	AS	0.28	0/667	0.54	0/900
19	CS	0.30	0/661	0.68	0/893
20	AT	0.27	0/730	0.58	0/965
20	CT	0.27	0/729	0.52	0/965
21	AU	0.29	0/203	0.56	0/266
21	CU	0.32	0/203	0.48	0/266
22	AV	0.49	0/310	0.95	1/480 (0.2%)
22	CV	1.15	3/144 (2.1%)	3.12	11/222 (5.0%)
23	AW	0.45	0/40	1.07	0/60
23	CW	0.35	0/40	1.09	0/60
24	AX	0.53	2/1700 (0.1%)	1.24	23/2650 (0.9%)
24	CX	0.54	0/1700	1.36	19/2650 (0.7%)
25	AY	0.33	0/115	0.82	0/176
25	CY	0.29	0/115	0.95	0/176
26	BA	0.50	4/68013 (0.0%)	0.93	70/106165 (0.1%)
26	DA	0.42	0/67542	0.94	88/105428 (0.1%)
27	BB	0.41	0/2878	0.91	2/4490 (0.0%)
27	DB	0.41	0/2878	1.00	8/4490 (0.2%)
28	BD	0.37	0/2186	0.57	0/2944
28	DD	0.34	0/2186	0.56	0/2944
29	BE	0.36	0/1592	0.53	0/2149
29	DE	0.34	0/1592	0.59	1/2149 (0.0%)
30	BF	0.35	0/1619	0.53	0/2193
30	DF	0.33	0/1615	0.56	0/2188
31	BG	0.29	0/1450	0.54	0/1959
31	DG	0.32	0/1449	0.57	0/1958
32	BH	0.30	0/1356	0.51	0/1834
32	DH	0.29	0/1356	0.51	0/1834
33	BI	0.31	0/1100	0.59	0/1501
33	DI	0.37	0/1076	0.78	4/1471 (0.3%)
34	BN	0.34	0/1144	0.54	0/1543
34	DN	0.31	0/1144	0.52	0/1543
35	BO	0.34	0/943	0.56	0/1269
35	DO	0.33	0/943	0.55	1/1269 (0.1%)
36	BP	0.35	0/1152	0.57	0/1533
36	DP	0.32	0/1152	0.63	0/1533
37	BQ	0.35	0/1143	0.59	1/1527 (0.1%)
37	DQ	0.32	0/1143	0.54	0/1527
38	BR	0.36	0/982	0.57	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.29	0/982	0.55	0/1312
39	BS	0.32	0/887	0.57	1/1180 (0.1%)
39	DS	0.29	0/880	0.57	0/1172
40	BT	0.34	0/1105	0.61	0/1477
40	DT	0.30	0/1097	0.53	0/1468
41	BU	0.35	0/977	0.53	0/1301
41	DU	0.28	0/977	0.50	0/1301
42	BV	0.36	0/782	0.55	0/1049
42	DV	0.29	0/782	0.54	0/1049
43	BW	0.35	0/897	0.53	0/1205
43	DW	0.30	0/897	0.49	0/1205
44	BX	0.39	0/764	0.58	1/1025 (0.1%)
44	DX	0.32	0/764	0.53	1/1025 (0.1%)
45	BY	0.34	0/819	0.59	0/1095
45	DY	0.30	0/819	0.55	0/1095
46	BZ	0.32	0/1379	0.58	0/1873
46	DZ	0.29	0/1390	0.54	0/1890
47	B0	0.36	0/662	0.60	0/881
47	D0	0.30	0/662	0.50	0/881
48	B1	0.32	0/762	0.53	0/1014
48	D1	0.31	0/762	0.53	0/1014
49	B2	0.32	0/590	0.57	0/781
49	D2	0.26	0/590	0.49	0/781
50	B3	0.35	0/474	0.52	0/635
50	D3	0.31	0/469	0.54	0/630
51	B4	0.34	0/565	0.70	0/761
51	D4	0.32	0/545	0.67	0/737
52	B5	0.37	0/469	0.62	1/635 (0.2%)
52	D5	0.32	0/469	0.54	0/635
53	B6	0.36	0/460	0.53	0/613
53	D6	0.34	0/456	0.51	0/608
54	B7	0.36	0/426	0.56	0/561
54	D7	0.34	0/426	0.49	0/561
55	B8	0.37	0/519	0.54	0/684
55	D8	0.31	0/525	0.50	0/691
56	B9	0.43	0/310	0.65	0/407
56	D9	0.33	0/310	0.59	0/407
All	All	0.41	20/310421 (0.0%)	0.88	455/464361 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	1
7	AG	0	1
20	AT	0	1
29	DE	0	1
33	DI	0	1
39	BS	0	1
46	BZ	0	1
51	B4	0	2
51	D4	0	1
All	All	0	10

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	C6-N1	-12.37	1.30	1.39
1	AA	1172	C	N3-C4	-10.50	1.26	1.33
1	CA	1154	G	N1-C2	-10.41	1.29	1.37
1	AA	1172	C	C2-N3	-8.49	1.28	1.35
1	AA	1164	G	N1-C2	-6.91	1.32	1.37

The worst 5 of 455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1172	C	N1-C2-O2	39.76	142.76	118.90
1	CA	1119	C	N1-C2-O2	26.84	135.00	118.90
1	AA	1172	C	N3-C2-O2	-25.31	104.18	121.90
1	CA	1154	G	C5-C6-O6	24.22	143.13	128.60
1	CA	1154	G	N1-C2-N2	-23.61	94.95	116.20

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	8	LYS	Peptide
7	AG	79	ARG	Peptide
20	AT	9	ASN	Peptide
39	BS	58	LEU	Peptide
46	BZ	158	PRO	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	32205	0	16255	743	1
1	CA	32312	0	16307	964	1
2	AB	1846	0	1867	74	0
2	CB	1825	0	1828	76	0
3	AC	1552	0	1546	49	0
3	CC	1542	0	1517	58	0
4	AD	1659	0	1676	74	0
4	CD	1674	0	1714	83	0
5	AE	1129	0	1184	33	0
5	CE	1133	0	1191	39	0
6	AF	806	0	793	16	0
6	CF	816	0	808	23	0
7	AG	1231	0	1238	37	0
7	CG	1235	0	1249	38	0
8	AH	1088	0	1126	35	0
8	CH	1088	0	1126	40	0
9	AI	983	0	986	48	0
9	CI	978	0	966	53	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	38	0
11	AK	829	0	825	23	0
11	CK	833	0	836	20	0
12	AL	930	0	980	21	0
12	CL	930	0	980	33	0
13	AM	958	0	1002	37	0
13	CM	950	0	988	47	0
14	AN	492	0	529	27	0
14	CN	492	0	529	23	0
15	AO	728	0	760	22	0
15	CO	728	0	760	27	0
16	AP	681	0	697	27	0
16	CP	677	0	686	26	0
17	AQ	823	0	891	23	0
17	CQ	823	0	891	18	0
18	AR	555	0	618	11	0
18	CR	555	0	618	23	0
19	AS	652	0	662	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	646	0	644	40	0
20	AT	728	0	798	27	0
20	CT	727	0	796	23	0
21	AU	199	0	208	5	0
21	CU	199	0	208	8	0
22	AV	277	0	140	7	0
22	CV	129	0	65	16	0
23	AW	74	0	51	5	0
23	CW	74	0	51	11	0
24	AX	1633	0	836	35	0
24	CX	1635	0	838	83	0
25	AY	104	0	56	3	0
25	CY	104	0	56	2	0
26	BA	60729	0	30620	950	0
26	DA	60311	0	30412	1223	1
27	BB	2573	0	1306	32	0
27	DB	2573	0	1306	87	0
28	BD	2136	0	2218	67	0
28	DD	2136	0	2218	74	0
29	BE	1559	0	1618	43	0
29	DE	1559	0	1618	56	0
30	BF	1584	0	1625	49	0
30	DF	1580	0	1619	55	0
31	BG	1425	0	1443	37	0
31	DG	1424	0	1434	73	0
32	BH	1330	0	1407	29	0
32	DH	1330	0	1407	44	0
33	BI	1085	0	1114	28	1
33	DI	1061	0	1080	50	0
34	BN	1117	0	1184	21	0
34	DN	1117	0	1184	29	0
35	BO	933	0	996	27	0
35	DO	933	0	996	38	0
36	BP	1135	0	1212	53	0
36	DP	1135	0	1212	61	0
37	BQ	1122	0	1179	38	0
37	DQ	1122	0	1179	33	0
38	BR	968	0	1033	26	1
38	DR	968	0	1033	36	0
39	BS	877	0	938	28	0
39	DS	870	0	923	29	0
40	BT	1091	0	1151	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DT	1083	0	1136	39	0
41	BU	959	0	1019	24	0
41	DU	959	0	1018	29	0
42	BV	771	0	830	21	1
42	DV	771	0	830	24	0
43	BW	886	0	940	15	0
43	DW	886	0	940	20	0
44	BX	750	0	814	24	0
44	DX	750	0	814	19	0
45	BY	806	0	881	24	0
45	DY	806	0	881	19	0
46	BZ	1349	0	1355	38	0
46	DZ	1360	0	1363	47	0
47	B0	653	0	674	20	0
47	D0	653	0	674	19	0
48	B1	755	0	826	19	0
48	D1	755	0	826	20	0
49	B2	588	0	643	8	0
49	D2	588	0	643	9	0
50	B3	469	0	518	15	0
50	D3	464	0	514	15	0
51	B4	552	0	533	32	0
51	D4	532	0	503	28	0
52	B5	455	0	465	8	0
52	D5	455	0	465	10	0
53	B6	453	0	473	13	0
53	D6	449	0	469	6	0
54	B7	418	0	467	19	0
54	D7	418	0	467	15	0
55	B8	511	0	571	29	0
55	D8	517	0	582	14	0
56	B9	307	0	335	8	0
56	D9	307	0	335	10	0
57	AA	207	0	0	0	0
57	AD	2	0	0	0	0
57	AE	2	0	0	0	0
57	AF	1	0	0	0	0
57	AJ	1	0	0	0	0
57	AK	1	0	0	0	0
57	AM	1	0	0	0	0
57	AN	2	0	0	0	0
57	AS	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AV	1	0	0	0	0
57	AW	1	0	0	0	0
57	AX	11	0	0	0	0
57	B0	4	0	0	0	0
57	B1	1	0	0	0	0
57	B2	1	0	0	0	0
57	B3	2	0	0	0	0
57	B5	2	0	0	0	0
57	B7	3	0	0	0	0
57	B8	1	0	0	0	0
57	B9	1	0	0	0	0
57	BA	720	0	0	0	0
57	BB	20	0	0	0	0
57	BD	11	0	0	0	0
57	BE	7	0	0	0	0
57	BF	10	0	0	0	0
57	BG	2	0	0	0	0
57	BN	6	0	0	0	0
57	BO	1	0	0	0	0
57	BP	4	0	0	0	0
57	BQ	5	0	0	0	0
57	BR	3	0	0	0	0
57	BU	8	0	0	0	0
57	BV	4	0	0	0	0
57	BW	5	0	0	0	0
57	BX	1	0	0	0	0
57	BY	1	0	0	0	0
57	BZ	1	0	0	0	0
57	CA	160	0	0	0	0
57	CE	1	0	0	0	0
57	CF	1	0	0	0	0
57	CJ	1	0	0	0	0
57	CK	1	0	0	0	0
57	CT	1	0	0	0	0
57	CW	1	0	0	0	0
57	CX	2	0	0	0	0
57	D3	1	0	0	0	0
57	D5	1	0	0	0	0
57	D8	2	0	0	0	0
57	DA	629	0	0	0	0
57	DB	10	0	0	0	0
57	DD	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DE	4	0	0	0	0
57	DF	4	0	0	0	0
57	DG	1	0	0	0	0
57	DN	1	0	0	0	0
57	DO	1	0	0	0	0
57	DP	2	0	0	0	0
57	DQ	3	0	0	0	0
57	DR	2	0	0	0	0
57	DU	4	0	0	0	0
57	DV	2	0	0	0	0
57	DW	2	0	0	0	0
57	DY	1	0	0	0	0
58	AD	8	0	0	1	0
58	CD	8	0	0	1	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	170	0	0	16	0
61	AL	2	0	0	1	0
61	AO	1	0	0	0	0
61	AU	1	0	0	1	0
61	AV	2	0	0	0	0
61	AW	3	0	0	0	0
61	B0	4	0	0	0	0
61	B1	1	0	0	0	0
61	B3	1	0	0	0	0
61	B5	5	0	0	0	0
61	B7	1	0	0	1	0
61	B8	7	0	0	0	0
61	BA	1102	0	0	59	0
61	BB	36	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BD	8	0	0	1	0
61	BE	13	0	0	5	0
61	BF	4	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BP	15	0	0	1	0
61	BQ	3	0	0	0	0
61	BR	1	0	0	1	0
61	BS	1	0	0	0	0
61	BT	3	0	0	0	0
61	BU	1	0	0	1	0
61	BV	4	0	0	0	0
61	BW	2	0	0	0	0
61	BX	2	0	0	0	0
61	CA	130	0	0	8	0
61	CE	1	0	0	0	0
61	CJ	2	0	0	0	0
61	CN	1	0	0	0	0
61	CT	1	0	0	0	0
61	CV	1	0	0	0	0
61	CW	1	0	0	0	0
61	CX	1	0	0	1	0
61	D0	5	0	0	1	0
61	D1	1	0	0	0	0
61	D3	2	0	0	0	0
61	D7	1	0	0	0	0
61	D8	4	0	0	0	0
61	DA	767	0	0	55	0
61	DB	9	0	0	0	0
61	DD	9	0	0	3	0
61	DE	5	0	0	0	0
61	DF	6	0	0	0	0
61	DN	2	0	0	0	0
61	DP	12	0	0	3	0
61	DR	2	0	0	1	0
61	DT	1	0	0	0	0
61	DU	2	0	0	0	0
61	DV	1	0	0	1	0
61	DX	2	0	0	0	0
61	DY	1	0	0	1	0
All	All	290205	0	193167	6242	3

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 14.

The worst 5 of 6242 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:CA:1002:G:H1	1:CA:1038:C:N4	1.48	1.11
26:DA:2121:G:H1	26:DA:2177:C:N4	1.52	1.06
1:AA:1164:G:N2	1:AA:1165:C:C5	2.24	1.06
1:CA:72:C:N4	1:CA:97:G:N1	2.04	1.05
26:DA:2139:C:N4	26:DA:2152:G:H1	1.55	1.04

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1043:C:O2'	26:DA:2137:C:O2'[2_655]	2.08	0.12
33:BI:89:TYR:O	1:CA:357:G:O2'[3_654]	2.10	0.10
38:BR:33:ARG:NH2	42:BV:53:GLU:OE2[4_445]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	229/256 (90%)	204 (89%)	21 (9%)	4 (2%)	9	29
2	CB	229/256 (90%)	204 (89%)	14 (6%)	11 (5%)	2	7
3	AC	204/239 (85%)	189 (93%)	13 (6%)	2 (1%)	15	44
3	CC	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	29	61
4	AD	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	29	61
4	CD	206/209 (99%)	196 (95%)	7 (3%)	3 (2%)	10	33
5	AE	146/162 (90%)	136 (93%)	9 (6%)	1 (1%)	22	53
5	CE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	22	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
6	CF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
7	AG	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	7	24
7	CG	153/156 (98%)	143 (94%)	9 (6%)	1 (1%)	22	53
8	AH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
8	CH	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	22	53
9	AI	125/128 (98%)	118 (94%)	7 (6%)	0	100	100
9	CI	125/128 (98%)	118 (94%)	6 (5%)	1 (1%)	19	49
10	AJ	95/105 (90%)	83 (87%)	5 (5%)	7 (7%)	1	2
10	CJ	94/105 (90%)	83 (88%)	6 (6%)	5 (5%)	2	6
11	AK	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17	46
11	CK	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	17	46
12	AL	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
13	AM	121/126 (96%)	113 (93%)	6 (5%)	2 (2%)	9	29
13	CM	120/126 (95%)	110 (92%)	9 (8%)	1 (1%)	19	49
14	AN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
14	CN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	AO	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
15	CO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	AP	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
16	CP	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
17	AQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	CQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
18	AR	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
18	CR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
19	AS	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
19	CS	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	5	19
20	AT	94/106 (89%)	85 (90%)	3 (3%)	6 (6%)	1	3
20	CT	94/106 (89%)	84 (89%)	6 (6%)	4 (4%)	2	8
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	CU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
28	BD	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	34	66
28	DD	273/276 (99%)	261 (96%)	10 (4%)	2 (1%)	22	53
29	BE	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	61
29	DE	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	15	44
30	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	29	61
30	DF	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	15	44
31	BG	179/182 (98%)	166 (93%)	9 (5%)	4 (2%)	6	22
31	DG	179/182 (98%)	166 (93%)	9 (5%)	4 (2%)	6	22
32	BH	172/180 (96%)	161 (94%)	9 (5%)	2 (1%)	13	39
32	DH	172/180 (96%)	163 (95%)	7 (4%)	2 (1%)	13	39
33	BI	144/148 (97%)	132 (92%)	9 (6%)	3 (2%)	7	23
33	DI	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	11	34
34	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
34	DN	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	22	53
35	BO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	19	49
35	DO	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	19	49
36	BP	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	22	53
36	DP	147/150 (98%)	133 (90%)	13 (9%)	1 (1%)	22	53
37	BQ	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
37	DQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
38	BR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
39	BS	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
39	DS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	46
40	BT	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
40	DT	129/146 (88%)	125 (97%)	3 (2%)	1 (1%)	19	49
41	BU	114/118 (97%)	114 (100%)	0	0	100	100
41	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
42	BV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	44
42	DV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
43	DW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
44	BX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
44	DX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
45	BY	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
45	DY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
46	BZ	169/206 (82%)	148 (88%)	19 (11%)	2 (1%)	13	39
46	DZ	172/206 (84%)	156 (91%)	14 (8%)	2 (1%)	13	39
47	B0	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
47	D0	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
48	B1	95/98 (97%)	94 (99%)	0	1 (1%)	14	41
48	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	41
49	B2	68/72 (94%)	68 (100%)	0	0	100	100
49	D2	68/72 (94%)	68 (100%)	0	0	100	100
50	B3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
50	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	B4	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	2
51	D4	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	4
52	B5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
52	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
53	B6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
53	D6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
54	B7	46/49 (94%)	46 (100%)	0	0	100	100
54	D7	46/49 (94%)	45 (98%)	0	1 (2%)	6	22
55	B8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
55	D8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
56	B9	35/37 (95%)	35 (100%)	0	0	100	100
56	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11409/12128 (94%)	10783 (94%)	516 (4%)	110 (1%)	15	44

5 of 110 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	231	GLU
4	AD	166	LYS
7	AG	80	VAL
10	AJ	55	LYS
20	AT	10	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	192/220 (87%)	161 (84%)	31 (16%)	2	7
2	CB	187/220 (85%)	161 (86%)	26 (14%)	3	11
3	AC	143/188 (76%)	131 (92%)	12 (8%)	11	31
3	CC	140/188 (74%)	127 (91%)	13 (9%)	9	26
4	AD	170/181 (94%)	153 (90%)	17 (10%)	7	22
4	CD	173/181 (96%)	157 (91%)	16 (9%)	9	27
5	AE	113/123 (92%)	106 (94%)	7 (6%)	18	47
5	CE	114/123 (93%)	105 (92%)	9 (8%)	12	34
6	AF	83/90 (92%)	78 (94%)	5 (6%)	19	48
6	CF	85/90 (94%)	79 (93%)	6 (7%)	14	39
7	AG	119/127 (94%)	107 (90%)	12 (10%)	7	22
7	CG	120/127 (94%)	108 (90%)	12 (10%)	7	22
8	AH	114/119 (96%)	109 (96%)	5 (4%)	28	61
8	CH	114/119 (96%)	106 (93%)	8 (7%)	15	40
9	AI	90/99 (91%)	76 (84%)	14 (16%)	2	8
9	CI	89/99 (90%)	78 (88%)	11 (12%)	4	14
10	AJ	66/92 (72%)	60 (91%)	6 (9%)	9	27
10	CJ	69/92 (75%)	63 (91%)	6 (9%)	10	30
11	AK	82/99 (83%)	76 (93%)	6 (7%)	14	38
11	CK	83/99 (84%)	79 (95%)	4 (5%)	25	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	97/109 (89%)	91 (94%)	6 (6%)	18	47
12	CL	97/109 (89%)	94 (97%)	3 (3%)	40	74
13	AM	93/101 (92%)	82 (88%)	11 (12%)	5	16
13	CM	92/101 (91%)	81 (88%)	11 (12%)	5	15
14	AN	49/50 (98%)	43 (88%)	6 (12%)	5	15
14	CN	49/50 (98%)	43 (88%)	6 (12%)	5	15
15	AO	78/80 (98%)	66 (85%)	12 (15%)	2	8
15	CO	78/80 (98%)	70 (90%)	8 (10%)	7	21
16	AP	69/74 (93%)	60 (87%)	9 (13%)	4	13
16	CP	68/74 (92%)	62 (91%)	6 (9%)	10	29
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	39	73
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	13	37
18	AR	59/77 (77%)	54 (92%)	5 (8%)	10	31
18	CR	59/77 (77%)	54 (92%)	5 (8%)	10	31
19	AS	69/80 (86%)	61 (88%)	8 (12%)	5	17
19	CS	67/80 (84%)	62 (92%)	5 (8%)	13	37
20	AT	70/82 (85%)	60 (86%)	10 (14%)	3	10
20	CT	70/82 (85%)	63 (90%)	7 (10%)	7	22
21	AU	18/22 (82%)	16 (89%)	2 (11%)	6	19
21	CU	18/22 (82%)	17 (94%)	1 (6%)	21	51
28	BD	215/218 (99%)	201 (94%)	14 (6%)	17	44
28	DD	215/218 (99%)	200 (93%)	15 (7%)	15	40
29	BE	164/166 (99%)	144 (88%)	20 (12%)	5	15
29	DE	164/166 (99%)	147 (90%)	17 (10%)	7	21
30	BF	160/166 (96%)	145 (91%)	15 (9%)	8	26
30	DF	159/166 (96%)	146 (92%)	13 (8%)	11	33
31	BG	143/156 (92%)	128 (90%)	15 (10%)	7	20
31	DG	142/156 (91%)	122 (86%)	20 (14%)	3	10
32	BH	144/148 (97%)	138 (96%)	6 (4%)	30	63
32	DH	144/148 (97%)	132 (92%)	12 (8%)	11	32
33	BI	110/124 (89%)	90 (82%)	20 (18%)	1	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DI	104/124 (84%)	87 (84%)	17 (16%)	2	7
34	BN	118/119 (99%)	103 (87%)	15 (13%)	4	14
34	DN	118/119 (99%)	108 (92%)	10 (8%)	10	31
35	BO	100/100 (100%)	94 (94%)	6 (6%)	19	48
35	DO	100/100 (100%)	96 (96%)	4 (4%)	31	65
36	BP	115/116 (99%)	105 (91%)	10 (9%)	10	30
36	DP	115/116 (99%)	103 (90%)	12 (10%)	7	21
37	BQ	111/111 (100%)	100 (90%)	11 (10%)	8	23
37	DQ	111/111 (100%)	100 (90%)	11 (10%)	8	23
38	BR	101/101 (100%)	82 (81%)	19 (19%)	1	5
38	DR	101/101 (100%)	84 (83%)	17 (17%)	2	6
39	BS	87/88 (99%)	79 (91%)	8 (9%)	9	27
39	DS	85/88 (97%)	75 (88%)	10 (12%)	5	16
40	BT	115/127 (91%)	106 (92%)	9 (8%)	12	35
40	DT	113/127 (89%)	103 (91%)	10 (9%)	10	29
41	BU	93/94 (99%)	86 (92%)	7 (8%)	13	37
41	DU	93/94 (99%)	88 (95%)	5 (5%)	22	53
42	BV	80/82 (98%)	68 (85%)	12 (15%)	3	9
42	DV	80/82 (98%)	72 (90%)	8 (10%)	7	22
43	BW	90/92 (98%)	84 (93%)	6 (7%)	16	43
43	DW	90/92 (98%)	82 (91%)	8 (9%)	9	28
44	BX	77/78 (99%)	74 (96%)	3 (4%)	32	66
44	DX	77/78 (99%)	72 (94%)	5 (6%)	17	44
45	BY	85/91 (93%)	77 (91%)	8 (9%)	8	26
45	DY	85/91 (93%)	78 (92%)	7 (8%)	11	33
46	BZ	145/179 (81%)	131 (90%)	14 (10%)	8	24
46	DZ	145/179 (81%)	127 (88%)	18 (12%)	4	14
47	B0	65/67 (97%)	62 (95%)	3 (5%)	27	60
47	D0	65/67 (97%)	62 (95%)	3 (5%)	27	60
48	B1	80/83 (96%)	72 (90%)	8 (10%)	7	22
48	D1	80/83 (96%)	73 (91%)	7 (9%)	10	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	B2	65/67 (97%)	56 (86%)	9 (14%)	3	11
49	D2	65/67 (97%)	59 (91%)	6 (9%)	9	27
50	B3	51/52 (98%)	45 (88%)	6 (12%)	5	16
50	D3	50/52 (96%)	47 (94%)	3 (6%)	19	48
51	B4	59/63 (94%)	47 (80%)	12 (20%)	1	4
51	D4	53/63 (84%)	46 (87%)	7 (13%)	4	12
52	B5	50/52 (96%)	48 (96%)	2 (4%)	31	65
52	D5	50/52 (96%)	48 (96%)	2 (4%)	31	65
53	B6	51/52 (98%)	44 (86%)	7 (14%)	3	11
53	D6	50/52 (96%)	48 (96%)	2 (4%)	31	65
54	B7	41/42 (98%)	38 (93%)	3 (7%)	14	38
54	D7	41/42 (98%)	38 (93%)	3 (7%)	14	38
55	B8	53/55 (96%)	49 (92%)	4 (8%)	13	37
55	D8	54/55 (98%)	53 (98%)	1 (2%)	57	85
56	B9	34/34 (100%)	31 (91%)	3 (9%)	10	29
56	D9	34/34 (100%)	33 (97%)	1 (3%)	42	76
All	All	9319/10066 (93%)	8433 (90%)	886 (10%)	8	25

