



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 09:40 am BST

PDB ID : 4V8G
Title : Crystal structure of RMF bound to the 70S ribosome.
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.
Deposited on : 2011-12-11
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
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

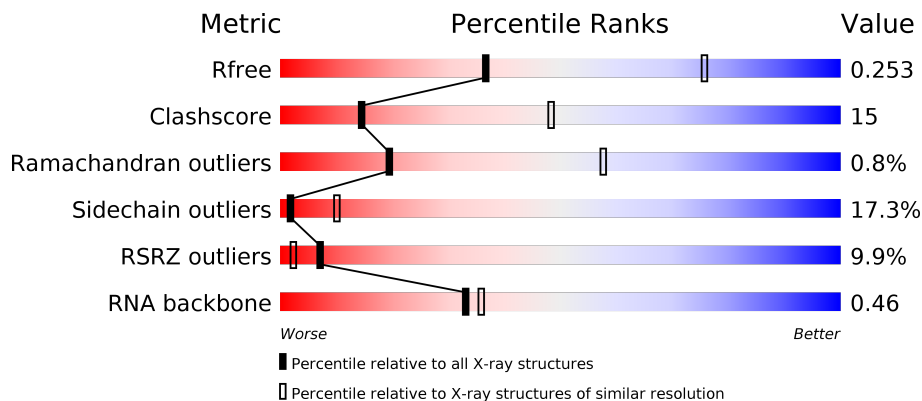
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	1522	
1	CA	1522	
2	AB	256	
2	CB	256	


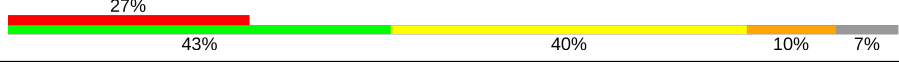
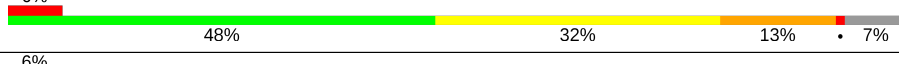


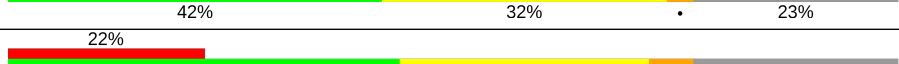
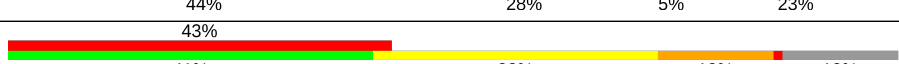
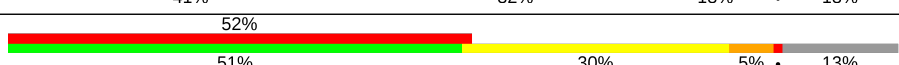
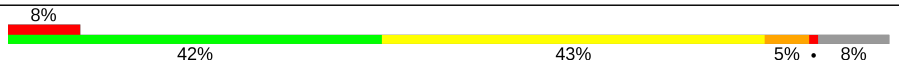

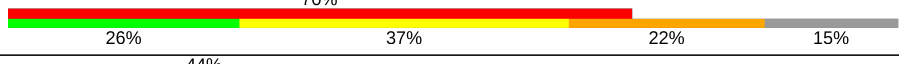



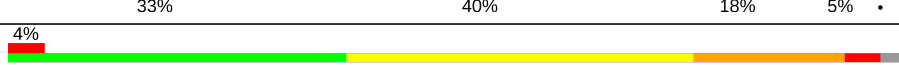
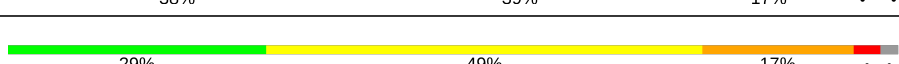
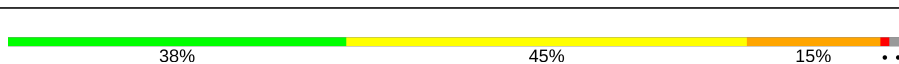








Continued on next page...

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	






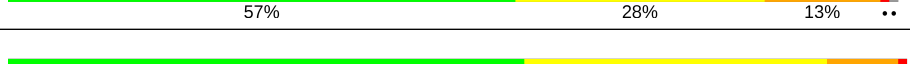
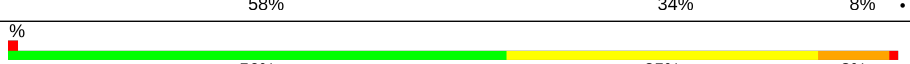
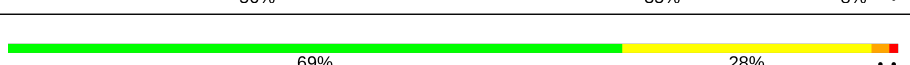
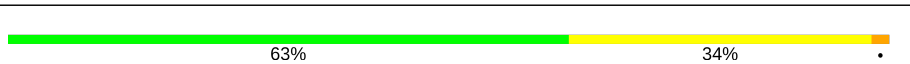