5 of 886 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	BZ	136	PHE
3	CC	115	LEU
43	DW	51	LEU
48	B1	75	GLU
53	B6	28	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
41	BU	117	GLN
2	CB	40	HIS
38	DR	71	GLN
45	BY	6	HIS
49	B2	48	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	407 (27%)	26 (1%)
1	CA	1501/1521 (98%)	413 (27%)	28 (1%)
22	AV	12/24 (50%)	7 (58%)	0
22	CV	5/24 (20%)	4 (80%)	0
23	AW	1/3 (33%)	0	0
23	CW	1/3 (33%)	0	0
24	AX	74/77 (96%)	26 (35%)	2 (2%)
24	CX	74/77 (96%)	31 (41%)	4 (5%)
25	AY	4/76 (5%)	1 (25%)	0
25	CY	4/76 (5%)	1 (25%)	0
26	BA	2811/2915 (96%)	529 (18%)	30 (1%)
26	DA	2791/2915 (95%)	595 (21%)	30 (1%)
27	BB	120/121 (99%)	16 (13%)	2 (1%)
27	DB	119/121 (98%)	31 (26%)	0
All	All	9012/9474 (95%)	2061 (22%)	122 (1%)

5 of 2061 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	15	G
1	AA	22	G

5 of 122 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2689	U
1	CA	509	A
26	DA	2104	G
26	BA	2756	U
1	CA	65	U

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

12 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
23	PPU	AW	76	26,23	32,40,41	0.97	1 (3%)	33,57,60	1.53	7 (21%)
24	5MC	CX	32	24	15,22,23	1.32	1 (6%)	19,32,35	1.36	2 (10%)
24	PSU	AX	55	24	17,21,22	1.51	3 (17%)	20,30,33	3.08	6 (30%)
24	PSU	CX	55	24	17,21,22	1.59	2 (11%)	20,30,33	3.23	6 (30%)
24	5MU	CX	54	24	15,22,23	1.08	2 (13%)	16,32,35	1.85	2 (12%)
24	5MC	AX	32	24	15,22,23	1.27	1 (6%)	19,32,35	1.47	3 (15%)
24	5MU	AX	54	24	15,22,23	1.05	2 (13%)	16,32,35	1.73	2 (12%)
24	4SU	AX	8	24	14,21,22	1.42	2 (14%)	15,30,33	2.72	2 (13%)
24	31H	AX	76	24,57	26,32,35	1.15	3 (11%)	22,45,50	1.70	3 (13%)
23	PPU	CW	76	26,23	32,40,41	0.92	1 (3%)	33,57,60	1.76	9 (27%)
24	4SU	CX	8	24	14,21,22	1.29	1 (7%)	15,30,33	1.89	2 (13%)
24	31H	CX	76	24,60,57	28,34,35	1.26	4 (14%)	23,47,50	1.67	3 (13%)

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
23	PPU	AW	76	26,23	-	4/21/43/44	0/4/4/4
24	5MC	CX	32	24	-	0/5/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/5/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/5/25/26	0/2/2/2
24	5MU	AX	54	24	-	0/5/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/5/25/26	0/2/2/2
24	31H	AX	76	24,57	-	7/15/37/41	0/3/3/3
23	PPU	CW	76	26,23	-	5/21/43/44	0/4/4/4
24	4SU	CX	8	24	-	0/5/25/26	0/2/2/2
24	31H	CX	76	24,60,57	-	9/18/40/41	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CX	32	5MC	C5-C4	4.66	1.48	1.41
24	AX	32	5MC	C5-C4	4.51	1.48	1.41
24	CX	55	PSU	C5-C1'	-4.50	1.48	1.52
24	CX	8	4SU	C4-S4	-4.09	1.60	1.67
24	AX	8	4SU	C4-S4	-4.04	1.60	1.67

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	8	4SU	C2-N3-C4	9.25	128.57	115.15
24	CX	55	PSU	N1-C2-N3	-8.74	121.48	128.43
24	AX	55	PSU	N1-C2-N3	-8.26	121.86	128.43
24	CX	55	PSU	C4-N3-C2	6.75	120.84	115.14
24	AX	55	PSU	C4-N3-C2	6.61	120.72	115.14

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AX	76	31H	C3'-C4'-C5'-O5'
24	CX	76	31H	C3'-C4'-C5'-O5'
24	CX	76	31H	C-CA-CB-CG
24	CX	76	31H	N-CA-CB-CG
24	CX	76	31H	OCN-CN-N-CA

There are no ring outliers.

11 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	76	PPU	5	0
24	CX	32	5MC	3	0
24	AX	55	PSU	1	0
24	CX	55	PSU	1	0
24	CX	54	5MU	2	0
24	AX	32	5MC	2	0
24	AX	54	5MU	1	0
24	AX	8	4SU	2	0
23	CW	76	PPU	11	0
24	CX	8	4SU	2	0
24	CX	76	31H	4	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1916 ligands modelled in this entry, 1914 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SF4	AD	302	4	0,12,12	0.00	-	-		
58	SF4	CD	501	4	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	AD	302	4	-	-	0/6/5/5
58	SF4	CD	501	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AD	302	SF4	1	0
58	CD	501	SF4	1	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	1498/1521 (98%)	0.20	23 (1%) 73 68	39, 73, 93, 105	0
1	CA	1503/1521 (98%)	0.15	27 (1%) 68 61	41, 75, 94, 106	0
2	AB	231/256 (90%)	0.52	15 (6%) 18 11	69, 82, 91, 101	0
2	CB	231/256 (90%)	2.17	109 (47%) 0 0	71, 84, 93, 101	0
3	AC	206/239 (86%)	0.45	6 (2%) 51 41	67, 79, 89, 95	0
3	CC	206/239 (86%)	1.88	84 (40%) 0 0	70, 81, 91, 95	0
4	AD	208/209 (99%)	0.58	13 (6%) 20 12	57, 74, 85, 91	0
4	CD	208/209 (99%)	0.80	21 (10%) 7 4	57, 75, 85, 92	0
5	AE	148/162 (91%)	0.51	5 (3%) 45 35	59, 71, 82, 90	0
5	CE	148/162 (91%)	1.02	29 (19%) 1 0	59, 73, 84, 91	0
6	AF	100/101 (99%)	0.43	4 (4%) 38 28	54, 69, 78, 83	0
6	CF	100/101 (99%)	0.26	5 (5%) 28 19	56, 71, 80, 83	0
7	AG	155/156 (99%)	0.57	14 (9%) 9 5	64, 76, 86, 92	0
7	CG	155/156 (99%)	1.08	25 (16%) 1 1	67, 78, 88, 92	0
8	AH	137/138 (99%)	0.41	6 (4%) 34 24	60, 72, 80, 85	0
8	CH	137/138 (99%)	1.35	34 (24%) 0 0	62, 74, 82, 85	0
9	AI	127/128 (99%)	0.83	17 (13%) 3 1	64, 83, 91, 96	0
9	CI	127/128 (99%)	1.62	46 (36%) 0 0	69, 84, 91, 98	0
10	AJ	97/105 (92%)	0.72	10 (10%) 6 3	66, 83, 92, 94	0
10	CJ	96/105 (91%)	2.07	54 (56%) 0 0	69, 85, 93, 94	0
11	AK	114/129 (88%)	0.68	9 (7%) 12 7	46, 70, 81, 85	0
11	CK	114/129 (88%)	0.62	13 (11%) 5 3	50, 71, 82, 85	0
12	AL	122/132 (92%)	0.53	3 (2%) 57 47	50, 64, 73, 81	0
12	CL	122/132 (92%)	0.71	12 (9%) 7 4	52, 65, 75, 81	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%)	0.64	13 (10%) 6 3	58, 72, 83, 90	0
13	CM	122/126 (96%)	1.49	33 (27%) 0 0	72, 85, 93, 100	0
14	AN	60/61 (98%)	0.63	6 (10%) 7 4	65, 75, 81, 82	0
14	CN	60/61 (98%)	2.22	31 (51%) 0 0	69, 78, 83, 86	0
15	AO	88/89 (98%)	0.75	2 (2%) 60 51	54, 69, 81, 85	0
15	CO	88/89 (98%)	0.60	9 (10%) 6 3	53, 71, 82, 87	0
16	AP	82/88 (93%)	0.81	10 (12%) 4 2	59, 72, 82, 85	0
16	CP	82/88 (93%)	0.52	4 (4%) 29 20	57, 71, 81, 85	0
17	AQ	99/105 (94%)	0.62	3 (3%) 50 40	58, 71, 80, 83	0
17	CQ	99/105 (94%)	1.13	17 (17%) 1 1	56, 72, 81, 83	0
18	AR	68/88 (77%)	0.82	8 (11%) 4 2	59, 70, 80, 84	0
18	CR	68/88 (77%)	0.55	7 (10%) 6 3	60, 71, 82, 85	0
19	AS	83/93 (89%)	0.84	12 (14%) 2 1	72, 82, 89, 93	0
19	CS	83/93 (89%)	2.22	43 (51%) 0 0	73, 84, 91, 95	0
20	AT	96/106 (90%)	1.07	19 (19%) 1 0	60, 71, 83, 85	0
20	CT	96/106 (90%)	1.09	20 (20%) 1 0	56, 71, 83, 85	0
21	AU	23/27 (85%)	0.88	1 (4%) 35 25	69, 74, 79, 85	0
21	CU	23/27 (85%)	0.56	2 (8%) 10 5	71, 76, 84, 86	0
22	AV	13/24 (54%)	1.75	4 (30%) 0 0	56, 88, 93, 97	0
22	CV	6/24 (25%)	1.12	2 (33%) 0 0	59, 76, 95, 96	0
23	AW	2/3 (66%)	0.33	0 100 100	30, 30, 30, 37	0
23	CW	2/3 (66%)	0.65	0 100 100	50, 50, 50, 57	0
24	AX	71/77 (92%)	0.18	0 100 100	27, 70, 84, 92	0
24	CX	71/77 (92%)	0.24	0 100 100	30, 75, 86, 93	0
25	AY	5/76 (6%)	0.06	0 100 100	51, 76, 87, 94	0
25	CY	5/76 (6%)	1.35	0 100 100	60, 79, 90, 91	0
26	BA	2819/2915 (96%)	0.22	22 (0%) 86 81	20, 42, 89, 107	0
26	DA	2800/2915 (96%)	-0.04	50 (1%) 68 61	22, 46, 90, 107	0
27	BB	120/121 (99%)	0.07	0 100 100	37, 63, 77, 88	0
27	DB	120/121 (99%)	0.10	5 (4%) 36 26	42, 68, 80, 91	0
28	BD	275/276 (99%)	0.20	2 (0%) 87 84	21, 41, 58, 78	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DD	275/276 (99%)	0.00	1 (0%) 92 91	23, 43, 61, 80	0
29	BE	204/206 (99%)	0.20	1 (0%) 91 88	21, 46, 65, 82	0
29	DE	204/206 (99%)	-0.06	1 (0%) 91 88	23, 48, 67, 84	0
30	BF	203/210 (96%)	0.22	3 (1%) 73 68	22, 51, 73, 87	0
30	DF	203/210 (96%)	0.06	1 (0%) 91 88	24, 54, 74, 86	0
31	BG	181/182 (99%)	0.36	6 (3%) 46 36	55, 70, 82, 93	0
31	DG	181/182 (99%)	1.34	49 (27%) 0 0	59, 74, 85, 93	0
32	BH	174/180 (96%)	0.13	1 (0%) 89 86	49, 65, 77, 81	0
32	DH	174/180 (96%)	1.24	37 (21%) 0 0	52, 70, 80, 84	0
33	BI	146/148 (98%)	0.71	13 (8%) 9 5	47, 81, 90, 95	0
33	DI	146/148 (98%)	3.00	79 (54%) 0 0	46, 84, 94, 99	0
34	BN	140/140 (100%)	0.25	1 (0%) 87 84	29, 49, 72, 82	0
34	DN	140/140 (100%)	0.08	2 (1%) 75 70	33, 53, 74, 83	0
35	BO	122/122 (100%)	-0.02	0 100 100	26, 42, 61, 65	0
35	DO	122/122 (100%)	-0.04	0 100 100	36, 57, 70, 79	0
36	BP	149/150 (99%)	0.32	2 (1%) 77 72	25, 52, 76, 85	0
36	DP	149/150 (99%)	0.52	6 (4%) 38 28	28, 54, 78, 86	0
37	BQ	141/141 (100%)	0.24	0 100 100	29, 51, 65, 78	0
37	DQ	141/141 (100%)	0.70	16 (11%) 5 3	31, 55, 69, 79	0
38	BR	118/118 (100%)	-0.11	0 100 100	23, 37, 56, 63	0
38	DR	118/118 (100%)	0.17	0 100 100	31, 50, 64, 71	0
39	BS	110/112 (98%)	0.18	1 (0%) 84 80	33, 51, 63, 76	0
39	DS	110/112 (98%)	0.79	11 (10%) 7 4	55, 76, 86, 89	0
40	BT	131/146 (89%)	-0.19	0 100 100	27, 44, 73, 86	0
40	DT	131/146 (89%)	0.04	0 100 100	42, 59, 78, 86	0
41	BU	116/118 (98%)	-0.07	1 (0%) 84 80	18, 32, 52, 73	0
41	DU	116/118 (98%)	0.26	2 (1%) 70 63	37, 58, 75, 80	0
42	BV	101/101 (100%)	-0.03	0 100 100	20, 43, 61, 76	0
42	DV	101/101 (100%)	0.84	13 (12%) 3 2	36, 67, 81, 87	0
43	BW	112/113 (99%)	0.05	1 (0%) 84 80	20, 33, 51, 84	0
43	DW	112/113 (99%)	0.29	1 (0%) 84 80	32, 47, 65, 100	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	95/96 (98%)	0.11	0 100 100	22, 37, 57, 82	0
44	DX	95/96 (98%)	0.69	8 (8%) 11 5	39, 59, 73, 82	0
45	BY	107/110 (97%)	0.00	0 100 100	32, 48, 70, 81	0
45	DY	107/110 (97%)	0.97	14 (13%) 3 2	48, 68, 78, 89	0
46	BZ	171/206 (83%)	0.46	4 (2%) 60 51	40, 63, 83, 88	0
46	DZ	174/206 (84%)	1.68	59 (33%) 0 0	64, 82, 94, 97	0
47	B0	83/85 (97%)	-0.07	0 100 100	23, 38, 52, 66	0
47	D0	83/85 (97%)	0.77	6 (7%) 15 8	36, 61, 72, 81	0
48	B1	97/98 (98%)	0.02	1 (1%) 82 77	21, 42, 65, 74	0
48	D1	97/98 (98%)	0.41	3 (3%) 49 39	30, 54, 76, 82	0
49	B2	70/72 (97%)	0.10	0 100 100	32, 48, 63, 87	0
49	D2	70/72 (97%)	0.48	4 (5%) 23 15	50, 67, 78, 83	0
50	B3	59/60 (98%)	-0.12	0 100 100	21, 37, 62, 81	0
50	D3	59/60 (98%)	0.99	6 (10%) 6 3	44, 60, 77, 87	0
51	B4	69/71 (97%)	0.62	11 (15%) 1 1	54, 76, 91, 98	0
51	D4	69/71 (97%)	1.54	24 (34%) 0 0	80, 90, 95, 99	0
52	B5	59/60 (98%)	-0.10	1 (1%) 70 63	19, 33, 53, 65	0
52	D5	59/60 (98%)	-0.04	0 100 100	28, 48, 69, 72	0
53	B6	53/54 (98%)	-0.06	0 100 100	28, 40, 60, 64	0
53	D6	53/54 (98%)	0.45	3 (5%) 23 15	43, 59, 72, 82	0
54	B7	48/49 (97%)	-0.06	0 100 100	18, 25, 54, 63	0
54	D7	48/49 (97%)	-0.00	1 (2%) 63 54	29, 39, 63, 81	0
55	B8	64/65 (98%)	-0.04	0 100 100	23, 32, 46, 61	0
55	D8	64/65 (98%)	0.42	0 100 100	37, 55, 66, 70	0
56	B9	37/37 (100%)	0.48	1 (2%) 54 44	27, 49, 67, 71	0
56	D9	37/37 (100%)	0.88	5 (13%) 3 1	46, 54, 67, 74	0
All	All	20640/21602 (95%)	0.40	1309 (6%) 20 12	18, 63, 89, 107	0

The worst 5 of 1309 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	DI	65	ALA	11.9
33	DI	119	PRO	11.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	DI	146	ALA	10.9
33	DI	128	LEU	10.8
33	DI	85	GLU	10.6

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	5MC	CX	32	21/22	0.85	0.22	68,80,88,99	0
24	4SU	CX	8	20/21	0.90	0.17	61,80,93,118	0
24	PSU	CX	55	20/21	0.91	0.16	61,72,81,89	0
24	5MU	CX	54	21/22	0.92	0.13	71,79,92,107	0
24	PSU	AX	55	20/21	0.93	0.16	58,70,77,82	0
24	5MU	AX	54	21/22	0.95	0.16	57,67,82,96	0
24	4SU	AX	8	20/21	0.95	0.17	47,59,67,84	0
24	31H	CX	76	32/33	0.95	0.23	23,42,61,84	10
24	5MC	AX	32	21/22	0.95	0.18	46,55,75,77	0
24	31H	AX	76	30/33	0.96	0.26	14,31,55,77	8
23	PPU	AW	76	37/38	0.97	0.20	12,29,37,42	0
23	PPU	CW	76	37/38	0.97	0.23	27,41,53,63	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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
57	MG	AA	3063	1/1	0.17	0.12	89,89,89,89	0
57	MG	DA	3553	1/1	0.35	0.40	75,75,75,75	0
57	MG	BA	3502	1/1	0.50	0.23	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
57	MG	BA	3674	1/1	0.55	0.19	59,59,59,59	0
57	MG	DA	3160	1/1	0.57	0.11	65,65,65,65	0
57	MG	AA	3166	1/1	0.61	0.20	70,70,70,70	0
57	MG	DW	201	1/1	0.62	0.20	70,70,70,70	0
57	MG	DV	202	1/1	0.63	0.79	75,75,75,75	0
57	MG	CA	3148	1/1	0.63	0.18	81,81,81,81	0
57	MG	DA	3069	1/1	0.63	0.49	59,59,59,59	0
57	MG	CA	3116	1/1	0.64	0.33	74,74,74,74	0
57	MG	DA	3135	1/1	0.65	0.18	61,61,61,61	0
57	MG	CA	3025	1/1	0.66	0.18	66,66,66,66	0
57	MG	DA	3548	1/1	0.66	0.15	58,58,58,58	0
57	MG	DA	3519	1/1	0.67	0.17	60,60,60,60	0
57	MG	DA	3609	1/1	0.67	0.26	55,55,55,55	0
57	MG	AA	3041	1/1	0.67	0.19	62,62,62,62	0
57	MG	AA	3007	1/1	0.68	0.20	47,47,47,47	0
57	MG	BA	3233	1/1	0.68	0.31	55,55,55,55	0
57	MG	CA	3004	1/1	0.68	0.23	70,70,70,70	0
57	MG	AA	3100	1/1	0.69	0.17	69,69,69,69	0
57	MG	AA	3064	1/1	0.69	0.14	65,65,65,65	0
57	MG	DA	3390	1/1	0.70	0.17	54,54,54,54	0
57	MG	BA	3113	1/1	0.71	0.23	57,57,57,57	0
57	MG	BA	3306	1/1	0.71	0.20	32,32,32,32	0
57	MG	AA	3054	1/1	0.71	0.16	62,62,62,62	0
57	MG	BF	309	1/1	0.71	0.41	61,61,61,61	0
57	MG	BA	3603	1/1	0.71	0.18	42,42,42,42	0
57	MG	BA	3003	1/1	0.72	0.16	44,44,44,44	0
57	MG	CA	3008	1/1	0.72	0.13	67,67,67,67	0
57	MG	DA	3580	1/1	0.73	0.11	47,47,47,47	0
57	MG	BA	3639	1/1	0.73	0.15	46,46,46,46	0
57	MG	CX	3002	1/1	0.73	0.35	75,75,75,75	0
57	MG	AA	3198	1/1	0.73	0.12	66,66,66,66	0
57	MG	AA	3085	1/1	0.73	0.15	69,69,69,69	0
57	MG	DA	3550	1/1	0.73	0.28	63,63,63,63	0
57	MG	AA	3122	1/1	0.73	0.10	52,52,52,52	0
57	MG	AF	3001	1/1	0.73	0.20	58,58,58,58	0
57	MG	DA	3102	1/1	0.74	0.14	64,64,64,64	0
57	MG	DA	3130	1/1	0.74	0.23	55,55,55,55	0
57	MG	DA	3260	1/1	0.74	0.20	43,43,43,43	0
57	MG	DA	3106	1/1	0.74	0.21	52,52,52,52	0
57	MG	AA	3109	1/1	0.75	0.26	75,75,75,75	0
57	MG	AN	502	1/1	0.75	0.17	61,61,61,61	0
57	MG	CA	3056	1/1	0.75	0.12	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
57	MG	CA	3044	1/1	0.75	0.14	59,59,59,59	0
57	MG	DB	3008	1/1	0.75	0.10	59,59,59,59	0
57	MG	BA	3062	1/1	0.75	0.26	52,52,52,52	0
57	MG	AA	3040	1/1	0.75	0.21	67,67,67,67	0
57	MG	AA	3114	1/1	0.75	0.31	57,57,57,57	0
57	MG	AA	3126	1/1	0.76	0.18	52,52,52,52	0
57	MG	DA	3027	1/1	0.76	0.18	42,42,42,42	0
57	MG	DA	3407	1/1	0.76	0.16	67,67,67,67	0
57	MG	BA	3293	1/1	0.76	0.16	43,43,43,43	0
59	ZN	D4	501	1/1	0.76	0.19	154,154,154,154	0
57	MG	DA	3374	1/1	0.76	0.15	42,42,42,42	0
57	MG	DA	3342	1/1	0.76	0.15	49,49,49,49	0
57	MG	CA	3158	1/1	0.76	0.18	66,66,66,66	0
57	MG	DA	3578	1/1	0.76	0.23	63,63,63,63	0
57	MG	AA	3190	1/1	0.77	0.12	75,75,75,75	0
57	MG	DA	3111	1/1	0.77	0.25	54,54,54,54	0
57	MG	CA	3107	1/1	0.77	0.21	89,89,89,89	0
57	MG	DA	3457	1/1	0.78	0.22	45,45,45,45	0
57	MG	AA	3080	1/1	0.78	0.16	82,82,82,82	0
57	MG	DA	3328	1/1	0.78	0.15	66,66,66,66	0
57	MG	BA	3470	1/1	0.78	0.13	69,69,69,69	0
57	MG	BA	3303	1/1	0.78	0.23	39,39,39,39	0
57	MG	DG	3001	1/1	0.78	0.09	49,49,49,49	0
57	MG	CA	3085	1/1	0.78	0.32	71,71,71,71	0
57	MG	CA	3082	1/1	0.78	0.14	71,71,71,71	0
57	MG	DA	3158	1/1	0.78	0.13	52,52,52,52	0
57	MG	DA	3565	1/1	0.78	0.20	49,49,49,49	0
57	MG	AA	3145	1/1	0.78	0.23	71,71,71,71	0
57	MG	DA	3545	1/1	0.79	0.18	70,70,70,70	0
57	MG	BA	3587	1/1	0.79	0.18	51,51,51,51	0
57	MG	AA	3146	1/1	0.79	0.11	81,81,81,81	0
57	MG	BA	3328	1/1	0.79	0.09	55,55,55,55	0
57	MG	DE	303	1/1	0.79	0.17	49,49,49,49	0
57	MG	BA	3604	1/1	0.79	0.10	62,62,62,62	0
57	MG	CA	3040	1/1	0.79	0.26	67,67,67,67	0
57	MG	AA	3111	1/1	0.79	0.13	70,70,70,70	0
57	MG	DA	3276	1/1	0.79	0.17	56,56,56,56	0
57	MG	BA	3216	1/1	0.79	0.17	35,35,35,35	0
57	MG	DA	3303	1/1	0.79	0.19	57,57,57,57	0
57	MG	BA	3158	1/1	0.79	0.29	48,48,48,48	0
57	MG	AA	3042	1/1	0.79	0.17	52,52,52,52	0
57	MG	BA	3467	1/1	0.80	0.23	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
57	MG	BA	3422	1/1	0.80	0.15	39,39,39,39	0
57	MG	AA	3125	1/1	0.80	0.11	60,60,60,60	0
57	MG	BA	3487	1/1	0.80	0.11	70,70,70,70	0
57	MG	AA	3181	1/1	0.80	0.07	82,82,82,82	0
57	MG	DA	3520	1/1	0.80	0.20	51,51,51,51	0
57	MG	DA	3307	1/1	0.80	0.21	51,51,51,51	0
57	MG	CA	3113	1/1	0.80	0.17	75,75,75,75	0
57	MG	AA	3001	1/1	0.80	0.13	72,72,72,72	0
57	MG	CA	3042	1/1	0.80	0.16	68,68,68,68	0
57	MG	BA	3261	1/1	0.80	0.19	52,52,52,52	0
57	MG	DA	3134	1/1	0.81	0.16	59,59,59,59	0
57	MG	DA	3003	1/1	0.81	0.19	56,56,56,56	0
57	MG	DA	3436	1/1	0.81	0.12	61,61,61,61	0
57	MG	DA	3304	1/1	0.81	0.14	44,44,44,44	0
57	MG	CA	3066	1/1	0.81	0.18	69,69,69,69	0
57	MG	BA	3570	1/1	0.81	0.11	48,48,48,48	0
57	MG	AA	3043	1/1	0.81	0.27	59,59,59,59	0
57	MG	CA	3137	1/1	0.81	0.17	81,81,81,81	0
57	MG	BB	3020	1/1	0.81	0.16	55,55,55,55	0
57	MG	DA	3162	1/1	0.81	0.43	58,58,58,58	0
57	MG	AX	3008	1/1	0.81	0.11	58,58,58,58	0
57	MG	CA	3015	1/1	0.81	0.11	61,61,61,61	0
57	MG	BZ	3001	1/1	0.81	0.28	56,56,56,56	0
57	MG	CE	3001	1/1	0.81	0.19	80,80,80,80	0
57	MG	DD	307	1/1	0.81	0.12	50,50,50,50	0
57	MG	BA	3579	1/1	0.81	0.32	44,44,44,44	0
57	MG	BA	3651	1/1	0.81	0.25	62,62,62,62	0
57	MG	DA	3054	1/1	0.81	0.17	40,40,40,40	0
57	MG	BA	3608	1/1	0.81	0.09	50,50,50,50	0
57	MG	DA	3533	1/1	0.81	0.49	47,47,47,47	0
57	MG	BA	3199	1/1	0.81	0.27	60,60,60,60	0
57	MG	BA	3002	1/1	0.82	0.14	45,45,45,45	0
57	MG	BA	3331	1/1	0.82	0.26	39,39,39,39	0
57	MG	CA	3030	1/1	0.82	0.10	75,75,75,75	0
57	MG	CA	3005	1/1	0.82	0.12	81,81,81,81	0
57	MG	CA	3133	1/1	0.82	0.19	69,69,69,69	0
57	MG	CA	3038	1/1	0.82	0.13	68,68,68,68	0
57	MG	DA	3410	1/1	0.82	0.23	37,37,37,37	0
57	MG	DA	3555	1/1	0.82	0.15	70,70,70,70	0
57	MG	BA	3396	1/1	0.82	0.24	20,20,20,20	0
57	MG	BA	3020	1/1	0.82	0.30	55,55,55,55	0
57	MG	BA	3351	1/1	0.82	0.11	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
57	MG	AA	3008	1/1	0.82	0.11	65,65,65,65	0
57	MG	AA	3097	1/1	0.82	0.17	45,45,45,45	0
57	MG	DA	3087	1/1	0.82	0.14	65,65,65,65	0
57	MG	BA	3079	1/1	0.82	0.23	55,55,55,55	0
57	MG	DA	3132	1/1	0.82	0.14	53,53,53,53	0
57	MG	BA	3109	1/1	0.82	0.14	53,53,53,53	0
57	MG	DA	3446	1/1	0.82	0.23	37,37,37,37	0
57	MG	AA	3105	1/1	0.82	0.26	59,59,59,59	0
57	MG	AA	3127	1/1	0.82	0.28	73,73,73,73	0
57	MG	DA	3608	1/1	0.82	0.15	61,61,61,61	0
57	MG	DA	3119	1/1	0.82	0.20	52,52,52,52	0
57	MG	DA	3406	1/1	0.82	0.15	62,62,62,62	0
59	ZN	CN	501	1/1	0.82	0.07	101,101,101,101	0
57	MG	BA	3175	1/1	0.82	0.18	55,55,55,55	0
57	MG	AA	3069	1/1	0.82	0.11	75,75,75,75	0
57	MG	BA	3180	1/1	0.83	0.27	32,32,32,32	0
57	MG	DA	3105	1/1	0.83	0.21	37,37,37,37	0
57	MG	CA	3126	1/1	0.83	0.36	73,73,73,73	0
57	MG	DF	3001	1/1	0.83	0.12	36,36,36,36	0
57	MG	CA	3019	1/1	0.83	0.12	57,57,57,57	0
57	MG	AA	3170	1/1	0.83	0.15	70,70,70,70	0
57	MG	DA	3546	1/1	0.83	0.14	41,41,41,41	0
57	MG	DA	3439	1/1	0.83	0.17	44,44,44,44	0
57	MG	CA	3052	1/1	0.83	0.09	61,61,61,61	0
57	MG	DA	3193	1/1	0.83	0.21	43,43,43,43	0
57	MG	BA	3258	1/1	0.83	0.22	35,35,35,35	0
57	MG	DA	3297	1/1	0.83	0.14	48,48,48,48	0
57	MG	BA	3130	1/1	0.83	0.38	39,39,39,39	0
57	MG	CA	3092	1/1	0.83	0.16	76,76,76,76	0
57	MG	DA	3283	1/1	0.83	0.14	40,40,40,40	0
57	MG	BA	3366	1/1	0.83	0.22	38,38,38,38	0
57	MG	CA	3055	1/1	0.83	0.13	66,66,66,66	0
57	MG	DA	3217	1/1	0.83	0.35	50,50,50,50	0
57	MG	BQ	3003	1/1	0.83	0.74	68,68,68,68	0
57	MG	CA	3023	1/1	0.83	0.10	88,88,88,88	0
57	MG	CA	3058	1/1	0.83	0.35	70,70,70,70	0
57	MG	DA	3624	1/1	0.83	0.28	66,66,66,66	0
57	MG	CA	3096	1/1	0.83	0.17	51,51,51,51	0
57	MG	BA	3221	1/1	0.83	0.25	59,59,59,59	0
57	MG	BA	3700	1/1	0.83	0.20	69,69,69,69	0
57	MG	BA	3166	1/1	0.83	0.27	45,45,45,45	0
57	MG	DA	3224	1/1	0.83	0.29	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3252	1/1	0.83	0.12	63,63,63,63	0
57	MG	BA	3611	1/1	0.83	0.12	61,61,61,61	0
57	MG	CA	3033	1/1	0.83	0.15	67,67,67,67	0
57	MG	DA	3013	1/1	0.84	0.15	43,43,43,43	0
57	MG	DA	3072	1/1	0.84	0.37	46,46,46,46	0
57	MG	DA	3368	1/1	0.84	0.09	58,58,58,58	0
57	MG	CA	3043	1/1	0.84	0.13	68,68,68,68	0
57	MG	BA	3347	1/1	0.84	0.22	32,32,32,32	0
57	MG	CA	3035	1/1	0.84	0.28	63,63,63,63	0
57	MG	DA	3337	1/1	0.84	0.22	46,46,46,46	0
57	MG	BA	3136	1/1	0.84	0.21	56,56,56,56	0
57	MG	BA	3178	1/1	0.84	0.24	52,52,52,52	0
57	MG	CA	3059	1/1	0.84	0.18	60,60,60,60	0
57	MG	CA	3031	1/1	0.84	0.10	55,55,55,55	0
57	MG	BA	3543	1/1	0.84	0.11	69,69,69,69	0
57	MG	DA	3148	1/1	0.84	0.20	45,45,45,45	0
57	MG	CA	3067	1/1	0.84	0.15	45,45,45,45	0
57	MG	DA	3547	1/1	0.84	0.25	68,68,68,68	0
57	MG	BA	3177	1/1	0.84	0.20	39,39,39,39	0
57	MG	CA	3135	1/1	0.84	0.11	85,85,85,85	0
57	MG	AA	3051	1/1	0.84	0.27	51,51,51,51	0
57	MG	AA	3004	1/1	0.84	0.17	61,61,61,61	0
57	MG	CA	3007	1/1	0.84	0.14	55,55,55,55	0
57	MG	DA	3495	1/1	0.84	0.11	48,48,48,48	0
57	MG	BA	3474	1/1	0.84	0.17	64,64,64,64	0
57	MG	AA	3056	1/1	0.84	0.31	66,66,66,66	0
57	MG	DA	3554	1/1	0.84	0.18	46,46,46,46	0
57	MG	DA	3191	1/1	0.84	0.08	54,54,54,54	0
57	MG	BA	3507	1/1	0.84	0.17	48,48,48,48	0
57	MG	CA	3041	1/1	0.85	0.10	62,62,62,62	0
57	MG	AA	3047	1/1	0.85	0.21	59,59,59,59	0
57	MG	DA	3110	1/1	0.85	0.10	60,60,60,60	0
57	MG	DA	3369	1/1	0.85	0.26	36,36,36,36	0
57	MG	AA	3141	1/1	0.85	0.11	54,54,54,54	0
57	MG	BA	3494	1/1	0.85	0.22	30,30,30,30	0
57	MG	BA	3334	1/1	0.85	0.18	37,37,37,37	0
57	MG	DA	3083	1/1	0.85	0.24	30,30,30,30	0
57	MG	DA	3090	1/1	0.85	0.16	52,52,52,52	0
57	MG	CA	3120	1/1	0.85	0.27	72,72,72,72	0
57	MG	DA	3430	1/1	0.85	0.21	26,26,26,26	0
57	MG	B7	103	1/1	0.85	0.21	51,51,51,51	0
57	MG	BA	3445	1/1	0.85	0.21	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
57	MG	CA	3017	1/1	0.85	0.29	69,69,69,69	0
57	MG	DA	3114	1/1	0.85	0.14	51,51,51,51	0
57	MG	BA	3406	1/1	0.85	0.22	24,24,24,24	0
57	MG	BA	3618	1/1	0.85	0.10	64,64,64,64	0
57	MG	BA	3094	1/1	0.85	0.15	46,46,46,46	0
57	MG	CA	3003	1/1	0.85	0.13	74,74,74,74	0
57	MG	DA	3266	1/1	0.85	0.14	45,45,45,45	0
57	MG	DA	3197	1/1	0.85	0.15	35,35,35,35	0
57	MG	BA	3112	1/1	0.85	0.29	58,58,58,58	0
57	MG	BA	3304	1/1	0.85	0.26	49,49,49,49	0
57	MG	CA	3114	1/1	0.85	0.24	96,96,96,96	0
57	MG	BA	3299	1/1	0.85	0.20	27,27,27,27	0
57	MG	DA	3577	1/1	0.85	0.18	25,25,25,25	0
57	MG	DA	3070	1/1	0.85	0.22	35,35,35,35	0
57	MG	BA	3610	1/1	0.85	0.19	60,60,60,60	0
57	MG	BA	3091	1/1	0.85	0.18	56,56,56,56	0
57	MG	BD	308	1/1	0.85	0.32	41,41,41,41	0
57	MG	BA	3326	1/1	0.85	0.15	40,40,40,40	0
57	MG	DA	3568	1/1	0.85	0.14	45,45,45,45	0
57	MG	CA	3130	1/1	0.85	0.16	88,88,88,88	0
57	MG	CA	3012	1/1	0.85	0.34	45,45,45,45	0
57	MG	DA	3628	1/1	0.85	0.56	59,59,59,59	0
57	MG	DA	3367	1/1	0.85	0.15	24,24,24,24	0
57	MG	DA	3425	1/1	0.85	0.13	40,40,40,40	0
57	MG	BA	3052	1/1	0.85	0.25	44,44,44,44	0
57	MG	BA	3549	1/1	0.85	0.18	55,55,55,55	0
57	MG	CA	3054	1/1	0.85	0.36	53,53,53,53	0
57	MG	BA	3287	1/1	0.85	0.27	42,42,42,42	0
57	MG	AA	3121	1/1	0.85	0.10	66,66,66,66	0
57	MG	BA	3355	1/1	0.85	0.12	30,30,30,30	0
57	MG	AA	3172	1/1	0.85	0.28	54,54,54,54	0
57	MG	BA	3413	1/1	0.85	0.09	50,50,50,50	0
57	MG	BA	3416	1/1	0.86	0.15	73,73,73,73	0
57	MG	BA	3144	1/1	0.86	0.19	42,42,42,42	0
57	MG	DA	3499	1/1	0.86	0.14	47,47,47,47	0
57	MG	BA	3103	1/1	0.86	0.49	62,62,62,62	0
57	MG	DA	3223	1/1	0.86	0.11	56,56,56,56	0
57	MG	CW	101	1/1	0.86	0.19	43,43,43,43	0
57	MG	BA	3263	1/1	0.86	0.30	50,50,50,50	0
57	MG	AX	3003	1/1	0.86	0.33	66,66,66,66	0
57	MG	CA	3081	1/1	0.86	0.13	67,67,67,67	0
57	MG	BA	3182	1/1	0.86	0.18	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
57	MG	AA	3058	1/1	0.86	0.21	48,48,48,48	0
57	MG	AA	3123	1/1	0.86	0.11	59,59,59,59	0
57	MG	AA	3205	1/1	0.86	0.25	48,48,48,48	0
57	MG	DA	3311	1/1	0.86	0.18	42,42,42,42	0
57	MG	DA	3059	1/1	0.86	0.17	60,60,60,60	0
57	MG	DA	3366	1/1	0.86	0.16	40,40,40,40	0
57	MG	DB	3002	1/1	0.86	0.07	75,75,75,75	0
57	MG	DA	3043	1/1	0.86	0.15	44,44,44,44	0
57	MG	BA	3005	1/1	0.86	0.19	44,44,44,44	0
57	MG	BA	3380	1/1	0.86	0.16	55,55,55,55	0
57	MG	DA	3244	1/1	0.86	0.22	43,43,43,43	0
57	MG	DA	3625	1/1	0.86	0.26	57,57,57,57	0
57	MG	DA	3444	1/1	0.86	0.25	37,37,37,37	0
57	MG	CA	3062	1/1	0.86	0.09	73,73,73,73	0
57	MG	BA	3623	1/1	0.86	0.14	42,42,42,42	0
57	MG	DA	3189	1/1	0.86	0.19	57,57,57,57	0
57	MG	CA	3127	1/1	0.86	0.33	76,76,76,76	0
57	MG	AA	3151	1/1	0.86	0.16	72,72,72,72	0
57	MG	DA	3139	1/1	0.86	0.20	49,49,49,49	0
57	MG	DA	3602	1/1	0.86	0.25	50,50,50,50	0
57	MG	DA	3513	1/1	0.86	0.11	49,49,49,49	0
57	MG	DA	3619	1/1	0.86	0.41	63,63,63,63	0
57	MG	BA	3029	1/1	0.86	0.19	53,53,53,53	0
57	MG	DA	3566	1/1	0.86	0.08	40,40,40,40	0
57	MG	BA	3021	1/1	0.86	0.19	35,35,35,35	0
57	MG	AA	3163	1/1	0.86	0.17	70,70,70,70	0
57	MG	AA	3011	1/1	0.86	0.16	67,67,67,67	0
57	MG	BA	3066	1/1	0.86	0.20	53,53,53,53	0
57	MG	AA	3087	1/1	0.86	0.13	57,57,57,57	0
57	MG	BA	3385	1/1	0.86	0.27	34,34,34,34	0
57	MG	DA	3491	1/1	0.86	0.16	43,43,43,43	0
57	MG	BG	3002	1/1	0.86	0.12	65,65,65,65	0
57	MG	AA	3134	1/1	0.86	0.15	59,59,59,59	0
57	MG	CA	3001	1/1	0.86	0.09	53,53,53,53	0
57	MG	DA	3284	1/1	0.86	0.20	51,51,51,51	0
57	MG	DA	3154	1/1	0.86	0.16	40,40,40,40	0
57	MG	BA	3625	1/1	0.86	0.12	46,46,46,46	0
57	MG	CA	3084	1/1	0.86	0.15	58,58,58,58	0
57	MG	BA	3680	1/1	0.86	0.13	46,46,46,46	0
57	MG	CA	3142	1/1	0.87	0.20	55,55,55,55	0
57	MG	DA	3120	1/1	0.87	0.26	55,55,55,55	0
57	MG	BA	3492	1/1	0.87	0.18	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
57	MG	BA	3548	1/1	0.87	0.18	54,54,54,54	0
57	MG	DA	3088	1/1	0.87	0.20	41,41,41,41	0
57	MG	DA	3412	1/1	0.87	0.09	60,60,60,60	0
57	MG	CA	3154	1/1	0.87	0.14	68,68,68,68	0
57	MG	BA	3482	1/1	0.87	0.13	56,56,56,56	0
57	MG	AA	3066	1/1	0.87	0.09	66,66,66,66	0
57	MG	DA	3259	1/1	0.87	0.14	39,39,39,39	0
57	MG	BA	3164	1/1	0.87	0.28	44,44,44,44	0
57	MG	DA	3558	1/1	0.87	0.09	45,45,45,45	0
57	MG	BA	3298	1/1	0.87	0.25	50,50,50,50	0
57	MG	DA	3141	1/1	0.87	0.23	37,37,37,37	0
57	MG	BA	3425	1/1	0.87	0.20	28,28,28,28	0
57	MG	BA	3691	1/1	0.87	0.32	54,54,54,54	0
57	MG	BA	3689	1/1	0.87	0.14	46,46,46,46	0
57	MG	CA	3050	1/1	0.87	0.11	56,56,56,56	0
57	MG	DA	3011	1/1	0.87	0.12	36,36,36,36	0
57	MG	AA	3028	1/1	0.87	0.17	58,58,58,58	0
57	MG	BA	3243	1/1	0.87	0.23	46,46,46,46	0
57	MG	CA	3060	1/1	0.87	0.16	78,78,78,78	0
57	MG	BA	3566	1/1	0.87	0.17	31,31,31,31	0
57	MG	DA	3046	1/1	0.87	0.33	50,50,50,50	0
57	MG	CA	3124	1/1	0.87	0.17	57,57,57,57	0
57	MG	CA	3139	1/1	0.87	0.09	82,82,82,82	0
57	MG	BA	3295	1/1	0.87	0.14	56,56,56,56	0
57	MG	DA	3312	1/1	0.87	0.20	30,30,30,30	0
57	MG	DA	3036	1/1	0.87	0.14	48,48,48,48	0
57	MG	BU	201	1/1	0.87	0.11	36,36,36,36	0
57	MG	CA	3149	1/1	0.87	0.10	49,49,49,49	0
57	MG	BA	3360	1/1	0.87	0.16	60,60,60,60	0
57	MG	BA	3527	1/1	0.87	0.17	37,37,37,37	0
57	MG	DA	3187	1/1	0.87	0.23	39,39,39,39	0
57	MG	AA	3076	1/1	0.87	0.19	62,62,62,62	0
57	MG	CA	3032	1/1	0.87	0.42	58,58,58,58	0
57	MG	BA	3078	1/1	0.87	0.20	55,55,55,55	0
57	MG	BA	3412	1/1	0.87	0.40	44,44,44,44	0
57	MG	AA	3113	1/1	0.87	0.29	54,54,54,54	0
57	MG	BA	3281	1/1	0.87	0.26	46,46,46,46	0
57	MG	CA	3155	1/1	0.87	0.16	66,66,66,66	0
57	MG	DA	3600	1/1	0.87	0.10	45,45,45,45	0
57	MG	CA	3029	1/1	0.87	0.16	48,48,48,48	0
57	MG	DA	3205	1/1	0.87	0.12	52,52,52,52	0
57	MG	AA	3156	1/1	0.87	0.15	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3060	1/1	0.87	0.22	59,59,59,59	0
57	MG	DA	3037	1/1	0.87	0.16	41,41,41,41	0
57	MG	DA	3587	1/1	0.87	0.20	35,35,35,35	0
57	MG	BA	3515	1/1	0.87	0.17	44,44,44,44	0
57	MG	AA	3062	1/1	0.87	0.23	57,57,57,57	0
57	MG	BA	3514	1/1	0.87	0.37	36,36,36,36	0
57	MG	BA	3153	1/1	0.87	0.12	53,53,53,53	0
57	MG	AA	3180	1/1	0.87	0.21	61,61,61,61	0
57	MG	DA	3291	1/1	0.87	0.21	56,56,56,56	0
57	MG	DA	3370	1/1	0.87	0.12	72,72,72,72	0
57	MG	B5	101	1/1	0.87	0.21	30,30,30,30	0
57	MG	BA	3104	1/1	0.87	0.20	54,54,54,54	0
57	MG	BA	3097	1/1	0.87	0.20	44,44,44,44	0
57	MG	DA	3421	1/1	0.87	0.07	31,31,31,31	0
57	MG	CA	3026	1/1	0.87	0.13	59,59,59,59	0
57	MG	DA	3137	1/1	0.87	0.28	48,48,48,48	0
57	MG	DA	3077	1/1	0.88	0.19	58,58,58,58	0
57	MG	BA	3242	1/1	0.88	0.22	45,45,45,45	0
57	MG	BA	3143	1/1	0.88	0.19	41,41,41,41	0
57	MG	DA	3596	1/1	0.88	0.25	71,71,71,71	0
57	MG	BA	3350	1/1	0.88	0.16	43,43,43,43	0
57	MG	BA	3683	1/1	0.88	0.27	44,44,44,44	0
57	MG	DA	3402	1/1	0.88	0.15	47,47,47,47	0
57	MG	DA	3455	1/1	0.88	0.35	34,34,34,34	0
57	MG	DA	3496	1/1	0.88	0.19	63,63,63,63	0
57	MG	BA	3719	1/1	0.88	0.09	53,53,53,53	0
57	MG	AS	101	1/1	0.88	0.09	55,55,55,55	0
57	MG	BA	3291	1/1	0.88	0.18	44,44,44,44	0
57	MG	DA	3503	1/1	0.88	0.19	51,51,51,51	0
57	MG	DA	3226	1/1	0.88	0.18	54,54,54,54	0
57	MG	DA	3023	1/1	0.88	0.21	35,35,35,35	0
57	MG	BA	3636	1/1	0.88	0.29	45,45,45,45	0
57	MG	BA	3063	1/1	0.88	0.14	39,39,39,39	0
57	MG	DA	3601	1/1	0.88	0.12	43,43,43,43	0
57	MG	DA	3605	1/1	0.88	0.08	64,64,64,64	0
57	MG	DA	3293	1/1	0.88	0.19	41,41,41,41	0
57	MG	DA	3591	1/1	0.88	0.10	69,69,69,69	0
57	MG	CA	3098	1/1	0.88	0.07	76,76,76,76	0
57	MG	BA	3542	1/1	0.88	0.12	40,40,40,40	0
57	MG	DA	3509	1/1	0.88	0.24	42,42,42,42	0
57	MG	BA	3709	1/1	0.88	0.33	45,45,45,45	0
57	MG	DA	3204	1/1	0.88	0.19	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
57	MG	BA	3615	1/1	0.88	0.13	60,60,60,60	0
57	MG	CA	3102	1/1	0.88	0.12	56,56,56,56	0
57	MG	DA	3353	1/1	0.88	0.12	42,42,42,42	0
57	MG	DA	3574	1/1	0.88	0.14	59,59,59,59	0
57	MG	BA	3235	1/1	0.88	0.18	52,52,52,52	0
57	MG	BE	3002	1/1	0.88	0.45	50,50,50,50	0
57	MG	DA	3305	1/1	0.88	0.07	48,48,48,48	0
57	MG	CA	3099	1/1	0.88	0.22	50,50,50,50	0
57	MG	BA	3234	1/1	0.88	0.43	39,39,39,39	0
57	MG	AA	3065	1/1	0.88	0.11	48,48,48,48	0
57	MG	CA	3022	1/1	0.88	0.28	55,55,55,55	0
57	MG	AA	3104	1/1	0.88	0.15	47,47,47,47	0
57	MG	DA	3345	1/1	0.88	0.19	28,28,28,28	0
57	MG	DA	3117	1/1	0.88	0.12	40,40,40,40	0
57	MG	BA	3534	1/1	0.88	0.28	23,23,23,23	0
57	MG	DD	305	1/1	0.88	0.35	48,48,48,48	0
57	MG	BA	3333	1/1	0.88	0.10	58,58,58,58	0
57	MG	BF	305	1/1	0.88	0.15	33,33,33,33	0
57	MG	DA	3356	1/1	0.88	0.23	53,53,53,53	0
57	MG	CA	3106	1/1	0.88	0.14	65,65,65,65	0
57	MG	DA	3615	1/1	0.88	0.15	36,36,36,36	0
57	MG	BA	3583	1/1	0.88	0.10	54,54,54,54	0
57	MG	AX	3010	1/1	0.88	0.14	61,61,61,61	0
57	MG	DA	3564	1/1	0.88	0.17	48,48,48,48	0
57	MG	BA	3129	1/1	0.88	0.13	30,30,30,30	0
57	MG	AA	3143	1/1	0.88	0.15	32,32,32,32	0
57	MG	DA	3122	1/1	0.88	0.13	58,58,58,58	0
57	MG	DA	3452	1/1	0.88	0.19	40,40,40,40	0
57	MG	DA	3461	1/1	0.88	0.13	55,55,55,55	0
57	MG	DA	3219	1/1	0.88	0.22	54,54,54,54	0
57	MG	CA	3152	1/1	0.88	0.15	66,66,66,66	0
57	MG	BA	3247	1/1	0.88	0.18	37,37,37,37	0
57	MG	BA	3070	1/1	0.88	0.20	44,44,44,44	0
57	MG	CA	3088	1/1	0.88	0.11	61,61,61,61	0
57	MG	DA	3458	1/1	0.88	0.08	44,44,44,44	0
57	MG	DA	3597	1/1	0.88	0.09	42,42,42,42	0
57	MG	BA	3601	1/1	0.89	0.18	69,69,69,69	0
57	MG	BA	3519	1/1	0.89	0.16	26,26,26,26	0
57	MG	DA	3292	1/1	0.89	0.12	29,29,29,29	0
57	MG	BA	3361	1/1	0.89	0.08	38,38,38,38	0
57	MG	DA	3256	1/1	0.89	0.12	52,52,52,52	0
57	MG	BA	3146	1/1	0.89	0.19	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3610	1/1	0.89	0.16	42,42,42,42	0
57	MG	CA	3129	1/1	0.89	0.21	83,83,83,83	0
57	MG	BA	3665	1/1	0.89	0.14	50,50,50,50	0
57	MG	DA	3146	1/1	0.89	0.11	44,44,44,44	0
57	MG	DA	3626	1/1	0.89	0.22	38,38,38,38	0
57	MG	AA	3073	1/1	0.89	0.13	59,59,59,59	0
57	MG	BA	3577	1/1	0.89	0.24	35,35,35,35	0
57	MG	DA	3592	1/1	0.89	0.14	62,62,62,62	0
57	MG	AA	3150	1/1	0.89	0.09	65,65,65,65	0
57	MG	BA	3525	1/1	0.89	0.18	49,49,49,49	0
57	MG	BA	3429	1/1	0.89	0.13	37,37,37,37	0
57	MG	BA	3204	1/1	0.89	0.13	61,61,61,61	0
57	MG	BA	3533	1/1	0.89	0.28	45,45,45,45	0
57	MG	BA	3011	1/1	0.89	0.18	32,32,32,32	0
57	MG	CA	3095	1/1	0.89	0.25	52,52,52,52	0
57	MG	BA	3047	1/1	0.89	0.23	44,44,44,44	0
57	MG	BA	3337	1/1	0.89	0.15	51,51,51,51	0
57	MG	DO	5001	1/1	0.89	0.17	53,53,53,53	0
57	MG	AA	3168	1/1	0.89	0.09	56,56,56,56	0
57	MG	BA	3183	1/1	0.89	0.25	50,50,50,50	0
57	MG	AD	303	1/1	0.89	0.21	60,60,60,60	0
57	MG	BA	3388	1/1	0.89	0.15	31,31,31,31	0
57	MG	DA	3064	1/1	0.89	0.31	52,52,52,52	0
57	MG	DA	3047	1/1	0.89	0.19	44,44,44,44	0
57	MG	BA	3033	1/1	0.89	0.16	39,39,39,39	0
57	MG	BA	3372	1/1	0.89	0.09	58,58,58,58	0
57	MG	DA	3267	1/1	0.89	0.28	45,45,45,45	0
57	MG	BA	3595	1/1	0.89	0.21	52,52,52,52	0
57	MG	BA	3349	1/1	0.89	0.19	55,55,55,55	0
57	MG	CA	3109	1/1	0.89	0.19	61,61,61,61	0
57	MG	AA	3090	1/1	0.89	0.20	70,70,70,70	0
57	MG	DA	3063	1/1	0.89	0.10	40,40,40,40	0
57	MG	DA	3595	1/1	0.89	0.14	65,65,65,65	0
57	MG	CA	3048	1/1	0.89	0.18	48,48,48,48	0
57	MG	AA	3162	1/1	0.89	0.10	40,40,40,40	0
57	MG	BA	3523	1/1	0.89	0.14	31,31,31,31	0
57	MG	BA	3571	1/1	0.89	0.20	24,24,24,24	0
57	MG	D8	102	1/1	0.89	0.25	63,63,63,63	0
57	MG	DA	3281	1/1	0.89	0.13	37,37,37,37	0
57	MG	DA	3061	1/1	0.89	0.28	36,36,36,36	0
57	MG	BA	3316	1/1	0.89	0.18	49,49,49,49	0
57	MG	DA	3066	1/1	0.89	0.10	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3308	1/1	0.89	0.14	52,52,52,52	0
57	MG	DA	3562	1/1	0.89	0.10	58,58,58,58	0
57	MG	DA	3287	1/1	0.89	0.29	58,58,58,58	0
57	MG	DA	3248	1/1	0.89	0.20	59,59,59,59	0
57	MG	AA	3053	1/1	0.89	0.17	54,54,54,54	0
57	MG	AA	3193	1/1	0.89	0.31	77,77,77,77	0
57	MG	BA	3162	1/1	0.89	0.20	39,39,39,39	0
57	MG	DA	3001	1/1	0.89	0.37	45,45,45,45	0
57	MG	DA	3314	1/1	0.89	0.14	56,56,56,56	0
57	MG	BA	3231	1/1	0.89	0.21	42,42,42,42	0
57	MG	BA	3565	1/1	0.89	0.10	50,50,50,50	0
57	MG	BA	3229	1/1	0.89	0.51	52,52,52,52	0
57	MG	DA	3161	1/1	0.89	0.23	35,35,35,35	0
57	MG	DA	3362	1/1	0.89	0.27	48,48,48,48	0
57	MG	CA	3027	1/1	0.89	0.08	62,62,62,62	0
57	MG	DA	3575	1/1	0.89	0.21	19,19,19,19	0
57	MG	BA	3447	1/1	0.89	0.13	44,44,44,44	0
57	MG	BA	3088	1/1	0.89	0.42	59,59,59,59	0
57	MG	DA	3056	1/1	0.89	0.08	35,35,35,35	0
57	MG	BB	3004	1/1	0.89	0.11	43,43,43,43	0
57	MG	BA	3027	1/1	0.89	1.04	36,36,36,36	0
57	MG	BA	3203	1/1	0.89	0.23	56,56,56,56	0
57	MG	AA	3188	1/1	0.89	0.10	62,62,62,62	0
57	MG	DA	3322	1/1	0.89	0.18	51,51,51,51	0
57	MG	DA	3138	1/1	0.89	0.21	39,39,39,39	0
57	MG	CA	3094	1/1	0.89	0.09	80,80,80,80	0
57	MG	BA	3223	1/1	0.89	0.15	38,38,38,38	0
57	MG	BA	3501	1/1	0.90	0.07	67,67,67,67	0
57	MG	DA	3095	1/1	0.90	0.25	45,45,45,45	0
57	MG	AA	3089	1/1	0.90	0.20	61,61,61,61	0
57	MG	CA	3064	1/1	0.90	0.16	64,64,64,64	0
57	MG	AA	3017	1/1	0.90	0.15	63,63,63,63	0
57	MG	AA	3033	1/1	0.90	0.19	43,43,43,43	0
57	MG	DA	3380	1/1	0.90	0.13	65,65,65,65	0
57	MG	DA	3143	1/1	0.90	0.21	47,47,47,47	0
57	MG	BA	3581	1/1	0.90	0.08	55,55,55,55	0
57	MG	DA	3116	1/1	0.90	0.22	36,36,36,36	0
57	MG	BF	304	1/1	0.90	0.26	35,35,35,35	0
57	MG	B7	102	1/1	0.90	0.32	53,53,53,53	0
57	MG	DA	3196	1/1	0.90	0.23	46,46,46,46	0
57	MG	AA	3005	1/1	0.90	0.16	66,66,66,66	0
57	MG	CA	3147	1/1	0.90	0.12	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
57	MG	BA	3381	1/1	0.90	0.17	30,30,30,30	0
57	MG	BA	3526	1/1	0.90	0.16	48,48,48,48	0
57	MG	CA	3110	1/1	0.90	0.19	56,56,56,56	0
57	MG	DA	3067	1/1	0.90	0.13	54,54,54,54	0
57	MG	DA	3028	1/1	0.90	0.15	52,52,52,52	0
57	MG	BA	3466	1/1	0.90	0.25	57,57,57,57	0
57	MG	DA	3280	1/1	0.90	0.19	49,49,49,49	0
57	MG	BE	3006	1/1	0.90	0.34	72,72,72,72	0
57	MG	DA	3007	1/1	0.90	0.08	48,48,48,48	0
57	MG	BA	3371	1/1	0.90	0.16	53,53,53,53	0
57	MG	BA	3632	1/1	0.90	0.11	43,43,43,43	0
57	MG	BA	3238	1/1	0.90	0.27	26,26,26,26	0
57	MG	BA	3650	1/1	0.90	0.10	49,49,49,49	0
59	ZN	D9	501	1/1	0.90	0.07	75,75,75,75	0
57	MG	AA	3155	1/1	0.90	0.24	65,65,65,65	0
57	MG	BA	3139	1/1	0.90	0.32	45,45,45,45	0
57	MG	BA	3031	1/1	0.90	0.13	51,51,51,51	0
57	MG	AA	3014	1/1	0.90	0.14	73,73,73,73	0
57	MG	DW	202	1/1	0.90	0.18	43,43,43,43	0
57	MG	DE	301	1/1	0.90	0.10	52,52,52,52	0
57	MG	BA	3669	1/1	0.90	0.19	34,34,34,34	0
57	MG	CJ	5001	1/1	0.90	0.12	51,51,51,51	0
57	MG	BA	3532	1/1	0.90	0.24	39,39,39,39	0
57	MG	BR	202	1/1	0.90	0.18	49,49,49,49	0
57	MG	CA	3057	1/1	0.90	0.11	48,48,48,48	0
57	MG	DA	3034	1/1	0.90	0.26	46,46,46,46	0
57	MG	AA	3124	1/1	0.90	0.21	58,58,58,58	0
57	MG	DA	3201	1/1	0.90	0.27	42,42,42,42	0
57	MG	DA	3008	1/1	0.90	0.22	26,26,26,26	0
57	MG	DA	3448	1/1	0.90	0.25	36,36,36,36	0
57	MG	AA	3039	1/1	0.90	0.28	62,62,62,62	0
57	MG	BA	3061	1/1	0.90	0.10	58,58,58,58	0
57	MG	DA	3103	1/1	0.90	0.32	55,55,55,55	0
57	MG	DA	3598	1/1	0.90	0.11	48,48,48,48	0
57	MG	DA	3364	1/1	0.90	0.17	49,49,49,49	0
57	MG	DA	3557	1/1	0.90	0.07	54,54,54,54	0
57	MG	DA	3539	1/1	0.90	0.26	52,52,52,52	0
57	MG	BA	3419	1/1	0.90	0.24	58,58,58,58	0
57	MG	BA	3214	1/1	0.90	0.22	48,48,48,48	0
57	MG	AA	3154	1/1	0.90	0.19	46,46,46,46	0
57	MG	BA	3257	1/1	0.90	0.30	40,40,40,40	0
57	MG	BB	3005	1/1	0.90	0.17	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
57	MG	B0	103	1/1	0.90	0.12	38,38,38,38	0
57	MG	BA	3111	1/1	0.90	0.29	51,51,51,51	0
57	MG	AA	3098	1/1	0.90	0.14	42,42,42,42	0
57	MG	DA	3255	1/1	0.90	0.28	34,34,34,34	0
57	MG	AA	3173	1/1	0.90	0.20	53,53,53,53	0
57	MG	DA	3508	1/1	0.90	0.10	58,58,58,58	0
57	MG	BA	3426	1/1	0.90	0.18	30,30,30,30	0
57	MG	BN	3002	1/1	0.90	0.25	46,46,46,46	0
57	MG	BA	3574	1/1	0.90	0.12	41,41,41,41	0
57	MG	DQ	3003	1/1	0.90	0.28	59,59,59,59	0
57	MG	DA	3426	1/1	0.90	0.34	38,38,38,38	0
57	MG	BA	3232	1/1	0.90	0.18	31,31,31,31	0
57	MG	BA	3322	1/1	0.90	0.18	40,40,40,40	0
57	MG	CA	3078	1/1	0.90	0.18	63,63,63,63	0
57	MG	CA	3140	1/1	0.90	0.07	48,48,48,48	0
57	MG	BB	3001	1/1	0.90	0.16	44,44,44,44	0
57	MG	BA	3453	1/1	0.90	0.11	47,47,47,47	0
57	MG	CA	3119	1/1	0.90	0.09	74,74,74,74	0
57	MG	BA	3217	1/1	0.90	0.36	57,57,57,57	0
57	MG	BA	3712	1/1	0.90	0.11	30,30,30,30	0
57	MG	DA	3375	1/1	0.90	0.23	30,30,30,30	0
57	MG	DA	3515	1/1	0.90	0.17	53,53,53,53	0
57	MG	DA	3627	1/1	0.90	0.21	56,56,56,56	0
57	MG	DA	3068	1/1	0.90	0.17	48,48,48,48	0
57	MG	BA	3465	1/1	0.90	0.17	44,44,44,44	0
57	MG	DA	3428	1/1	0.90	0.19	46,46,46,46	0
57	MG	DA	3263	1/1	0.91	0.13	47,47,47,47	0
57	MG	DA	3613	1/1	0.91	0.38	45,45,45,45	0
57	MG	BA	3218	1/1	0.91	0.59	52,52,52,52	0
57	MG	BA	3500	1/1	0.91	0.10	54,54,54,54	0
57	MG	DA	3394	1/1	0.91	0.11	48,48,48,48	0
57	MG	BA	3152	1/1	0.91	0.25	45,45,45,45	0
57	MG	BA	3584	1/1	0.91	0.10	59,59,59,59	0
57	MG	AA	3096	1/1	0.91	0.06	57,57,57,57	0
57	MG	DA	3572	1/1	0.91	0.13	46,46,46,46	0
57	MG	BA	3149	1/1	0.91	0.19	40,40,40,40	0
57	MG	BA	3556	1/1	0.91	0.16	52,52,52,52	0
57	MG	BA	3656	1/1	0.91	0.15	57,57,57,57	0
57	MG	DA	3147	1/1	0.91	0.18	42,42,42,42	0
57	MG	DA	3129	1/1	0.91	0.12	41,41,41,41	0
57	MG	BA	3509	1/1	0.91	0.32	34,34,34,34	0
57	MG	DA	3417	1/1	0.91	0.20	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3069	1/1	0.91	0.33	56,56,56,56	0
57	MG	DA	3484	1/1	0.91	0.10	41,41,41,41	0
57	MG	DA	3133	1/1	0.91	0.14	52,52,52,52	0
57	MG	BA	3018	1/1	0.91	0.21	58,58,58,58	0
57	MG	AA	3072	1/1	0.91	0.08	65,65,65,65	0
57	MG	CA	3036	1/1	0.91	0.11	47,47,47,47	0
57	MG	BD	310	1/1	0.91	0.39	34,34,34,34	0
57	MG	AA	3070	1/1	0.91	0.24	43,43,43,43	0
57	MG	CA	3075	1/1	0.91	0.17	48,48,48,48	0
57	MG	BA	3616	1/1	0.91	0.17	32,32,32,32	0
57	MG	DA	3257	1/1	0.91	0.34	46,46,46,46	0
57	MG	B9	502	1/1	0.91	0.12	31,31,31,31	0
57	MG	DA	3569	1/1	0.91	0.15	42,42,42,42	0
57	MG	AA	3149	1/1	0.91	0.14	48,48,48,48	0
57	MG	CA	3083	1/1	0.91	0.27	71,71,71,71	0
57	MG	BA	3692	1/1	0.91	0.17	64,64,64,64	0
57	MG	AA	3086	1/1	0.91	0.13	45,45,45,45	0
57	MG	BA	3173	1/1	0.91	0.27	28,28,28,28	0
57	MG	DA	3178	1/1	0.91	0.21	39,39,39,39	0
57	MG	BB	3019	1/1	0.91	0.15	62,62,62,62	0
57	MG	DA	3611	1/1	0.91	0.18	58,58,58,58	0
57	MG	DA	3265	1/1	0.91	0.14	33,33,33,33	0
57	MG	BA	3174	1/1	0.91	0.16	44,44,44,44	0
57	MG	DB	3009	1/1	0.91	0.21	55,55,55,55	0
57	MG	AA	3027	1/1	0.91	0.18	55,55,55,55	0
57	MG	DA	3019	1/1	0.91	0.18	54,54,54,54	0
57	MG	DA	3492	1/1	0.91	0.10	45,45,45,45	0
57	MG	AX	3006	1/1	0.91	0.27	59,59,59,59	0
57	MG	DA	3622	1/1	0.91	1.08	58,58,58,58	0
57	MG	CA	3097	1/1	0.91	0.23	43,43,43,43	0
57	MG	BA	3210	1/1	0.91	0.15	42,42,42,42	0
57	MG	DA	3527	1/1	0.91	0.26	52,52,52,52	0
57	MG	CA	3122	1/1	0.91	0.09	50,50,50,50	0
57	MG	DA	3018	1/1	0.91	0.33	51,51,51,51	0
57	MG	AA	3084	1/1	0.91	0.14	43,43,43,43	0
57	MG	DA	3319	1/1	0.91	0.33	45,45,45,45	0
57	MG	AJ	201	1/1	0.91	0.08	67,67,67,67	0
57	MG	DA	3617	1/1	0.91	0.18	40,40,40,40	0
57	MG	BA	3379	1/1	0.91	0.10	69,69,69,69	0
57	MG	BA	3598	1/1	0.91	0.22	54,54,54,54	0
57	MG	DA	3449	1/1	0.91	0.09	52,52,52,52	0
57	MG	AA	3160	1/1	0.91	0.24	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
57	MG	BA	3001	1/1	0.91	0.20	48,48,48,48	0
57	MG	DA	3576	1/1	0.91	0.27	46,46,46,46	0
57	MG	CA	3125	1/1	0.91	0.14	64,64,64,64	0
57	MG	BA	3613	1/1	0.91	0.09	74,74,74,74	0
57	MG	DA	3327	1/1	0.91	0.12	49,49,49,49	0
57	MG	DA	3326	1/1	0.91	0.10	40,40,40,40	0
57	MG	AA	3185	1/1	0.91	0.15	50,50,50,50	0
57	MG	DA	3497	1/1	0.91	0.18	61,61,61,61	0
57	MG	BU	206	1/1	0.91	0.36	39,39,39,39	0
57	MG	DA	3021	1/1	0.91	0.13	50,50,50,50	0
57	MG	DA	3038	1/1	0.91	0.11	39,39,39,39	0
57	MG	DA	3093	1/1	0.91	0.13	45,45,45,45	0
57	MG	DA	3524	1/1	0.91	0.10	40,40,40,40	0
57	MG	AA	3016	1/1	0.91	0.14	52,52,52,52	0
57	MG	DA	3091	1/1	0.91	0.21	37,37,37,37	0
57	MG	BA	3024	1/1	0.91	0.15	42,42,42,42	0
57	MG	DA	3081	1/1	0.91	0.31	45,45,45,45	0
57	MG	CA	3013	1/1	0.91	0.17	45,45,45,45	0
57	MG	DA	3563	1/1	0.91	0.15	55,55,55,55	0
57	MG	DA	3427	1/1	0.91	0.20	26,26,26,26	0
57	MG	DA	3511	1/1	0.91	0.18	40,40,40,40	0
57	MG	BA	3658	1/1	0.91	0.22	16,16,16,16	0
57	MG	DA	3522	1/1	0.91	0.17	41,41,41,41	0
57	MG	BA	3699	1/1	0.91	0.10	33,33,33,33	0
57	MG	BA	3099	1/1	0.91	0.33	36,36,36,36	0
57	MG	BA	3374	1/1	0.91	0.15	48,48,48,48	0
57	MG	BA	3590	1/1	0.91	0.23	62,62,62,62	0
57	MG	DA	3032	1/1	0.91	0.18	34,34,34,34	0
57	MG	DA	3453	1/1	0.91	0.22	44,44,44,44	0
57	MG	BA	3241	1/1	0.91	0.32	53,53,53,53	0
57	MG	BD	306	1/1	0.91	0.30	30,30,30,30	0
57	MG	AA	3055	1/1	0.91	0.31	53,53,53,53	0
57	MG	DA	3389	1/1	0.91	0.15	31,31,31,31	0
57	MG	BB	3009	1/1	0.91	0.18	63,63,63,63	0
57	MG	AA	3171	1/1	0.91	0.16	45,45,45,45	0
57	MG	DA	3288	1/1	0.91	0.25	32,32,32,32	0
57	MG	AA	3026	1/1	0.91	0.08	61,61,61,61	0
57	MG	CA	3053	1/1	0.91	0.17	59,59,59,59	0
57	MG	BA	3092	1/1	0.91	0.14	32,32,32,32	0
57	MG	CA	3117	1/1	0.91	0.13	100,100,100,100	0
57	MG	BA	3032	1/1	0.91	0.23	30,30,30,30	0
57	MG	AA	3046	1/1	0.91	0.18	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
57	MG	BA	3535	1/1	0.91	0.25	29,29,29,29	0
57	MG	BA	3404	1/1	0.91	0.22	30,30,30,30	0
57	MG	BA	3635	1/1	0.91	0.11	59,59,59,59	0
57	MG	DA	3194	1/1	0.92	0.28	43,43,43,43	0
57	MG	DA	3075	1/1	0.92	0.11	40,40,40,40	0
57	MG	BA	3262	1/1	0.92	0.27	38,38,38,38	0
57	MG	DA	3530	1/1	0.92	0.10	43,43,43,43	0
57	MG	DA	3521	1/1	0.92	0.09	57,57,57,57	0
57	MG	BA	3511	1/1	0.92	0.20	41,41,41,41	0
57	MG	BW	201	1/1	0.92	0.18	48,48,48,48	0
57	MG	DA	3347	1/1	0.92	0.19	32,32,32,32	0
57	MG	B0	102	1/1	0.92	0.13	53,53,53,53	0
57	MG	BA	3075	1/1	0.92	0.35	45,45,45,45	0
57	MG	DA	3473	1/1	0.92	0.20	32,32,32,32	0
57	MG	BA	3284	1/1	0.92	0.12	41,41,41,41	0
57	MG	BA	3476	1/1	0.92	0.14	37,37,37,37	0
57	MG	BA	3017	1/1	0.92	0.23	48,48,48,48	0
57	MG	DA	3422	1/1	0.92	0.26	40,40,40,40	0
57	MG	BA	3704	1/1	0.92	0.13	31,31,31,31	0
57	MG	DA	3450	1/1	0.92	0.17	34,34,34,34	0
57	MG	DA	3346	1/1	0.92	0.12	39,39,39,39	0
57	MG	BA	3513	1/1	0.92	0.12	55,55,55,55	0
57	MG	DA	3035	1/1	0.92	0.19	45,45,45,45	0
57	MG	BA	3597	1/1	0.92	0.30	56,56,56,56	0
57	MG	DA	3415	1/1	0.92	0.37	55,55,55,55	0
57	MG	CF	3001	1/1	0.92	0.17	51,51,51,51	0
57	MG	DA	3285	1/1	0.92	0.12	50,50,50,50	0
57	MG	BA	3022	1/1	0.92	0.22	47,47,47,47	0
57	MG	DA	3212	1/1	0.92	0.08	47,47,47,47	0
57	MG	AA	3176	1/1	0.92	0.09	43,43,43,43	0
57	MG	DA	3113	1/1	0.92	0.24	42,42,42,42	0
57	MG	DA	3062	1/1	0.92	0.24	49,49,49,49	0
57	MG	BA	3300	1/1	0.92	0.12	55,55,55,55	0
57	MG	DA	3344	1/1	0.92	0.13	42,42,42,42	0
57	MG	BA	3266	1/1	0.92	0.21	53,53,53,53	0
57	MG	BA	3510	1/1	0.92	0.24	20,20,20,20	0
57	MG	BA	3230	1/1	0.92	0.35	45,45,45,45	0
57	MG	DA	3104	1/1	0.92	0.19	47,47,47,47	0
57	MG	AA	3199	1/1	0.92	0.17	58,58,58,58	0
57	MG	BA	3675	1/1	0.92	0.19	41,41,41,41	0
57	MG	AA	3031	1/1	0.92	0.10	41,41,41,41	0
57	MG	BA	3015	1/1	0.92	0.15	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
57	MG	DA	3514	1/1	0.92	0.20	34,34,34,34	0
57	MG	BA	3176	1/1	0.92	0.23	35,35,35,35	0
57	MG	AA	3158	1/1	0.92	0.09	72,72,72,72	0
57	MG	BA	3342	1/1	0.92	0.20	38,38,38,38	0
57	MG	DA	3153	1/1	0.92	0.15	34,34,34,34	0
57	MG	BA	3397	1/1	0.92	0.11	33,33,33,33	0
57	MG	DA	3107	1/1	0.92	0.17	39,39,39,39	0
57	MG	DA	3155	1/1	0.92	0.22	34,34,34,34	0
57	MG	AA	3018	1/1	0.92	0.14	62,62,62,62	0
57	MG	DA	3125	1/1	0.92	0.11	48,48,48,48	0
57	MG	D8	101	1/1	0.92	0.15	60,60,60,60	0
57	MG	BA	3455	1/1	0.92	0.17	44,44,44,44	0
57	MG	BA	3168	1/1	0.92	0.19	32,32,32,32	0
57	MG	DA	3246	1/1	0.92	0.30	57,57,57,57	0
57	MG	BU	208	1/1	0.92	0.43	39,39,39,39	0
57	MG	BA	3317	1/1	0.92	0.14	49,49,49,49	0
57	MG	BA	3237	1/1	0.92	0.15	36,36,36,36	0
57	MG	DA	3099	1/1	0.92	0.15	40,40,40,40	0
57	MG	AV	3001	1/1	0.92	0.20	59,59,59,59	0
57	MG	DA	3488	1/1	0.92	0.14	47,47,47,47	0
57	MG	DA	3543	1/1	0.92	0.14	61,61,61,61	0
57	MG	DA	3607	1/1	0.92	0.18	73,73,73,73	0
57	MG	AA	3059	1/1	0.92	0.30	61,61,61,61	0
57	MG	BB	3018	1/1	0.92	0.10	43,43,43,43	0
57	MG	DA	3264	1/1	0.92	0.10	33,33,33,33	0
57	MG	BB	3012	1/1	0.92	0.16	33,33,33,33	0
57	MG	BA	3497	1/1	0.92	0.19	41,41,41,41	0
57	MG	AM	201	1/1	0.92	0.05	43,43,43,43	0
57	MG	BA	3105	1/1	0.92	0.25	45,45,45,45	0
57	MG	BA	3344	1/1	0.92	0.19	48,48,48,48	0
57	MG	DA	3517	1/1	0.92	0.18	36,36,36,36	0
57	MG	DA	3250	1/1	0.92	0.16	41,41,41,41	0
57	MG	BA	3559	1/1	0.92	0.17	36,36,36,36	0
57	MG	BA	3135	1/1	0.92	0.19	48,48,48,48	0
57	MG	DA	3182	1/1	0.92	0.39	52,52,52,52	0
57	MG	CA	3136	1/1	0.92	0.11	68,68,68,68	0
57	MG	BA	3155	1/1	0.92	0.20	44,44,44,44	0
57	MG	BB	3008	1/1	0.92	0.11	60,60,60,60	0
57	MG	BW	203	1/1	0.92	0.17	39,39,39,39	0
57	MG	DA	3383	1/1	0.92	0.13	45,45,45,45	0
57	MG	AA	3192	1/1	0.92	0.12	72,72,72,72	0
57	MG	BA	3120	1/1	0.92	0.36	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
57	MG	DA	3317	1/1	0.92	0.24	42,42,42,42	0
57	MG	BA	3698	1/1	0.92	0.30	51,51,51,51	0
57	MG	DA	3216	1/1	0.92	0.29	43,43,43,43	0
57	MG	DB	3010	1/1	0.92	0.20	55,55,55,55	0
57	MG	AA	3003	1/1	0.92	0.10	53,53,53,53	0
57	MG	CA	3010	1/1	0.92	0.20	56,56,56,56	0
57	MG	DA	3498	1/1	0.92	0.07	66,66,66,66	0
57	MG	CA	3045	1/1	0.92	0.15	53,53,53,53	0
57	MG	BA	3115	1/1	0.92	0.48	49,49,49,49	0
57	MG	BA	3702	1/1	0.92	0.12	41,41,41,41	0
57	MG	BD	311	1/1	0.92	0.36	60,60,60,60	0
57	MG	CA	3018	1/1	0.92	0.13	47,47,47,47	0
57	MG	BA	3684	1/1	0.92	0.10	47,47,47,47	0
57	MG	BA	3324	1/1	0.92	0.21	61,61,61,61	0
57	MG	BF	302	1/1	0.92	0.18	59,59,59,59	0
57	MG	DA	3268	1/1	0.92	0.12	35,35,35,35	0
57	MG	DB	3003	1/1	0.92	0.06	76,76,76,76	0
57	MG	BA	3068	1/1	0.92	0.15	46,46,46,46	0
57	MG	BA	3279	1/1	0.92	0.21	48,48,48,48	0
57	MG	BA	3437	1/1	0.92	0.23	52,52,52,52	0
57	MG	CT	3001	1/1	0.92	0.07	59,59,59,59	0
57	MG	BA	3122	1/1	0.92	0.21	39,39,39,39	0
57	MG	BA	3454	1/1	0.92	0.14	45,45,45,45	0
57	MG	DA	3431	1/1	0.92	0.15	56,56,56,56	0
57	MG	BA	3207	1/1	0.92	0.16	55,55,55,55	0
57	MG	AA	3068	1/1	0.92	0.12	64,64,64,64	0
57	MG	AX	3011	1/1	0.92	0.37	73,73,73,73	0
57	MG	CA	3020	1/1	0.92	0.06	51,51,51,51	0
57	MG	BA	3123	1/1	0.92	0.12	56,56,56,56	0
57	MG	AA	3032	1/1	0.92	0.11	80,80,80,80	0
57	MG	DA	3109	1/1	0.92	0.18	45,45,45,45	0
57	MG	BA	3411	1/1	0.92	0.23	24,24,24,24	0
57	MG	CA	3024	1/1	0.92	0.07	58,58,58,58	0
57	MG	DA	3343	1/1	0.92	0.10	37,37,37,37	0
57	MG	DA	3221	1/1	0.92	0.13	49,49,49,49	0
57	MG	BA	3688	1/1	0.92	0.34	46,46,46,46	0
57	MG	DU	3004	1/1	0.92	0.18	69,69,69,69	0
57	MG	DA	3379	1/1	0.92	0.16	37,37,37,37	0
57	MG	DA	3094	1/1	0.92	0.19	38,38,38,38	0
57	MG	DA	3198	1/1	0.92	0.08	41,41,41,41	0
57	MG	DA	3271	1/1	0.92	0.21	47,47,47,47	0
57	MG	BA	3415	1/1	0.92	0.22	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
57	MG	DA	3371	1/1	0.92	0.23	47,47,47,47	0
57	MG	CA	3070	1/1	0.92	0.24	42,42,42,42	0
57	MG	DA	3040	1/1	0.92	0.42	48,48,48,48	0
57	MG	BA	3547	1/1	0.93	0.18	33,33,33,33	0
57	MG	BA	3516	1/1	0.93	0.14	32,32,32,32	0
57	MG	DA	3170	1/1	0.93	0.37	47,47,47,47	0
57	MG	BA	3108	1/1	0.93	0.15	36,36,36,36	0
57	MG	BA	3301	1/1	0.93	0.23	43,43,43,43	0
57	MG	DA	3262	1/1	0.93	0.08	39,39,39,39	0
57	MG	BA	3522	1/1	0.93	0.11	34,34,34,34	0
57	MG	BA	3715	1/1	0.93	0.15	33,33,33,33	0
57	MG	DA	3537	1/1	0.93	0.21	45,45,45,45	0
57	MG	BA	3313	1/1	0.93	0.15	30,30,30,30	0
57	MG	BA	3228	1/1	0.93	0.28	33,33,33,33	0
57	MG	DA	3331	1/1	0.93	0.26	54,54,54,54	0
57	MG	BA	3378	1/1	0.93	0.18	45,45,45,45	0
57	MG	DA	3089	1/1	0.93	0.19	36,36,36,36	0
57	MG	DA	3167	1/1	0.93	0.17	26,26,26,26	0
57	MG	BA	3268	1/1	0.93	0.16	45,45,45,45	0
57	MG	DA	3338	1/1	0.93	0.11	36,36,36,36	0
57	MG	BA	3156	1/1	0.93	0.13	43,43,43,43	0
57	MG	AA	3006	1/1	0.93	0.17	62,62,62,62	0
57	MG	BA	3250	1/1	0.93	0.15	47,47,47,47	0
57	MG	BA	3399	1/1	0.93	0.15	26,26,26,26	0
57	MG	BA	3499	1/1	0.93	0.22	51,51,51,51	0
57	MG	BA	3460	1/1	0.93	0.14	43,43,43,43	0
57	MG	BA	3098	1/1	0.93	0.59	50,50,50,50	0
57	MG	DA	3384	1/1	0.93	0.09	41,41,41,41	0
57	MG	CA	3105	1/1	0.93	0.16	76,76,76,76	0
57	MG	BA	3049	1/1	0.93	0.25	53,53,53,53	0
57	MG	DA	3115	1/1	0.93	0.13	58,58,58,58	0
57	MG	BA	3336	1/1	0.93	0.09	47,47,47,47	0
57	MG	DA	3048	1/1	0.93	0.16	53,53,53,53	0
57	MG	DA	3590	1/1	0.93	0.10	58,58,58,58	0
57	MG	DA	3571	1/1	0.93	0.19	54,54,54,54	0
57	MG	BA	3065	1/1	0.93	0.27	43,43,43,43	0
57	MG	DA	3616	1/1	0.93	0.13	28,28,28,28	0
57	MG	AA	3020	1/1	0.93	0.19	62,62,62,62	0
57	MG	BA	3557	1/1	0.93	0.17	35,35,35,35	0
57	MG	BA	3224	1/1	0.93	0.45	48,48,48,48	0
57	MG	DP	202	1/1	0.93	0.28	48,48,48,48	0
57	MG	BA	3433	1/1	0.93	0.12	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
57	MG	BA	3357	1/1	0.93	0.20	31,31,31,31	0
57	MG	BA	3205	1/1	0.93	0.12	52,52,52,52	0
57	MG	BA	3660	1/1	0.93	0.11	62,62,62,62	0
57	MG	BA	3107	1/1	0.93	0.28	49,49,49,49	0
57	MG	DA	3388	1/1	0.93	0.21	33,33,33,33	0
57	MG	BA	3213	1/1	0.93	0.15	48,48,48,48	0
57	MG	BA	3521	1/1	0.93	0.28	32,32,32,32	0
57	MG	BA	3409	1/1	0.93	0.27	27,27,27,27	0
57	MG	DA	3582	1/1	0.93	0.16	24,24,24,24	0
57	MG	AA	3202	1/1	0.93	0.06	60,60,60,60	0
57	MG	DA	3501	1/1	0.93	0.24	47,47,47,47	0
57	MG	BA	3524	1/1	0.93	0.12	39,39,39,39	0
57	MG	AA	3048	1/1	0.93	0.19	42,42,42,42	0
57	MG	DA	3432	1/1	0.93	0.12	33,33,33,33	0
57	MG	DF	3003	1/1	0.93	0.17	36,36,36,36	0
57	MG	BA	3286	1/1	0.93	0.15	33,33,33,33	0
57	MG	BA	3054	1/1	0.93	0.25	44,44,44,44	0
57	MG	BA	3642	1/1	0.93	0.17	50,50,50,50	0
57	MG	BA	3308	1/1	0.93	0.15	14,14,14,14	0
57	MG	CA	3151	1/1	0.93	0.12	58,58,58,58	0
57	MG	DA	3142	1/1	0.93	0.23	50,50,50,50	0
57	MG	BA	3093	1/1	0.93	0.16	23,23,23,23	0
57	MG	DA	3528	1/1	0.93	0.12	60,60,60,60	0
57	MG	DA	3278	1/1	0.93	0.07	38,38,38,38	0
57	MG	BA	3555	1/1	0.93	0.08	62,62,62,62	0
57	MG	DA	3360	1/1	0.93	0.11	54,54,54,54	0
57	MG	BA	3424	1/1	0.93	0.21	29,29,29,29	0
57	MG	BA	3410	1/1	0.93	0.19	40,40,40,40	0
57	MG	BA	3310	1/1	0.93	0.21	43,43,43,43	0
57	MG	DA	3581	1/1	0.93	0.17	53,53,53,53	0
57	MG	DA	3411	1/1	0.93	0.09	51,51,51,51	0
57	MG	BA	3585	1/1	0.93	0.16	45,45,45,45	0
57	MG	CA	3016	1/1	0.93	0.05	52,52,52,52	0
57	MG	AA	3034	1/1	0.93	0.08	47,47,47,47	0
57	MG	DA	3376	1/1	0.93	0.24	40,40,40,40	0
57	MG	DA	3419	1/1	0.93	0.20	37,37,37,37	0
57	MG	DF	3004	1/1	0.93	0.27	56,56,56,56	0
57	MG	DA	3350	1/1	0.93	0.36	44,44,44,44	0
57	MG	BN	3003	1/1	0.93	0.25	61,61,61,61	0
57	MG	BA	3179	1/1	0.93	0.20	49,49,49,49	0
57	MG	BA	3710	1/1	0.93	0.11	21,21,21,21	0
57	MG	BA	3064	1/1	0.93	0.16	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
57	MG	AA	3131	1/1	0.93	0.20	56,56,56,56	0
57	MG	BA	3673	1/1	0.93	0.11	55,55,55,55	0
57	MG	BA	3666	1/1	0.93	0.17	79,79,79,79	0
57	MG	BA	3552	1/1	0.93	0.11	59,59,59,59	0
57	MG	DA	3225	1/1	0.93	0.14	42,42,42,42	0
57	MG	BA	3055	1/1	0.93	0.20	43,43,43,43	0
57	MG	DA	3082	1/1	0.93	0.17	47,47,47,47	0
57	MG	BA	3591	1/1	0.93	0.10	42,42,42,42	0
57	MG	AX	3005	1/1	0.93	0.32	57,57,57,57	0
57	MG	CA	3128	1/1	0.93	0.12	43,43,43,43	0
57	MG	DA	3234	1/1	0.93	0.30	34,34,34,34	0
57	MG	DA	3112	1/1	0.93	0.14	63,63,63,63	0
57	MG	DA	3251	1/1	0.93	0.28	34,34,34,34	0
57	MG	BA	3138	1/1	0.93	0.26	57,57,57,57	0
57	MG	DA	3076	1/1	0.93	0.34	53,53,53,53	0
57	MG	DA	3213	1/1	0.93	0.30	51,51,51,51	0
57	MG	CA	3111	1/1	0.93	0.08	65,65,65,65	0
57	MG	BA	3249	1/1	0.93	0.22	44,44,44,44	0
57	MG	DA	3097	1/1	0.93	0.16	50,50,50,50	0
57	MG	BA	3320	1/1	0.93	0.12	56,56,56,56	0
57	MG	DA	3490	1/1	0.93	0.10	62,62,62,62	0
57	MG	AA	3195	1/1	0.93	0.10	58,58,58,58	0
57	MG	DA	3593	1/1	0.93	0.20	49,49,49,49	0
57	MG	CA	3068	1/1	0.93	0.12	53,53,53,53	0
57	MG	BA	3621	1/1	0.93	0.13	18,18,18,18	0
57	MG	BA	3222	1/1	0.93	0.20	52,52,52,52	0
57	MG	BA	3605	1/1	0.93	0.24	44,44,44,44	0
57	MG	AA	3197	1/1	0.93	0.14	50,50,50,50	0
57	MG	AA	3037	1/1	0.93	0.11	48,48,48,48	0
57	MG	BA	3717	1/1	0.93	0.43	40,40,40,40	0
57	MG	BA	3273	1/1	0.93	0.17	30,30,30,30	0
57	MG	CA	3093	1/1	0.93	0.16	69,69,69,69	0
57	MG	AA	3025	1/1	0.93	0.18	46,46,46,46	0
57	MG	AA	3021	1/1	0.93	0.16	58,58,58,58	0
57	MG	DA	3538	1/1	0.93	0.22	77,77,77,77	0
57	MG	BA	3505	1/1	0.93	0.20	16,16,16,16	0
57	MG	BA	3297	1/1	0.93	0.22	36,36,36,36	0
57	MG	CA	3051	1/1	0.93	0.30	57,57,57,57	0
57	MG	DA	3413	1/1	0.93	0.29	30,30,30,30	0
57	MG	AA	3106	1/1	0.93	0.07	53,53,53,53	0
57	MG	DA	3603	1/1	0.93	0.14	40,40,40,40	0
57	MG	AA	3019	1/1	0.93	0.12	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
57	MG	AA	3128	1/1	0.93	0.22	53,53,53,53	0
57	MG	CA	3091	1/1	0.93	0.20	75,75,75,75	0
57	MG	BA	3431	1/1	0.93	0.22	25,25,25,25	0
57	MG	BA	3215	1/1	0.93	0.10	53,53,53,53	0
57	MG	DA	3159	1/1	0.93	0.14	32,32,32,32	0
57	MG	BA	3006	1/1	0.93	0.14	38,38,38,38	0
57	MG	AE	3001	1/1	0.93	0.37	85,85,85,85	0
57	MG	BA	3401	1/1	0.93	0.28	31,31,31,31	0
57	MG	BA	3421	1/1	0.93	0.18	29,29,29,29	0
57	MG	BA	3450	1/1	0.93	0.07	45,45,45,45	0
57	MG	BA	3377	1/1	0.93	0.24	58,58,58,58	0
57	MG	BA	3564	1/1	0.93	0.19	44,44,44,44	0
57	MG	BA	3641	1/1	0.93	0.18	33,33,33,33	0
57	MG	CA	3090	1/1	0.93	0.43	64,64,64,64	0
57	MG	DA	3220	1/1	0.93	0.21	54,54,54,54	0
57	MG	AA	3050	1/1	0.93	0.17	49,49,49,49	0
57	MG	DA	3381	1/1	0.93	0.22	55,55,55,55	0
57	MG	BA	3628	1/1	0.93	0.18	60,60,60,60	0
57	MG	BR	203	1/1	0.93	0.28	31,31,31,31	0
57	MG	AA	3115	1/1	0.93	0.33	38,38,38,38	0
57	MG	DA	3318	1/1	0.93	0.19	39,39,39,39	0
57	MG	BA	3672	1/1	0.93	0.10	28,28,28,28	0
57	MG	BA	3434	1/1	0.93	0.21	27,27,27,27	0
57	MG	BA	3671	1/1	0.93	0.14	55,55,55,55	0
57	MG	BA	3134	1/1	0.93	0.17	43,43,43,43	0
57	MG	CA	3034	1/1	0.93	0.27	49,49,49,49	0
57	MG	DA	3200	1/1	0.93	0.18	38,38,38,38	0
57	MG	BU	205	1/1	0.93	0.15	32,32,32,32	0
57	MG	BA	3172	1/1	0.94	0.17	27,27,27,27	0
57	MG	BA	3708	1/1	0.94	0.16	38,38,38,38	0
57	MG	BA	3567	1/1	0.94	0.20	55,55,55,55	0
57	MG	CA	3039	1/1	0.94	0.10	52,52,52,52	0
57	MG	DA	3209	1/1	0.94	0.17	53,53,53,53	0
57	MG	BA	3282	1/1	0.94	0.10	44,44,44,44	0
57	MG	DA	3171	1/1	0.94	0.21	38,38,38,38	0
57	MG	BA	3019	1/1	0.94	0.15	30,30,30,30	0
57	MG	CA	3131	1/1	0.94	0.14	57,57,57,57	0
57	MG	BA	3446	1/1	0.94	0.09	49,49,49,49	0
57	MG	BA	3558	1/1	0.94	0.17	63,63,63,63	0
57	MG	BA	3530	1/1	0.94	0.26	20,20,20,20	0
57	MG	BA	3563	1/1	0.94	0.10	38,38,38,38	0
57	MG	DA	3467	1/1	0.94	0.16	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
57	MG	BA	3703	1/1	0.94	0.10	47,47,47,47	0
57	MG	BA	3089	1/1	0.94	0.13	30,30,30,30	0
57	MG	AA	3203	1/1	0.94	0.10	42,42,42,42	0
57	MG	BA	3200	1/1	0.94	0.24	39,39,39,39	0
57	MG	CA	3009	1/1	0.94	0.12	44,44,44,44	0
57	MG	DA	3525	1/1	0.94	0.08	40,40,40,40	0
57	MG	BA	3398	1/1	0.94	0.25	36,36,36,36	0
57	MG	BA	3132	1/1	0.94	0.18	52,52,52,52	0
57	MG	D5	101	1/1	0.94	0.20	42,42,42,42	0
57	MG	CX	3003	1/1	0.94	0.12	53,53,53,53	0
57	MG	BA	3080	1/1	0.94	0.19	51,51,51,51	0
57	MG	DA	3282	1/1	0.94	0.19	36,36,36,36	0
57	MG	BX	101	1/1	0.94	0.28	36,36,36,36	0
57	MG	DA	3559	1/1	0.94	0.21	31,31,31,31	0
57	MG	BA	3074	1/1	0.94	0.13	43,43,43,43	0
57	MG	DA	3358	1/1	0.94	0.53	45,45,45,45	0
57	MG	BA	3387	1/1	0.94	0.15	29,29,29,29	0
57	MG	DR	3001	1/1	0.94	1.12	66,66,66,66	0
57	MG	BA	3471	1/1	0.94	0.10	42,42,42,42	0
57	MG	BA	3137	1/1	0.94	0.17	57,57,57,57	0
57	MG	BA	3071	1/1	0.94	0.20	48,48,48,48	0
57	MG	BA	3392	1/1	0.94	0.18	27,27,27,27	0
57	MG	BD	302	1/1	0.94	0.24	38,38,38,38	0
57	MG	DA	3434	1/1	0.94	0.09	48,48,48,48	0
57	MG	DA	3045	1/1	0.94	0.13	39,39,39,39	0
60	K	AX	3001	1/1	0.94	0.10	39,39,39,39	0
57	MG	DA	3502	1/1	0.94	0.14	51,51,51,51	0
57	MG	BA	3369	1/1	0.94	0.16	57,57,57,57	0
57	MG	BA	3044	1/1	0.94	0.07	40,40,40,40	0
57	MG	BA	3540	1/1	0.94	0.20	24,24,24,24	0
57	MG	CA	3157	1/1	0.94	0.09	61,61,61,61	0
57	MG	CA	3159	1/1	0.94	0.14	46,46,46,46	0
57	MG	DA	3418	1/1	0.94	0.21	41,41,41,41	0
57	MG	BG	3001	1/1	0.94	0.18	44,44,44,44	0
57	MG	BA	3389	1/1	0.94	0.11	57,57,57,57	0
57	MG	AA	3147	1/1	0.94	0.06	51,51,51,51	0
57	MG	DA	3074	1/1	0.94	0.18	38,38,38,38	0
57	MG	BA	3059	1/1	0.94	0.29	50,50,50,50	0
57	MG	BA	3679	1/1	0.94	0.15	38,38,38,38	0
57	MG	BA	3443	1/1	0.94	0.24	38,38,38,38	0
57	MG	DA	3199	1/1	0.94	0.07	41,41,41,41	0
57	MG	DA	3409	1/1	0.94	0.08	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	3044	1/1	0.94	0.14	46,46,46,46	0
57	MG	DA	3485	1/1	0.94	0.20	41,41,41,41	0
57	MG	BA	3472	1/1	0.94	0.10	39,39,39,39	0
57	MG	DF	3002	1/1	0.94	0.12	51,51,51,51	0
57	MG	DA	3341	1/1	0.94	0.14	32,32,32,32	0
57	MG	AA	3030	1/1	0.94	0.28	41,41,41,41	0
57	MG	BA	3240	1/1	0.94	0.33	52,52,52,52	0
57	MG	BA	3148	1/1	0.94	0.20	44,44,44,44	0
57	MG	BA	3087	1/1	0.94	0.21	44,44,44,44	0
57	MG	BA	3544	1/1	0.94	0.17	52,52,52,52	0
57	MG	CA	3021	1/1	0.94	0.15	46,46,46,46	0
57	MG	DA	3058	1/1	0.94	0.21	47,47,47,47	0
57	MG	B1	101	1/1	0.94	0.41	37,37,37,37	0
57	MG	CA	3160	1/1	0.94	0.39	49,49,49,49	0
57	MG	DA	3144	1/1	0.94	0.08	48,48,48,48	0
57	MG	BA	3048	1/1	0.94	0.14	44,44,44,44	0
57	MG	DA	3118	1/1	0.94	0.09	46,46,46,46	0
57	MG	BA	3367	1/1	0.94	0.06	42,42,42,42	0
57	MG	BA	3072	1/1	0.94	0.12	32,32,32,32	0
57	MG	BA	3393	1/1	0.94	0.15	30,30,30,30	0
57	MG	BA	3119	1/1	0.94	0.24	41,41,41,41	0
57	MG	DA	3214	1/1	0.94	0.13	43,43,43,43	0
57	MG	BA	3116	1/1	0.94	0.28	54,54,54,54	0
57	MG	AA	3036	1/1	0.94	0.11	51,51,51,51	0
57	MG	DA	3185	1/1	0.94	0.20	57,57,57,57	0
57	MG	AA	3107	1/1	0.94	0.14	50,50,50,50	0
57	MG	DU	3002	1/1	0.94	0.42	67,67,67,67	0
57	MG	BA	3661	1/1	0.94	0.19	56,56,56,56	0
57	MG	BA	3364	1/1	0.94	0.21	37,37,37,37	0
57	MG	BA	3483	1/1	0.94	0.15	36,36,36,36	0
57	MG	AA	3092	1/1	0.94	0.15	36,36,36,36	0
57	MG	AA	3067	1/1	0.94	0.13	47,47,47,47	0
57	MG	DA	3459	1/1	0.94	0.43	40,40,40,40	0
57	MG	BA	3575	1/1	0.94	0.17	30,30,30,30	0
57	MG	BF	306	1/1	0.94	0.08	43,43,43,43	0
57	MG	DA	3060	1/1	0.94	0.11	50,50,50,50	0
57	MG	BO	5001	1/1	0.94	0.14	49,49,49,49	0
57	MG	BA	3251	1/1	0.94	0.27	48,48,48,48	0
57	MG	BA	3084	1/1	0.94	0.14	37,37,37,37	0
57	MG	BA	3417	1/1	0.94	0.17	49,49,49,49	0
57	MG	DA	3270	1/1	0.94	0.15	57,57,57,57	0
57	MG	DA	3002	1/1	0.94	0.31	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
57	MG	DA	3218	1/1	0.94	0.09	36,36,36,36	0
57	MG	DA	3437	1/1	0.94	0.17	48,48,48,48	0
57	MG	DA	3377	1/1	0.94	0.17	31,31,31,31	0
57	MG	BA	3260	1/1	0.94	0.26	45,45,45,45	0
57	MG	BB	3007	1/1	0.94	0.10	51,51,51,51	0
57	MG	DA	3051	1/1	0.94	0.09	54,54,54,54	0
57	MG	DA	3149	1/1	0.94	0.19	42,42,42,42	0
57	MG	DA	3510	1/1	0.94	0.13	52,52,52,52	0
57	MG	DA	3486	1/1	0.94	0.16	37,37,37,37	0
57	MG	DA	3210	1/1	0.94	0.44	57,57,57,57	0
57	MG	AX	3012	1/1	0.94	0.21	15,15,15,15	0
57	MG	AA	3099	1/1	0.94	0.11	59,59,59,59	0
57	MG	DA	3227	1/1	0.94	0.13	57,57,57,57	0
57	MG	DA	3017	1/1	0.94	0.17	58,58,58,58	0
57	MG	DA	3254	1/1	0.94	0.28	42,42,42,42	0
57	MG	BA	3626	1/1	0.94	0.22	48,48,48,48	0
57	MG	DA	3460	1/1	0.94	0.07	57,57,57,57	0
57	MG	BA	3682	1/1	0.94	0.19	30,30,30,30	0
57	MG	DA	3039	1/1	0.94	0.39	48,48,48,48	0
57	MG	BP	3001	1/1	0.94	0.43	49,49,49,49	0
57	MG	BA	3561	1/1	0.94	0.18	37,37,37,37	0
57	MG	BA	3100	1/1	0.94	0.20	40,40,40,40	0
57	MG	BA	3508	1/1	0.94	0.19	52,52,52,52	0
57	MG	BA	3073	1/1	0.94	0.29	39,39,39,39	0
57	MG	BA	3713	1/1	0.94	0.14	63,63,63,63	0
57	MG	DB	3005	1/1	0.94	0.20	54,54,54,54	0
57	MG	AA	3015	1/1	0.94	0.16	28,28,28,28	0
57	MG	DA	3506	1/1	0.94	0.21	38,38,38,38	0
57	MG	BA	3126	1/1	0.94	0.28	34,34,34,34	0
57	MG	BA	3459	1/1	0.94	0.28	44,44,44,44	0
57	MG	BA	3678	1/1	0.94	0.20	49,49,49,49	0
57	MG	DA	3188	1/1	0.94	0.21	48,48,48,48	0
57	MG	DA	3049	1/1	0.94	0.15	46,46,46,46	0
57	MG	DA	3552	1/1	0.94	0.23	43,43,43,43	0
57	MG	DA	3544	1/1	0.94	0.07	59,59,59,59	0
57	MG	BA	3614	1/1	0.94	0.12	64,64,64,64	0
57	MG	DA	3391	1/1	0.94	0.21	39,39,39,39	0
57	MG	BA	3201	1/1	0.94	0.17	44,44,44,44	0
57	MG	BA	3278	1/1	0.94	0.07	38,38,38,38	0
57	MG	CK	3001	1/1	0.94	0.18	57,57,57,57	0
57	MG	DA	3228	1/1	0.94	0.24	49,49,49,49	0
57	MG	BA	3353	1/1	0.94	0.08	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3535	1/1	0.94	0.23	21,21,21,21	0
57	MG	B0	101	1/1	0.94	0.11	33,33,33,33	0
57	MG	CA	3118	1/1	0.94	0.17	69,69,69,69	0
57	MG	DA	3108	1/1	0.94	0.15	50,50,50,50	0
57	MG	BA	3023	1/1	0.94	0.16	25,25,25,25	0
57	MG	BA	3090	1/1	0.94	0.20	50,50,50,50	0
57	MG	BA	3335	1/1	0.94	0.09	26,26,26,26	0
57	MG	AA	3133	1/1	0.94	0.16	59,59,59,59	0
57	MG	BA	3083	1/1	0.94	0.18	33,33,33,33	0
57	MG	BA	3664	1/1	0.94	0.14	66,66,66,66	0
57	MG	DA	3286	1/1	0.94	0.25	45,45,45,45	0
57	MG	DA	3442	1/1	0.94	0.23	34,34,34,34	0
57	MG	BA	3157	1/1	0.94	0.12	42,42,42,42	0
57	MG	BA	3318	1/1	0.94	0.18	39,39,39,39	0
57	MG	DA	3561	1/1	0.94	0.13	51,51,51,51	0
57	MG	AA	3135	1/1	0.94	0.08	52,52,52,52	0
57	MG	AA	3144	1/1	0.94	0.28	44,44,44,44	0
57	MG	AA	3130	1/1	0.94	0.16	52,52,52,52	0
57	MG	BA	3644	1/1	0.94	0.19	48,48,48,48	0
57	MG	BA	3711	1/1	0.94	0.19	46,46,46,46	0
57	MG	BA	3058	1/1	0.94	0.20	24,24,24,24	0
57	MG	BA	3537	1/1	0.94	0.18	35,35,35,35	0
57	MG	DA	3306	1/1	0.94	0.12	31,31,31,31	0
57	MG	AA	3079	1/1	0.94	0.06	62,62,62,62	0
57	MG	BA	3327	1/1	0.94	0.18	32,32,32,32	0
57	MG	AA	3200	1/1	0.94	0.09	58,58,58,58	0
57	MG	CA	3063	1/1	0.94	0.11	59,59,59,59	0
57	MG	AA	3175	1/1	0.94	0.32	61,61,61,61	0
57	MG	BA	3294	1/1	0.94	0.21	37,37,37,37	0
57	MG	DA	3435	1/1	0.94	0.14	59,59,59,59	0
57	MG	CA	3086	1/1	0.94	0.14	56,56,56,56	0
57	MG	BA	3469	1/1	0.94	0.18	42,42,42,42	0
57	MG	BA	3667	1/1	0.94	0.18	31,31,31,31	0
57	MG	AA	3094	1/1	0.94	0.19	54,54,54,54	0
57	MG	AX	3002	1/1	0.94	0.18	67,67,67,67	0
57	MG	DA	3236	1/1	0.94	0.10	45,45,45,45	0
57	MG	BA	3118	1/1	0.94	0.24	28,28,28,28	0
57	MG	BA	3323	1/1	0.94	0.11	59,59,59,59	0
57	MG	BA	3430	1/1	0.94	0.13	54,54,54,54	0
57	MG	BA	3458	1/1	0.94	0.14	40,40,40,40	0
57	MG	CA	3014	1/1	0.94	0.12	58,58,58,58	0
57	MG	BN	3006	1/1	0.94	0.63	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DD	306	1/1	0.94	0.38	44,44,44,44	0
57	MG	DE	302	1/1	0.94	0.61	51,51,51,51	0
57	MG	DA	3408	1/1	0.94	0.10	44,44,44,44	0
57	MG	DA	3443	1/1	0.94	0.18	27,27,27,27	0
57	MG	BA	3329	1/1	0.94	0.12	21,21,21,21	0
57	MG	BA	3181	1/1	0.94	0.19	49,49,49,49	0
57	MG	BA	3463	1/1	0.94	0.12	43,43,43,43	0
57	MG	AA	3060	1/1	0.94	0.38	49,49,49,49	0
57	MG	DA	3177	1/1	0.94	0.34	29,29,29,29	0
57	MG	BA	3448	1/1	0.94	0.08	42,42,42,42	0
57	MG	BA	3035	1/1	0.94	0.21	28,28,28,28	0
57	MG	CA	3134	1/1	0.94	0.18	72,72,72,72	0
57	MG	DD	302	1/1	0.94	0.15	50,50,50,50	0
57	MG	DA	3121	1/1	0.95	0.12	39,39,39,39	0
57	MG	DA	3084	1/1	0.95	0.17	42,42,42,42	0
57	MG	AA	3174	1/1	0.95	0.14	64,64,64,64	0
57	MG	BA	3576	1/1	0.95	0.26	29,29,29,29	0
57	MG	DA	3180	1/1	0.95	0.30	41,41,41,41	0
57	MG	DA	3325	1/1	0.95	0.12	43,43,43,43	0
57	MG	BA	3486	1/1	0.95	0.17	32,32,32,32	0
57	MG	BA	3312	1/1	0.95	0.15	44,44,44,44	0
57	MG	BA	3036	1/1	0.95	0.63	42,42,42,42	0
57	MG	BA	3012	1/1	0.95	0.16	38,38,38,38	0
57	MG	DA	3440	1/1	0.95	0.27	44,44,44,44	0
57	MG	BA	3638	1/1	0.95	0.09	41,41,41,41	0
57	MG	AA	3118	1/1	0.95	0.17	50,50,50,50	0
57	MG	AD	301	1/1	0.95	0.09	47,47,47,47	0
57	MG	BA	3395	1/1	0.95	0.18	19,19,19,19	0
57	MG	BA	3622	1/1	0.95	0.13	24,24,24,24	0
57	MG	AA	3189	1/1	0.95	0.12	69,69,69,69	0
57	MG	DA	3157	1/1	0.95	0.18	44,44,44,44	0
57	MG	BQ	3001	1/1	0.95	0.32	51,51,51,51	0
57	MG	CA	3132	1/1	0.95	0.13	51,51,51,51	0
57	MG	DA	3475	1/1	0.95	0.19	35,35,35,35	0
57	MG	BA	3271	1/1	0.95	0.34	45,45,45,45	0
57	MG	DA	3274	1/1	0.95	0.22	45,45,45,45	0
57	MG	DA	3332	1/1	0.95	0.11	52,52,52,52	0
57	MG	DA	3163	1/1	0.95	0.27	43,43,43,43	0
57	MG	DA	3079	1/1	0.95	0.14	41,41,41,41	0
57	MG	DA	3551	1/1	0.95	0.11	57,57,57,57	0
57	MG	BW	202	1/1	0.95	0.60	41,41,41,41	0
57	MG	DA	3532	1/1	0.95	0.10	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3138	1/1	0.95	0.15	66,66,66,66	0
57	MG	BE	3003	1/1	0.95	0.16	25,25,25,25	0
57	MG	DA	3404	1/1	0.95	0.08	48,48,48,48	0
57	MG	DA	3478	1/1	0.95	0.16	57,57,57,57	0
57	MG	DA	3041	1/1	0.95	0.18	36,36,36,36	0
57	MG	DA	3156	1/1	0.95	0.16	46,46,46,46	0
57	MG	BA	3067	1/1	0.95	0.25	26,26,26,26	0
57	MG	BA	3082	1/1	0.95	0.16	57,57,57,57	0
57	MG	BA	3539	1/1	0.95	0.22	18,18,18,18	0
57	MG	BA	3045	1/1	0.95	0.21	33,33,33,33	0
57	MG	DA	3313	1/1	0.95	0.05	51,51,51,51	0
57	MG	BF	308	1/1	0.95	0.19	46,46,46,46	0
57	MG	AA	3196	1/1	0.95	0.12	60,60,60,60	0
57	MG	BA	3560	1/1	0.95	0.16	54,54,54,54	0
57	MG	DA	3190	1/1	0.95	0.27	52,52,52,52	0
57	MG	AA	3035	1/1	0.95	0.38	52,52,52,52	0
59	ZN	AN	501	1/1	0.95	0.12	71,71,71,71	0
57	MG	DA	3323	1/1	0.95	0.11	39,39,39,39	0
57	MG	AA	3057	1/1	0.95	0.12	38,38,38,38	0
57	MG	BA	3096	1/1	0.95	0.18	39,39,39,39	0
57	MG	DQ	3001	1/1	0.95	0.08	58,58,58,58	0
57	MG	DA	3277	1/1	0.95	0.44	50,50,50,50	0
57	MG	AA	3045	1/1	0.95	0.11	44,44,44,44	0
57	MG	AA	3142	1/1	0.95	0.30	53,53,53,53	0
57	MG	CA	3145	1/1	0.95	0.10	49,49,49,49	0
57	MG	DA	3211	1/1	0.95	0.15	43,43,43,43	0
57	MG	AA	3074	1/1	0.95	0.26	38,38,38,38	0
57	MG	DA	3165	1/1	0.95	0.14	54,54,54,54	0
57	MG	BA	3631	1/1	0.95	0.12	53,53,53,53	0
57	MG	DA	3472	1/1	0.95	0.20	24,24,24,24	0
57	MG	BA	3028	1/1	0.95	0.13	31,31,31,31	0
57	MG	BA	3714	1/1	0.95	0.10	42,42,42,42	0
57	MG	BA	3449	1/1	0.95	0.15	31,31,31,31	0
57	MG	BA	3452	1/1	0.95	0.18	15,15,15,15	0
57	MG	BA	3668	1/1	0.95	0.19	39,39,39,39	0
57	MG	AA	3110	1/1	0.95	0.19	52,52,52,52	0
57	MG	DA	3186	1/1	0.95	0.08	33,33,33,33	0
57	MG	DA	3010	1/1	0.95	0.12	51,51,51,51	0
57	MG	BA	3013	1/1	0.95	0.28	36,36,36,36	0
57	MG	DA	3300	1/1	0.95	0.14	38,38,38,38	0
57	MG	BA	3538	1/1	0.95	0.17	25,25,25,25	0
57	MG	BA	3648	1/1	0.95	0.13	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
57	MG	BA	3069	1/1	0.95	0.21	48,48,48,48	0
57	MG	DA	3085	1/1	0.95	0.13	27,27,27,27	0
57	MG	DA	3128	1/1	0.95	0.20	45,45,45,45	0
57	MG	DA	3612	1/1	0.95	0.11	64,64,64,64	0
57	MG	BA	3582	1/1	0.95	0.16	23,23,23,23	0
57	MG	CA	3071	1/1	0.95	0.40	49,49,49,49	0
57	MG	DA	3208	1/1	0.95	0.13	50,50,50,50	0
57	MG	AN	503	1/1	0.95	0.13	61,61,61,61	0
57	MG	DA	3589	1/1	0.95	0.14	52,52,52,52	0
57	MG	DA	3352	1/1	0.95	0.24	25,25,25,25	0
57	MG	DA	3184	1/1	0.95	0.09	44,44,44,44	0
57	MG	DA	3540	1/1	0.95	0.09	43,43,43,43	0
57	MG	BA	3077	1/1	0.95	0.13	33,33,33,33	0
57	MG	DA	3299	1/1	0.95	0.13	32,32,32,32	0
57	MG	BA	3277	1/1	0.95	0.29	34,34,34,34	0
57	MG	DA	3586	1/1	0.95	0.13	21,21,21,21	0
57	MG	DA	3006	1/1	0.95	0.14	40,40,40,40	0
57	MG	BA	3633	1/1	0.95	0.14	54,54,54,54	0
57	MG	AA	3093	1/1	0.95	0.20	56,56,56,56	0
57	MG	BA	3345	1/1	0.95	0.12	36,36,36,36	0
57	MG	BA	3211	1/1	0.95	0.16	50,50,50,50	0
57	MG	BA	3375	1/1	0.95	0.27	46,46,46,46	0
57	MG	BA	3693	1/1	0.95	0.14	48,48,48,48	0
57	MG	BA	3338	1/1	0.95	0.08	50,50,50,50	0
57	MG	BA	3289	1/1	0.95	0.13	41,41,41,41	0
57	MG	BA	3151	1/1	0.95	0.13	42,42,42,42	0
57	MG	DA	3441	1/1	0.95	0.27	43,43,43,43	0
57	MG	B8	101	1/1	0.95	0.15	34,34,34,34	0
57	MG	DA	3055	1/1	0.95	0.08	35,35,35,35	0
57	MG	BA	3008	1/1	0.95	0.11	22,22,22,22	0
57	MG	CA	3065	1/1	0.95	0.09	60,60,60,60	0
57	MG	BA	3373	1/1	0.95	0.24	46,46,46,46	0
57	MG	BA	3612	1/1	0.95	0.23	58,58,58,58	0
57	MG	BA	3720	1/1	0.95	0.22	48,48,48,48	0
57	MG	DA	3230	1/1	0.95	0.22	46,46,46,46	0
57	MG	BA	3050	1/1	0.95	0.10	44,44,44,44	0
57	MG	CA	3112	1/1	0.95	0.10	31,31,31,31	0
57	MG	BA	3391	1/1	0.95	0.24	30,30,30,30	0
57	MG	AA	3152	1/1	0.95	0.09	64,64,64,64	0
57	MG	BA	3171	1/1	0.95	0.36	44,44,44,44	0
57	MG	DA	3080	1/1	0.95	0.10	64,64,64,64	0
57	MG	BA	3340	1/1	0.95	0.10	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BN	3004	1/1	0.95	0.56	49,49,49,49	0
57	MG	DA	3290	1/1	0.95	0.14	43,43,43,43	0
57	MG	BA	3189	1/1	0.95	0.19	33,33,33,33	0
57	MG	BA	3634	1/1	0.95	0.24	58,58,58,58	0
57	MG	DA	3174	1/1	0.95	0.19	38,38,38,38	0
57	MG	B2	3001	1/1	0.95	0.11	43,43,43,43	0
57	MG	CA	3150	1/1	0.95	0.12	66,66,66,66	0
57	MG	BA	3707	1/1	0.95	0.36	34,34,34,34	0
57	MG	BA	3267	1/1	0.95	0.36	33,33,33,33	0
57	MG	AA	3061	1/1	0.95	0.10	65,65,65,65	0
57	MG	AA	3112	1/1	0.95	0.14	44,44,44,44	0
57	MG	DA	3042	1/1	0.95	0.32	37,37,37,37	0
57	MG	DA	3414	1/1	0.95	0.15	37,37,37,37	0
57	MG	DP	201	1/1	0.95	0.24	61,61,61,61	0
57	MG	BA	3202	1/1	0.95	0.17	42,42,42,42	0
57	MG	BQ	3005	1/1	0.95	0.17	39,39,39,39	0
57	MG	BA	3165	1/1	0.95	0.22	34,34,34,34	0
57	MG	BA	3325	1/1	0.95	0.12	38,38,38,38	0
57	MG	BB	3011	1/1	0.95	0.12	40,40,40,40	0
57	MG	DA	3479	1/1	0.95	0.17	45,45,45,45	0
57	MG	AA	3191	1/1	0.95	0.22	56,56,56,56	0
57	MG	DA	3396	1/1	0.95	0.11	43,43,43,43	0
57	MG	BA	3400	1/1	0.95	0.20	33,33,33,33	0
57	MG	DA	3424	1/1	0.95	0.08	56,56,56,56	0
57	MG	BB	3006	1/1	0.95	0.20	42,42,42,42	0
57	MG	BA	3159	1/1	0.95	0.27	43,43,43,43	0
57	MG	DA	3275	1/1	0.95	0.18	36,36,36,36	0
57	MG	AA	3120	1/1	0.95	0.13	53,53,53,53	0
57	MG	BQ	3004	1/1	0.95	0.26	35,35,35,35	0
57	MG	AA	3159	1/1	0.95	0.14	31,31,31,31	0
57	MG	BA	3480	1/1	0.95	0.27	50,50,50,50	0
57	MG	CA	3061	1/1	0.95	0.10	87,87,87,87	0
57	MG	CA	3037	1/1	0.95	0.18	60,60,60,60	0
57	MG	BA	3649	1/1	0.95	0.13	65,65,65,65	0
57	MG	AA	3207	1/1	0.95	0.10	57,57,57,57	0
57	MG	DA	3355	1/1	0.95	0.20	48,48,48,48	0
57	MG	DA	3330	1/1	0.95	0.18	49,49,49,49	0
57	MG	DA	3504	1/1	0.95	0.17	46,46,46,46	0
57	MG	DA	3229	1/1	0.95	0.17	39,39,39,39	0
57	MG	BA	3198	1/1	0.95	0.19	45,45,45,45	0
57	MG	AA	3012	1/1	0.95	0.23	61,61,61,61	0
59	ZN	B4	501	1/1	0.95	0.06	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	3072	1/1	0.95	0.28	38,38,38,38	0
57	MG	DA	3447	1/1	0.95	0.14	48,48,48,48	0
57	MG	DA	3166	1/1	0.95	0.20	47,47,47,47	0
57	MG	BA	3464	1/1	0.95	0.20	26,26,26,26	0
57	MG	DA	3529	1/1	0.95	0.12	43,43,43,43	0
57	MG	BA	3462	1/1	0.95	0.23	51,51,51,51	0
57	MG	BA	3046	1/1	0.95	0.18	30,30,30,30	0
57	MG	AA	3010	1/1	0.95	0.05	54,54,54,54	0
57	MG	BA	3439	1/1	0.95	0.16	12,12,12,12	0
57	MG	CA	3103	1/1	0.95	0.16	71,71,71,71	0
57	MG	AX	3007	1/1	0.95	0.26	54,54,54,54	0
57	MG	BB	3014	1/1	0.95	0.08	41,41,41,41	0
57	MG	DA	3493	1/1	0.95	0.10	53,53,53,53	0
57	MG	DA	3052	1/1	0.95	0.11	33,33,33,33	0
57	MG	AA	3002	1/1	0.95	0.13	58,58,58,58	0
57	MG	BA	3578	1/1	0.95	0.14	43,43,43,43	0
57	MG	DA	3053	1/1	0.95	0.22	50,50,50,50	0
57	MG	BA	3253	1/1	0.95	0.23	28,28,28,28	0
57	MG	BA	3056	1/1	0.95	0.20	21,21,21,21	0
57	MG	BA	3677	1/1	0.95	0.24	30,30,30,30	0
57	MG	BA	3225	1/1	0.95	0.12	45,45,45,45	0
57	MG	BA	3629	1/1	0.95	0.19	37,37,37,37	0
57	MG	BA	3663	1/1	0.95	0.24	36,36,36,36	0
57	MG	BA	3594	1/1	0.95	0.11	34,34,34,34	0
57	MG	DA	3481	1/1	0.95	0.12	69,69,69,69	0
57	MG	BA	3630	1/1	0.95	0.13	72,72,72,72	0
57	MG	CA	3046	1/1	0.95	0.19	53,53,53,53	0
57	MG	DA	3202	1/1	0.95	0.48	41,41,41,41	0
57	MG	BA	3314	1/1	0.95	0.25	42,42,42,42	0
57	MG	AA	3049	1/1	0.95	0.19	43,43,43,43	0
57	MG	BA	3436	1/1	0.95	0.22	21,21,21,21	0
57	MG	BA	3589	1/1	0.95	0.14	35,35,35,35	0
57	MG	BA	3208	1/1	0.95	0.10	33,33,33,33	0
57	MG	BP	3002	1/1	0.95	0.20	32,32,32,32	0
57	MG	BA	3695	1/1	0.95	0.20	19,19,19,19	0
57	MG	BU	202	1/1	0.95	0.10	45,45,45,45	0
57	MG	DA	3405	1/1	0.96	0.08	45,45,45,45	0
57	MG	BA	3206	1/1	0.96	0.13	37,37,37,37	0
57	MG	DA	3279	1/1	0.96	0.32	50,50,50,50	0
57	MG	DA	3604	1/1	0.96	0.28	61,61,61,61	0
57	MG	DA	3334	1/1	0.96	0.13	31,31,31,31	0
57	MG	DQ	3002	1/1	0.96	0.15	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
57	MG	BA	3264	1/1	0.96	0.09	47,47,47,47	0
57	MG	BA	3701	1/1	0.96	0.19	17,17,17,17	0
57	MG	BA	3405	1/1	0.96	0.24	31,31,31,31	0
57	MG	DA	3465	1/1	0.96	0.14	45,45,45,45	0
57	MG	AA	3038	1/1	0.96	0.22	58,58,58,58	0
57	MG	AA	3119	1/1	0.96	0.13	50,50,50,50	0
57	MG	AA	3077	1/1	0.96	0.27	52,52,52,52	0
57	MG	DA	3549	1/1	0.96	0.20	47,47,47,47	0
57	MG	BA	3311	1/1	0.96	0.07	42,42,42,42	0
57	MG	CA	3146	1/1	0.96	0.15	74,74,74,74	0
57	MG	AA	3102	1/1	0.96	0.29	52,52,52,52	0
57	MG	BA	3359	1/1	0.96	0.14	56,56,56,56	0
57	MG	BA	3573	1/1	0.96	0.15	29,29,29,29	0
57	MG	BA	3408	1/1	0.96	0.21	42,42,42,42	0
57	MG	DA	3324	1/1	0.96	0.25	42,42,42,42	0
57	MG	BA	3081	1/1	0.96	0.14	26,26,26,26	0
57	MG	BA	3652	1/1	0.96	0.20	65,65,65,65	0
57	MG	BN	3001	1/1	0.96	0.47	46,46,46,46	0
57	MG	BA	3244	1/1	0.96	0.39	29,29,29,29	0
57	MG	DA	3086	1/1	0.96	0.08	41,41,41,41	0
57	MG	BA	3188	1/1	0.96	0.19	48,48,48,48	0
57	MG	AE	3002	1/1	0.96	0.16	61,61,61,61	0
57	MG	CA	3002	1/1	0.96	0.20	66,66,66,66	0
57	MG	DA	3476	1/1	0.96	0.14	49,49,49,49	0
57	MG	DA	3092	1/1	0.96	0.09	29,29,29,29	0
57	MG	AA	3178	1/1	0.96	0.19	67,67,67,67	0
57	MG	AA	3184	1/1	0.96	0.11	56,56,56,56	0
57	MG	DA	3065	1/1	0.96	0.14	38,38,38,38	0
57	MG	BA	3315	1/1	0.96	0.10	42,42,42,42	0
57	MG	AA	3204	1/1	0.96	0.23	64,64,64,64	0
57	MG	DA	3136	1/1	0.96	0.17	62,62,62,62	0
57	MG	BR	201	1/1	0.96	0.23	30,30,30,30	0
57	MG	DA	3621	1/1	0.96	0.46	61,61,61,61	0
57	MG	BA	3606	1/1	0.96	0.18	39,39,39,39	0
57	MG	BA	3491	1/1	0.96	0.16	33,33,33,33	0
57	MG	BA	3520	1/1	0.96	0.20	46,46,46,46	0
57	MG	BA	3442	1/1	0.96	0.13	51,51,51,51	0
57	MG	DA	3253	1/1	0.96	0.23	34,34,34,34	0
57	MG	AA	3161	1/1	0.96	0.20	28,28,28,28	0
57	MG	BA	3572	1/1	0.96	0.20	27,27,27,27	0
57	MG	BA	3288	1/1	0.96	0.10	37,37,37,37	0
57	MG	CA	3089	1/1	0.96	0.12	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3607	1/1	0.96	0.19	41,41,41,41	0
57	MG	BP	3003	1/1	0.96	0.14	42,42,42,42	0
57	MG	DA	3348	1/1	0.96	0.20	33,33,33,33	0
57	MG	BA	3568	1/1	0.96	0.26	43,43,43,43	0
57	MG	BA	3302	1/1	0.96	0.17	50,50,50,50	0
59	ZN	B9	501	1/1	0.96	0.13	59,59,59,59	0
57	MG	DA	3126	1/1	0.96	0.13	39,39,39,39	0
57	MG	CA	3028	1/1	0.96	0.31	57,57,57,57	0
57	MG	BA	3696	1/1	0.96	0.11	41,41,41,41	0
57	MG	DA	3020	1/1	0.96	0.19	32,32,32,32	0
57	MG	AA	3116	1/1	0.96	0.26	41,41,41,41	0
57	MG	BA	3489	1/1	0.96	0.22	36,36,36,36	0
57	MG	AA	3140	1/1	0.96	0.12	56,56,56,56	0
57	MG	BA	3647	1/1	0.96	0.12	41,41,41,41	0
57	MG	BA	3545	1/1	0.96	0.24	34,34,34,34	0
57	MG	BA	3550	1/1	0.96	0.15	60,60,60,60	0
57	MG	DA	3242	1/1	0.96	0.20	48,48,48,48	0
57	MG	DA	3057	1/1	0.96	0.25	22,22,22,22	0
57	MG	BA	3541	1/1	0.96	0.17	43,43,43,43	0
57	MG	BA	3246	1/1	0.96	0.23	46,46,46,46	0
57	MG	BA	3184	1/1	0.96	0.26	42,42,42,42	0
57	MG	AA	3023	1/1	0.96	0.07	60,60,60,60	0
57	MG	BA	3506	1/1	0.96	0.12	39,39,39,39	0
57	MG	BA	3169	1/1	0.96	0.15	40,40,40,40	0
57	MG	BA	3444	1/1	0.96	0.23	32,32,32,32	0
57	MG	DA	3531	1/1	0.96	0.07	40,40,40,40	0
57	MG	DA	3098	1/1	0.96	0.19	32,32,32,32	0
57	MG	AA	3103	1/1	0.96	0.15	42,42,42,42	0
57	MG	AA	3167	1/1	0.96	0.06	65,65,65,65	0
57	MG	CA	3006	1/1	0.96	0.13	43,43,43,43	0
57	MG	BD	305	1/1	0.96	0.16	41,41,41,41	0
57	MG	D3	3001	1/1	0.96	0.17	54,54,54,54	0
57	MG	BA	3365	1/1	0.96	0.14	40,40,40,40	0
57	MG	DA	3397	1/1	0.96	0.08	46,46,46,46	0
57	MG	BA	3051	1/1	0.96	0.18	36,36,36,36	0
60	K	CX	3001	1/1	0.96	0.08	54,54,54,54	0
57	MG	DA	3477	1/1	0.96	0.10	37,37,37,37	0
57	MG	BA	3438	1/1	0.96	0.16	19,19,19,19	0
57	MG	BA	3435	1/1	0.96	0.24	31,31,31,31	0
57	MG	DA	3526	1/1	0.96	0.10	41,41,41,41	0
57	MG	BA	3600	1/1	0.96	0.25	59,59,59,59	0
57	MG	BA	3403	1/1	0.96	0.23	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	3101	1/1	0.96	0.19	53,53,53,53	0
57	MG	BA	3248	1/1	0.96	0.24	32,32,32,32	0
57	MG	BA	3490	1/1	0.96	0.28	17,17,17,17	0
57	MG	BA	3339	1/1	0.96	0.40	52,52,52,52	0
57	MG	BA	3382	1/1	0.96	0.19	31,31,31,31	0
57	MG	CA	3074	1/1	0.96	0.23	51,51,51,51	0
57	MG	BA	3040	1/1	0.96	0.14	28,28,28,28	0
57	MG	DA	3249	1/1	0.96	0.18	48,48,48,48	0
57	MG	BA	3531	1/1	0.96	0.28	20,20,20,20	0
57	MG	BA	3517	1/1	0.96	0.14	20,20,20,20	0
57	MG	BA	3602	1/1	0.96	0.33	65,65,65,65	0
57	MG	CA	3143	1/1	0.96	0.12	59,59,59,59	0
57	MG	AA	3132	1/1	0.96	0.20	67,67,67,67	0
57	MG	AW	101	1/1	0.96	0.24	24,24,24,24	0
57	MG	DA	3468	1/1	0.96	0.26	64,64,64,64	0
57	MG	BA	3423	1/1	0.96	0.25	26,26,26,26	0
57	MG	BA	3562	1/1	0.96	0.16	47,47,47,47	0
57	MG	DA	3152	1/1	0.96	0.20	38,38,38,38	0
57	MG	DA	3542	1/1	0.96	0.10	44,44,44,44	0
57	MG	BE	3005	1/1	0.96	0.15	15,15,15,15	0
57	MG	DA	3456	1/1	0.96	0.35	59,59,59,59	0
57	MG	BA	3041	1/1	0.96	0.25	39,39,39,39	0
57	MG	BA	3038	1/1	0.96	0.06	38,38,38,38	0
57	MG	AA	3022	1/1	0.96	0.07	57,57,57,57	0
57	MG	DA	3357	1/1	0.96	0.19	29,29,29,29	0
57	MG	AA	3075	1/1	0.96	0.14	57,57,57,57	0
57	MG	BA	3484	1/1	0.96	0.08	50,50,50,50	0
57	MG	BA	3319	1/1	0.96	0.15	37,37,37,37	0
57	MG	DA	3471	1/1	0.96	0.23	23,23,23,23	0
57	MG	BA	3220	1/1	0.96	0.23	54,54,54,54	0
57	MG	BU	204	1/1	0.96	0.33	38,38,38,38	0
57	MG	DV	201	1/1	0.96	0.30	49,49,49,49	0
57	MG	BP	3004	1/1	0.96	0.11	41,41,41,41	0
57	MG	BA	3296	1/1	0.96	0.24	31,31,31,31	0
57	MG	CA	3011	1/1	0.96	0.28	39,39,39,39	0
57	MG	BA	3599	1/1	0.96	0.19	43,43,43,43	0
57	MG	DA	3623	1/1	0.96	0.16	31,31,31,31	0
57	MG	DA	3014	1/1	0.96	0.20	45,45,45,45	0
57	MG	CA	3153	1/1	0.96	0.14	57,57,57,57	0
57	MG	DA	3429	1/1	0.96	0.15	38,38,38,38	0
57	MG	CA	3076	1/1	0.96	0.20	59,59,59,59	0
57	MG	BA	3619	1/1	0.96	0.13	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
57	MG	B5	103	1/1	0.96	0.08	50,50,50,50	0
57	MG	BA	3114	1/1	0.96	0.24	41,41,41,41	0
57	MG	BA	3226	1/1	0.96	0.43	36,36,36,36	0
57	MG	DA	3351	1/1	0.96	0.34	45,45,45,45	0
57	MG	BA	3478	1/1	0.96	0.15	22,22,22,22	0
57	MG	DA	3025	1/1	0.96	0.18	35,35,35,35	0
57	MG	BA	3518	1/1	0.96	0.22	48,48,48,48	0
57	MG	BA	3551	1/1	0.96	0.24	17,17,17,17	0
57	MG	DA	3004	1/1	0.96	0.28	32,32,32,32	0
57	MG	BA	3681	1/1	0.96	0.22	42,42,42,42	0
57	MG	BF	310	1/1	0.96	0.12	51,51,51,51	0
57	MG	DY	502	1/1	0.96	0.11	56,56,56,56	0
57	MG	AA	3164	1/1	0.96	0.12	54,54,54,54	0
57	MG	DA	3400	1/1	0.96	0.13	33,33,33,33	0
57	MG	DA	3309	1/1	0.96	0.12	34,34,34,34	0
57	MG	BA	3195	1/1	0.96	0.28	46,46,46,46	0
57	MG	BA	3657	1/1	0.96	0.12	55,55,55,55	0
57	MG	BA	3390	1/1	0.96	0.09	31,31,31,31	0
57	MG	BA	3495	1/1	0.96	0.22	47,47,47,47	0
57	MG	BA	3127	1/1	0.96	0.24	41,41,41,41	0
57	MG	BA	3016	1/1	0.96	0.15	35,35,35,35	0
57	MG	AX	3009	1/1	0.96	0.12	50,50,50,50	0
57	MG	BA	3352	1/1	0.96	0.14	29,29,29,29	0
57	MG	DA	3500	1/1	0.96	0.16	32,32,32,32	0
57	MG	AA	3117	1/1	0.96	0.12	55,55,55,55	0
57	MG	DA	3438	1/1	0.96	0.13	42,42,42,42	0
57	MG	B3	3001	1/1	0.96	0.12	43,43,43,43	0
57	MG	BA	3170	1/1	0.96	0.18	41,41,41,41	0
57	MG	BA	3254	1/1	0.96	0.20	30,30,30,30	0
57	MG	BA	3646	1/1	0.96	0.09	43,43,43,43	0
57	MG	DA	3026	1/1	0.96	0.14	41,41,41,41	0
57	MG	DA	3372	1/1	0.96	0.10	49,49,49,49	0
57	MG	DA	3463	1/1	0.96	0.08	54,54,54,54	0
57	MG	DA	3222	1/1	0.96	0.22	38,38,38,38	0
57	MG	DA	3420	1/1	0.96	0.09	41,41,41,41	0
57	MG	DA	3401	1/1	0.96	0.12	36,36,36,36	0
57	MG	DA	3241	1/1	0.96	0.18	40,40,40,40	0
57	MG	DA	3175	1/1	0.96	0.24	42,42,42,42	0
57	MG	DA	3536	1/1	0.96	0.15	48,48,48,48	0
57	MG	DR	3002	1/1	0.96	0.14	51,51,51,51	0
57	MG	DA	3273	1/1	0.96	0.21	41,41,41,41	0
57	MG	DA	3516	1/1	0.96	0.07	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3133	1/1	0.96	0.24	29,29,29,29	0
57	MG	AA	3082	1/1	0.96	0.15	55,55,55,55	0
57	MG	DA	3494	1/1	0.96	0.19	56,56,56,56	0
57	MG	BA	3307	1/1	0.96	0.26	31,31,31,31	0
57	MG	BA	3451	1/1	0.96	0.17	59,59,59,59	0
57	MG	BA	3354	1/1	0.96	0.11	31,31,31,31	0
57	MG	AA	3187	1/1	0.96	0.14	47,47,47,47	0
57	MG	BA	3609	1/1	0.96	0.18	47,47,47,47	0
57	MG	BA	3034	1/1	0.96	0.11	21,21,21,21	0
57	MG	BA	3292	1/1	0.96	0.17	26,26,26,26	0
57	MG	BA	3686	1/1	0.96	0.21	36,36,36,36	0
57	MG	DA	3365	1/1	0.96	0.08	54,54,54,54	0
57	MG	DA	3583	1/1	0.96	0.14	44,44,44,44	0
57	MG	AA	3201	1/1	0.96	0.10	68,68,68,68	0
57	MG	DA	3261	1/1	0.96	0.23	38,38,38,38	0
57	MG	DA	3403	1/1	0.96	0.13	31,31,31,31	0
57	MG	BA	3007	1/1	0.96	0.13	39,39,39,39	0
57	MG	AK	3001	1/1	0.96	0.12	55,55,55,55	0
57	MG	DA	3387	1/1	0.96	0.18	29,29,29,29	0
57	MG	BA	3161	1/1	0.96	0.21	54,54,54,54	0
57	MG	BA	3468	1/1	0.96	0.14	42,42,42,42	0
57	MG	BA	3705	1/1	0.96	0.32	32,32,32,32	0
57	MG	BA	3368	1/1	0.96	0.32	26,26,26,26	0
57	MG	CA	3104	1/1	0.96	0.15	37,37,37,37	0
57	MG	BA	3236	1/1	0.96	0.15	39,39,39,39	0
57	MG	BA	3039	1/1	0.96	0.15	27,27,27,27	0
57	MG	DA	3145	1/1	0.96	0.20	38,38,38,38	0
57	MG	BA	3363	1/1	0.96	0.21	31,31,31,31	0
57	MG	AA	3206	1/1	0.96	0.06	62,62,62,62	0
57	MG	BD	301	1/1	0.96	0.38	37,37,37,37	0
57	MG	AA	3157	1/1	0.96	0.14	38,38,38,38	0
57	MG	DE	304	1/1	0.96	0.15	47,47,47,47	0
57	MG	AA	3088	1/1	0.96	0.22	40,40,40,40	0
57	MG	BA	3394	1/1	0.96	0.18	22,22,22,22	0
57	MG	DA	3295	1/1	0.96	0.08	58,58,58,58	0
57	MG	CA	3100	1/1	0.96	0.20	48,48,48,48	0
57	MG	AA	3153	1/1	0.96	0.09	46,46,46,46	0
57	MG	BA	3341	1/1	0.96	0.06	52,52,52,52	0
57	MG	DA	3232	1/1	0.96	0.07	48,48,48,48	0
57	MG	DA	3321	1/1	0.97	0.17	40,40,40,40	0
57	MG	DA	3483	1/1	0.97	0.28	41,41,41,41	0
57	MG	DA	3378	1/1	0.97	0.15	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3187	1/1	0.97	0.15	35,35,35,35	0
57	MG	BA	3659	1/1	0.97	0.21	47,47,47,47	0
57	MG	BD	303	1/1	0.97	0.32	42,42,42,42	0
57	MG	BA	3186	1/1	0.97	0.24	42,42,42,42	0
57	MG	DA	3315	1/1	0.97	0.16	57,57,57,57	0
57	MG	CA	3144	1/1	0.97	0.23	58,58,58,58	0
57	MG	BA	3076	1/1	0.97	0.24	34,34,34,34	0
57	MG	DA	3164	1/1	0.97	0.08	44,44,44,44	0
57	MG	BA	3356	1/1	0.97	0.11	36,36,36,36	0
57	MG	CA	3141	1/1	0.97	0.15	69,69,69,69	0
57	MG	CA	3049	1/1	0.97	0.11	42,42,42,42	0
57	MG	BA	3569	1/1	0.97	0.24	46,46,46,46	0
57	MG	AA	3024	1/1	0.97	0.24	49,49,49,49	0
57	MG	AA	3071	1/1	0.97	0.39	41,41,41,41	0
57	MG	DA	3030	1/1	0.97	0.39	32,32,32,32	0
57	MG	BA	3102	1/1	0.97	0.26	43,43,43,43	0
57	MG	DA	3606	1/1	0.97	0.19	54,54,54,54	0
57	MG	DA	3629	1/1	0.97	0.22	40,40,40,40	0
57	MG	DA	3181	1/1	0.97	0.21	36,36,36,36	0
57	MG	DA	3489	1/1	0.97	0.15	38,38,38,38	0
57	MG	DA	3233	1/1	0.97	0.28	41,41,41,41	0
57	MG	DA	3294	1/1	0.97	0.17	18,18,18,18	0
57	MG	B3	3002	1/1	0.97	0.17	58,58,58,58	0
57	MG	DA	3012	1/1	0.97	0.08	42,42,42,42	0
57	MG	BA	3676	1/1	0.97	0.18	44,44,44,44	0
57	MG	DA	3487	1/1	0.97	0.09	44,44,44,44	0
57	MG	DA	3361	1/1	0.97	0.18	32,32,32,32	0
57	MG	DA	3127	1/1	0.97	0.35	40,40,40,40	0
57	MG	BV	203	1/1	0.97	0.10	31,31,31,31	0
57	MG	DA	3507	1/1	0.97	0.24	33,33,33,33	0
57	MG	BA	3106	1/1	0.97	0.25	24,24,24,24	0
57	MG	DA	3272	1/1	0.97	0.08	29,29,29,29	0
57	MG	DD	304	1/1	0.97	0.15	40,40,40,40	0
57	MG	DA	3505	1/1	0.97	0.07	41,41,41,41	0
57	MG	DD	301	1/1	0.97	0.21	31,31,31,31	0
57	MG	DA	3192	1/1	0.97	0.23	31,31,31,31	0
57	MG	DA	3033	1/1	0.97	0.13	46,46,46,46	0
57	MG	BA	3209	1/1	0.97	0.22	32,32,32,32	0
57	MG	CA	3121	1/1	0.97	0.19	51,51,51,51	0
57	MG	AA	3183	1/1	0.97	0.19	43,43,43,43	0
57	MG	BA	3025	1/1	0.97	0.20	12,12,12,12	0
57	MG	BA	3414	1/1	0.97	0.24	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3627	1/1	0.97	0.09	28,28,28,28	0
57	MG	BA	3163	1/1	0.97	0.26	43,43,43,43	0
57	MG	BA	3697	1/1	0.97	0.16	23,23,23,23	0
57	MG	DA	3151	1/1	0.97	0.20	48,48,48,48	0
57	MG	DA	3176	1/1	0.97	0.15	42,42,42,42	0
57	MG	DU	3001	1/1	0.97	0.62	56,56,56,56	0
57	MG	DA	3245	1/1	0.97	0.12	46,46,46,46	0
57	MG	BA	3640	1/1	0.97	0.15	53,53,53,53	0
58	SF4	CD	501	8/8	0.97	0.12	59,71,83,91	0
57	MG	DB	3007	1/1	0.97	0.09	55,55,55,55	0
57	MG	BA	3536	1/1	0.97	0.11	42,42,42,42	0
57	MG	BA	3259	1/1	0.97	0.29	40,40,40,40	0
57	MG	BA	3124	1/1	0.97	0.12	31,31,31,31	0
57	MG	AA	3179	1/1	0.97	0.11	56,56,56,56	0
57	MG	DA	3333	1/1	0.97	0.12	41,41,41,41	0
57	MG	DA	3588	1/1	0.97	0.13	21,21,21,21	0
57	MG	CA	3108	1/1	0.97	0.15	51,51,51,51	0
57	MG	BA	3305	1/1	0.97	0.18	45,45,45,45	0
57	MG	DA	3416	1/1	0.97	0.09	46,46,46,46	0
57	MG	AA	3138	1/1	0.97	0.20	40,40,40,40	0
57	MG	DA	3243	1/1	0.97	0.30	41,41,41,41	0
57	MG	AA	3108	1/1	0.97	0.20	54,54,54,54	0
57	MG	DA	3215	1/1	0.97	0.18	35,35,35,35	0
57	MG	DA	3470	1/1	0.97	0.14	34,34,34,34	0
57	MG	DA	3480	1/1	0.97	0.11	28,28,28,28	0
57	MG	AA	3013	1/1	0.97	0.12	53,53,53,53	0
57	MG	AA	3136	1/1	0.97	0.15	43,43,43,43	0
57	MG	BA	3085	1/1	0.97	0.15	18,18,18,18	0
57	MG	DA	3195	1/1	0.97	0.26	42,42,42,42	0
57	MG	DA	3359	1/1	0.97	0.16	42,42,42,42	0
57	MG	AA	3078	1/1	0.97	0.17	66,66,66,66	0
57	MG	DA	3556	1/1	0.97	0.14	49,49,49,49	0
57	MG	BA	3498	1/1	0.97	0.23	45,45,45,45	0
57	MG	BA	3418	1/1	0.97	0.23	26,26,26,26	0
57	MG	DA	3173	1/1	0.97	0.34	42,42,42,42	0
57	MG	DA	3445	1/1	0.97	0.09	59,59,59,59	0
57	MG	BA	3010	1/1	0.97	0.20	45,45,45,45	0
57	MG	AA	3186	1/1	0.97	0.10	43,43,43,43	0
57	MG	BA	3121	1/1	0.97	0.24	48,48,48,48	0
57	MG	DA	3393	1/1	0.97	0.16	41,41,41,41	0
57	MG	BA	3432	1/1	0.97	0.26	35,35,35,35	0
57	MG	DA	3096	1/1	0.97	0.21	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
57	MG	DA	3203	1/1	0.97	0.17	46,46,46,46	0
57	MG	DA	3301	1/1	0.97	0.11	54,54,54,54	0
57	MG	BA	3197	1/1	0.97	0.19	32,32,32,32	0
57	MG	BA	3150	1/1	0.97	0.21	40,40,40,40	0
57	MG	BA	3461	1/1	0.97	0.26	32,32,32,32	0
57	MG	BA	3037	1/1	0.97	0.17	38,38,38,38	0
57	MG	BA	3191	1/1	0.97	0.09	22,22,22,22	0
57	MG	BA	3160	1/1	0.97	0.25	23,23,23,23	0
57	MG	BA	3358	1/1	0.97	0.10	35,35,35,35	0
57	MG	DA	3078	1/1	0.97	0.04	49,49,49,49	0
57	MG	DA	3567	1/1	0.97	0.09	49,49,49,49	0
57	MG	BA	3321	1/1	0.97	0.15	31,31,31,31	0
57	MG	AA	3139	1/1	0.97	0.13	51,51,51,51	0
57	MG	BA	3042	1/1	0.97	0.15	34,34,34,34	0
57	MG	BA	3362	1/1	0.97	0.13	43,43,43,43	0
57	MG	BA	3529	1/1	0.97	0.28	29,29,29,29	0
57	MG	AA	3177	1/1	0.97	0.14	66,66,66,66	0
57	MG	BA	3488	1/1	0.97	0.05	34,34,34,34	0
57	MG	BA	3475	1/1	0.97	0.09	31,31,31,31	0
57	MG	BA	3456	1/1	0.97	0.14	44,44,44,44	0
57	MG	DA	3258	1/1	0.97	0.26	32,32,32,32	0
57	MG	AA	3091	1/1	0.97	0.24	35,35,35,35	0
57	MG	BA	3142	1/1	0.97	0.20	35,35,35,35	0
57	MG	BB	3002	1/1	0.97	0.19	44,44,44,44	0
57	MG	AA	3148	1/1	0.97	0.16	61,61,61,61	0
57	MG	BD	307	1/1	0.97	0.18	40,40,40,40	0
57	MG	BA	3227	1/1	0.97	0.19	39,39,39,39	0
57	MG	DA	3016	1/1	0.97	0.13	34,34,34,34	0
57	MG	DU	3003	1/1	0.97	0.20	60,60,60,60	0
57	MG	DA	3541	1/1	0.97	0.15	40,40,40,40	0
57	MG	DA	3124	1/1	0.97	0.26	30,30,30,30	0
57	MG	BA	3420	1/1	0.97	0.11	23,23,23,23	0
57	MG	BD	309	1/1	0.97	0.25	33,33,33,33	0
57	MG	BA	3554	1/1	0.97	0.08	44,44,44,44	0
57	MG	AA	3052	1/1	0.97	0.15	53,53,53,53	0
57	MG	DA	3316	1/1	0.97	0.17	39,39,39,39	0
57	MG	BA	3654	1/1	0.97	0.19	42,42,42,42	0
57	MG	BN	3005	1/1	0.97	0.22	31,31,31,31	0
57	MG	BA	3493	1/1	0.97	0.13	39,39,39,39	0
57	MG	CA	3101	1/1	0.97	0.14	41,41,41,41	0
57	MG	DA	3523	1/1	0.97	0.15	45,45,45,45	0
57	MG	BA	3192	1/1	0.97	0.09	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
57	MG	CA	3077	1/1	0.97	0.13	63,63,63,63	0
57	MG	DA	3385	1/1	0.97	0.09	47,47,47,47	0
57	MG	CA	3080	1/1	0.97	0.16	61,61,61,61	0
57	MG	DA	3207	1/1	0.97	0.24	39,39,39,39	0
57	MG	DA	3573	1/1	0.97	0.08	49,49,49,49	0
57	MG	DA	3454	1/1	0.97	0.27	28,28,28,28	0
57	MG	BA	3348	1/1	0.97	0.12	17,17,17,17	0
57	MG	BA	3383	1/1	0.97	0.13	37,37,37,37	0
57	MG	AX	3004	1/1	0.97	0.13	45,45,45,45	0
57	MG	DA	3247	1/1	0.97	0.11	43,43,43,43	0
57	MG	DA	3235	1/1	0.97	0.36	48,48,48,48	0
57	MG	BA	3332	1/1	0.97	0.21	29,29,29,29	0
57	MG	BA	3196	1/1	0.97	0.27	51,51,51,51	0
57	MG	BQ	3002	1/1	0.97	0.30	39,39,39,39	0
57	MG	DA	3512	1/1	0.97	0.13	24,24,24,24	0
57	MG	BA	3440	1/1	0.97	0.23	40,40,40,40	0
57	MG	DB	3006	1/1	0.97	0.13	44,44,44,44	0
57	MG	CA	3115	1/1	0.97	0.14	59,59,59,59	0
57	MG	AA	3009	1/1	0.97	0.09	40,40,40,40	0
57	MG	DA	3172	1/1	0.97	0.09	32,32,32,32	0
57	MG	DA	3320	1/1	0.97	0.12	19,19,19,19	0
57	MG	BA	3009	1/1	0.97	0.09	34,34,34,34	0
57	MG	CA	3079	1/1	0.97	0.14	42,42,42,42	0
57	MG	BA	3485	1/1	0.97	0.11	40,40,40,40	0
57	MG	BA	3546	1/1	0.97	0.25	27,27,27,27	0
57	MG	DA	3296	1/1	0.97	0.20	46,46,46,46	0
57	MG	BA	3043	1/1	0.97	0.17	44,44,44,44	0
57	MG	DA	3614	1/1	0.97	0.50	56,56,56,56	0
57	MG	DA	3585	1/1	0.97	0.27	45,45,45,45	0
57	MG	BF	307	1/1	0.97	0.24	25,25,25,25	0
57	MG	BA	3131	1/1	0.97	0.38	31,31,31,31	0
57	MG	BA	3270	1/1	0.97	0.42	47,47,47,47	0
57	MG	DA	3462	1/1	0.97	0.27	35,35,35,35	0
57	MG	DB	3004	1/1	0.97	0.11	38,38,38,38	0
57	MG	BA	3512	1/1	0.97	0.10	32,32,32,32	0
57	MG	BA	3141	1/1	0.97	0.21	38,38,38,38	0
57	MG	AA	3029	1/1	0.97	0.07	42,42,42,42	0
57	MG	BA	3481	1/1	0.97	0.23	35,35,35,35	0
57	MG	BA	3402	1/1	0.97	0.21	39,39,39,39	0
57	MG	DA	3398	1/1	0.97	0.13	37,37,37,37	0
57	MG	BA	3194	1/1	0.97	0.21	42,42,42,42	0
57	MG	BA	3154	1/1	0.97	0.20	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
57	MG	BA	3384	1/1	0.97	0.29	19,19,19,19	0
57	MG	DA	3231	1/1	0.97	0.28	33,33,33,33	0
57	MG	BA	3276	1/1	0.97	0.16	19,19,19,19	0
57	MG	DA	3618	1/1	0.97	0.16	46,46,46,46	0
57	MG	DA	3474	1/1	0.97	0.21	52,52,52,52	0
57	MG	BA	3473	1/1	0.97	0.18	31,31,31,31	0
57	MG	BA	3283	1/1	0.97	0.23	22,22,22,22	0
57	MG	BA	3219	1/1	0.97	0.43	42,42,42,42	0
57	MG	BV	204	1/1	0.97	0.09	36,36,36,36	0
57	MG	BA	3095	1/1	0.97	0.23	29,29,29,29	0
57	MG	DA	3302	1/1	0.97	0.18	30,30,30,30	0
57	MG	BA	3343	1/1	0.97	0.18	18,18,18,18	0
57	MG	DA	3534	1/1	0.97	0.12	30,30,30,30	0
57	MG	DA	3237	1/1	0.97	0.31	41,41,41,41	0
57	MG	BA	3694	1/1	0.97	0.19	11,11,11,11	0
57	MG	BA	3617	1/1	0.97	0.13	59,59,59,59	0
57	MG	BA	3624	1/1	0.97	0.11	26,26,26,26	0
57	MG	DA	3101	1/1	0.97	0.28	45,45,45,45	0
57	MG	BA	3053	1/1	0.97	0.20	33,33,33,33	0
57	MG	AA	3165	1/1	0.97	0.24	47,47,47,47	0
57	MG	DA	3594	1/1	0.97	0.16	51,51,51,51	0
57	MG	BA	3428	1/1	0.97	0.17	54,54,54,54	0
57	MG	BE	3004	1/1	0.97	0.12	49,49,49,49	0
57	MG	BA	3580	1/1	0.98	0.27	13,13,13,13	0
57	MG	DA	3289	1/1	0.98	0.25	50,50,50,50	0
57	MG	DA	3123	1/1	0.98	0.16	45,45,45,45	0
57	MG	BA	3479	1/1	0.98	0.13	22,22,22,22	0
57	MG	BE	3001	1/1	0.98	0.33	48,48,48,48	0
57	MG	BA	3110	1/1	0.98	0.18	40,40,40,40	0
57	MG	BA	3653	1/1	0.98	0.21	51,51,51,51	0
57	MG	DA	3029	1/1	0.98	0.16	44,44,44,44	0
57	MG	DA	3570	1/1	0.98	0.18	28,28,28,28	0
57	MG	DA	3336	1/1	0.98	0.21	38,38,38,38	0
57	MG	DA	3335	1/1	0.98	0.13	48,48,48,48	0
57	MG	DA	3464	1/1	0.98	0.15	51,51,51,51	0
57	MG	BD	304	1/1	0.98	0.19	36,36,36,36	0
57	MG	CA	3073	1/1	0.98	0.09	57,57,57,57	0
57	MG	BV	202	1/1	0.98	0.20	29,29,29,29	0
57	MG	BA	3255	1/1	0.98	0.06	37,37,37,37	0
57	MG	BA	3190	1/1	0.98	0.23	24,24,24,24	0
57	MG	BU	203	1/1	0.98	0.17	35,35,35,35	0
57	MG	BB	3003	1/1	0.98	0.17	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
57	MG	BA	3370	1/1	0.98	0.21	32,32,32,32	0
57	MG	DA	3024	1/1	0.98	0.09	29,29,29,29	0
57	MG	DA	3340	1/1	0.98	0.17	38,38,38,38	0
57	MG	BA	3718	1/1	0.98	0.16	36,36,36,36	0
57	MG	DA	3140	1/1	0.98	0.25	38,38,38,38	0
57	MG	DA	3349	1/1	0.98	0.15	35,35,35,35	0
57	MG	BA	3265	1/1	0.98	0.14	30,30,30,30	0
57	MG	BA	3477	1/1	0.98	0.14	19,19,19,19	0
58	SF4	AD	302	8/8	0.98	0.14	59,71,78,78	0
57	MG	BA	3596	1/1	0.98	0.14	56,56,56,56	0
57	MG	BA	3185	1/1	0.98	0.49	34,34,34,34	0
57	MG	DA	3005	1/1	0.98	0.20	29,29,29,29	0
57	MG	DA	3469	1/1	0.98	0.31	41,41,41,41	0
57	MG	DA	3240	1/1	0.98	0.24	36,36,36,36	0
57	MG	DA	3050	1/1	0.98	0.14	48,48,48,48	0
57	MG	BA	3645	1/1	0.98	0.14	43,43,43,43	0
57	MG	BA	3280	1/1	0.98	0.17	46,46,46,46	0
57	MG	BA	3687	1/1	0.98	0.11	30,30,30,30	0
57	MG	CA	3087	1/1	0.98	0.15	50,50,50,50	0
57	MG	BW	205	1/1	0.98	0.14	30,30,30,30	0
57	MG	DA	3206	1/1	0.98	0.22	37,37,37,37	0
57	MG	BA	3706	1/1	0.98	0.25	27,27,27,27	0
59	ZN	BY	202	1/1	0.98	0.12	70,70,70,70	0
57	MG	AA	3182	1/1	0.98	0.15	40,40,40,40	0
57	MG	BA	3117	1/1	0.98	0.17	24,24,24,24	0
57	MG	DA	3310	1/1	0.98	0.16	43,43,43,43	0
57	MG	BB	3016	1/1	0.98	0.06	39,39,39,39	0
57	MG	DA	3339	1/1	0.98	0.17	23,23,23,23	0
57	MG	BB	3015	1/1	0.98	0.11	42,42,42,42	0
57	MG	BA	3252	1/1	0.98	0.22	30,30,30,30	0
57	MG	DA	3238	1/1	0.98	0.43	31,31,31,31	0
57	MG	BB	3010	1/1	0.98	0.10	28,28,28,28	0
57	MG	DA	3179	1/1	0.98	0.24	50,50,50,50	0
57	MG	AA	3083	1/1	0.98	0.30	38,38,38,38	0
57	MG	BA	3662	1/1	0.98	0.25	62,62,62,62	0
57	MG	BA	3193	1/1	0.98	0.20	30,30,30,30	0
57	MG	AA	3129	1/1	0.98	0.16	37,37,37,37	0
57	MG	BF	303	1/1	0.98	0.18	35,35,35,35	0
57	MG	BA	3716	1/1	0.98	0.16	53,53,53,53	0
57	MG	DA	3183	1/1	0.98	0.21	31,31,31,31	0
57	MG	BA	3593	1/1	0.98	0.11	36,36,36,36	0
57	MG	BA	3269	1/1	0.98	0.24	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
57	MG	BY	201	1/1	0.98	0.16	51,51,51,51	0
57	MG	BA	3685	1/1	0.98	0.18	40,40,40,40	0
57	MG	DB	3001	1/1	0.98	0.07	50,50,50,50	0
57	MG	AA	3194	1/1	0.98	0.21	41,41,41,41	0
57	MG	DN	5001	1/1	0.98	0.06	53,53,53,53	0
57	MG	DA	3392	1/1	0.98	0.23	40,40,40,40	0
57	MG	BB	3013	1/1	0.98	0.18	43,43,43,43	0
57	MG	DA	3466	1/1	0.98	0.24	41,41,41,41	0
57	MG	BA	3030	1/1	0.98	0.12	44,44,44,44	0
57	MG	BV	201	1/1	0.98	0.22	33,33,33,33	0
57	MG	BF	301	1/1	0.98	0.18	30,30,30,30	0
57	MG	BA	3145	1/1	0.98	0.16	41,41,41,41	0
57	MG	BA	3272	1/1	0.98	0.21	38,38,38,38	0
57	MG	B7	101	1/1	0.98	0.18	48,48,48,48	0
57	MG	DA	3131	1/1	0.98	0.11	34,34,34,34	0
57	MG	BA	3496	1/1	0.98	0.29	33,33,33,33	0
57	MG	DA	3382	1/1	0.98	0.22	20,20,20,20	0
57	MG	BA	3290	1/1	0.98	0.14	43,43,43,43	0
57	MG	DA	3269	1/1	0.98	0.16	40,40,40,40	0
57	MG	BA	3101	1/1	0.98	0.29	29,29,29,29	0
57	MG	BA	3407	1/1	0.98	0.19	29,29,29,29	0
57	MG	DA	3071	1/1	0.98	0.15	42,42,42,42	0
57	MG	BW	204	1/1	0.98	0.17	27,27,27,27	0
57	MG	AA	3081	1/1	0.98	0.09	44,44,44,44	0
57	MG	BA	3212	1/1	0.98	0.29	24,24,24,24	0
57	MG	BA	3346	1/1	0.98	0.23	29,29,29,29	0
57	MG	BA	3504	1/1	0.98	0.24	33,33,33,33	0
59	ZN	DY	501	1/1	0.98	0.10	88,88,88,88	0
57	MG	AA	3137	1/1	0.98	0.28	66,66,66,66	0
57	MG	BB	3017	1/1	0.98	0.09	28,28,28,28	0
57	MG	BA	3004	1/1	0.98	0.18	26,26,26,26	0
57	MG	BA	3125	1/1	0.98	0.39	30,30,30,30	0
57	MG	BA	3086	1/1	0.98	0.22	15,15,15,15	0
57	MG	BA	3620	1/1	0.98	0.12	35,35,35,35	0
57	MG	DA	3560	1/1	0.98	0.20	48,48,48,48	0
57	MG	DA	3433	1/1	0.98	0.23	27,27,27,27	0
57	MG	BA	3643	1/1	0.98	0.16	47,47,47,47	0
57	MG	BA	3285	1/1	0.98	0.18	21,21,21,21	0
57	MG	BA	3503	1/1	0.98	0.11	50,50,50,50	0
57	MG	DA	3584	1/1	0.98	0.14	63,63,63,63	0
57	MG	DA	3620	1/1	0.98	0.17	47,47,47,47	0
57	MG	BA	3690	1/1	0.98	0.17	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3128	1/1	0.98	0.16	33,33,33,33	0
57	MG	DA	3073	1/1	0.98	0.31	49,49,49,49	0
57	MG	DA	3009	1/1	0.98	0.14	39,39,39,39	0
57	MG	B0	104	1/1	0.98	0.10	49,49,49,49	0
57	MG	BA	3457	1/1	0.98	0.11	41,41,41,41	0
57	MG	DA	3373	1/1	0.98	0.23	43,43,43,43	0
59	ZN	D6	501	1/1	0.98	0.16	64,64,64,64	0
57	MG	DA	3518	1/1	0.98	0.08	42,42,42,42	0
57	MG	DA	3100	1/1	0.98	0.20	38,38,38,38	0
57	MG	BA	3670	1/1	0.98	0.11	25,25,25,25	0
57	MG	DA	3015	1/1	0.98	0.25	41,41,41,41	0
57	MG	DA	3150	1/1	0.98	0.36	41,41,41,41	0
57	MG	DA	3239	1/1	0.98	0.31	51,51,51,51	0
57	MG	BA	3245	1/1	0.98	0.31	37,37,37,37	0
57	MG	CA	3047	1/1	0.98	0.20	50,50,50,50	0
57	MG	DA	3423	1/1	0.98	0.24	33,33,33,33	0
57	MG	BA	3441	1/1	0.98	0.13	56,56,56,56	0
57	MG	BA	3057	1/1	0.98	0.18	21,21,21,21	0
57	MG	BA	3553	1/1	0.98	0.19	41,41,41,41	0
57	MG	DA	3168	1/1	0.98	0.32	50,50,50,50	0
57	MG	DA	3169	1/1	0.98	0.20	45,45,45,45	0
57	MG	BA	3014	1/1	0.98	0.13	46,46,46,46	0
57	MG	BA	3427	1/1	0.98	0.16	23,23,23,23	0
57	MG	CA	3123	1/1	0.98	0.09	53,53,53,53	0
57	MG	BA	3386	1/1	0.98	0.25	30,30,30,30	0
57	MG	AA	3095	1/1	0.98	0.15	44,44,44,44	0
57	MG	CA	3156	1/1	0.98	0.05	57,57,57,57	0
57	MG	DD	303	1/1	0.98	0.24	42,42,42,42	0
57	MG	DA	3363	1/1	0.99	0.21	35,35,35,35	0
57	MG	BU	207	1/1	0.99	0.16	23,23,23,23	0
57	MG	BA	3376	1/1	0.99	0.21	21,21,21,21	0
59	ZN	D5	102	1/1	0.99	0.17	58,58,58,58	0
57	MG	BA	3239	1/1	0.99	0.17	42,42,42,42	0
59	ZN	B5	102	1/1	0.99	0.16	41,41,41,41	0
57	MG	DA	3579	1/1	0.99	0.29	58,58,58,58	0
57	MG	DA	3482	1/1	0.99	0.25	31,31,31,31	0
59	ZN	B6	501	1/1	0.99	0.14	43,43,43,43	0
57	MG	BA	3586	1/1	0.99	0.11	33,33,33,33	0
57	MG	BA	3274	1/1	0.99	0.17	44,44,44,44	0
57	MG	DA	3031	1/1	0.99	0.14	36,36,36,36	0
57	MG	BA	3309	1/1	0.99	0.10	31,31,31,31	0
57	MG	BA	3637	1/1	0.99	0.15	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
57	MG	DA	3386	1/1	0.99	0.20	39,39,39,39	0
57	MG	AA	3169	1/1	0.99	0.13	48,48,48,48	0
57	MG	BA	3140	1/1	0.99	0.19	26,26,26,26	0
57	MG	BA	3588	1/1	0.99	0.18	19,19,19,19	0
57	MG	DA	3298	1/1	0.99	0.11	35,35,35,35	0
57	MG	BA	3167	1/1	0.99	0.23	51,51,51,51	0
57	MG	BA	3275	1/1	0.99	0.10	38,38,38,38	0
57	MG	BA	3026	1/1	0.99	0.24	36,36,36,36	0
57	MG	BA	3330	1/1	0.99	0.17	14,14,14,14	0
57	MG	BA	3592	1/1	0.99	0.18	14,14,14,14	0
57	MG	BA	3528	1/1	0.99	0.17	37,37,37,37	0
57	MG	DA	3395	1/1	0.99	0.11	31,31,31,31	0
57	MG	DA	3399	1/1	0.99	0.13	26,26,26,26	0
57	MG	BA	3147	1/1	0.99	0.23	34,34,34,34	0
57	MG	BE	3007	1/1	0.99	0.10	31,31,31,31	0
57	MG	DA	3044	1/1	0.99	0.18	38,38,38,38	0
57	MG	DA	3451	1/1	0.99	0.21	39,39,39,39	0
57	MG	BA	3256	1/1	0.99	0.10	36,36,36,36	0
57	MG	DA	3599	1/1	0.99	0.23	36,36,36,36	0
57	MG	DA	3354	1/1	0.99	0.26	25,25,25,25	0
57	MG	DA	3329	1/1	0.99	0.26	54,54,54,54	0
57	MG	DA	3022	1/1	0.99	0.09	27,27,27,27	0
57	MG	BA	3655	1/1	0.99	0.09	68,68,68,68	0

6.5 Other polymers

There are no such residues in this entry.