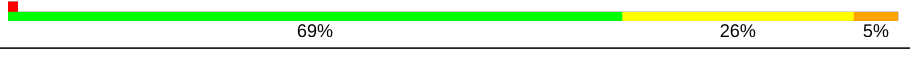

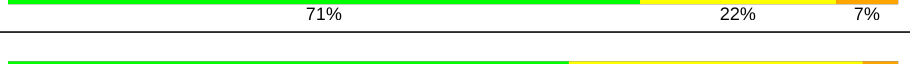
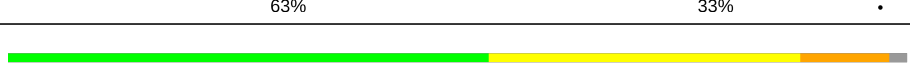

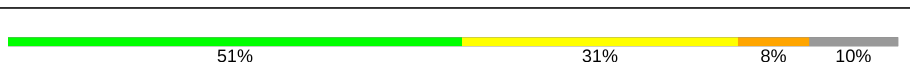








Continued on next page...

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	61	
22	CV	61	
23	BA	2915	
23	DA	2915	
24	BB	122	
24	DB	122	
25	BD	276	
25	DD	276	
26	BE	206	
26	DE	206	
27	BF	210	
27	DF	210	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	BG	182	
28	DG	182	
29	BH	180	
29	DH	180	
30	BI	148	
30	DI	148	
31	BN	140	
31	DN	140	
32	BO	122	
32	DO	122	
33	BP	150	
33	DP	150	
34	BQ	141	
34	DQ	141	
35	BR	118	
35	DR	118	
36	BS	112	
36	DS	112	
37	BT	146	
37	DT	146	
38	BU	118	
38	DU	118	
39	BV	101	
39	DV	101	
40	BW	113	



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	DW	113	69% 27% ..
41	BX	96	73% 23% ...
41	DX	96	72% 25% ...
42	BY	110	54% 39% 5% .
42	DY	110	57% 34% 5% ..
43	BZ	206	60% 31% 5% .
43	DZ	206	59% 31% 6% .
44	B0	85	60% 26% . 11%
44	D0	85	51% 35% . 11%
45	B1	98	64% 28% 6% ..
45	D1	98	65% 23% 9% ..
46	B2	72	57% 38% . .
46	D2	72	54% 39% . .
47	B3	60	72% 22% 5% .
47	D3	60	65% 27% 7% .
48	B4	71	30% 24% 8% . 35%
48	D4	71	30% 23% 11% . 35%
49	B5	60	70% 25% . .
49	D5	60	70% 23% 5% .
50	B6	54	46% 37% 15% .
50	D6	54	44% 37% 17% .
51	B7	49	59% 31% 8% .
51	D7	49	59% 35% . .
52	B8	65	55% 34% 9% .
52	D8	65	51% 40% 6% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	B9	37	
53	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
54	MG	AA	1616	-	-	-	X
54	MG	AA	1620	-	-	-	X
54	MG	AA	1622	-	-	-	X
54	MG	AA	1627	-	-	-	X
54	MG	AA	1630	-	-	-	X
54	MG	AA	1643	-	-	-	X
54	MG	AA	1652	-	-	-	X
54	MG	AA	1656	-	-	-	X
54	MG	AA	1661	-	-	-	X
54	MG	AA	1663	-	-	-	X
54	MG	AA	1665	-	-	-	X
54	MG	AA	1675	-	-	-	X
54	MG	AA	1678	-	-	-	X
54	MG	BA	3118	-	-	-	X
54	MG	BA	3145	-	-	-	X
54	MG	BA	3169	-	-	-	X
54	MG	BA	3201	-	-	-	X
54	MG	BA	3205	-	-	-	X
54	MG	BA	3267	-	-	-	X
54	MG	BA	3280	-	-	-	X
54	MG	BB	207	-	-	-	X
54	MG	CA	1606	-	-	-	X
54	MG	CA	1608	-	-	-	X
54	MG	CA	1609	-	-	-	X
54	MG	CA	1612	-	-	-	X
54	MG	CA	1619	-	-	-	X
54	MG	CA	1624	-	-	-	X
54	MG	CA	1631	-	-	-	X
54	MG	CA	1636	-	-	-	X
54	MG	DA	3037	-	-	-	X
54	MG	DA	3047	-	-	-	X
54	MG	DA	3048	-	-	-	X
54	MG	DA	3075	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3102	-	-	-	X
54	MG	DA	3143	-	-	-	X
54	MG	DA	3327	-	-	-	X
54	MG	DB	202	-	-	-	X
54	MG	DP	201	-	-	-	X

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 283930 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
			Total	C	N	O	P			
1	AA	1505	Total	C	N	O	P	0	0	0
			32353	14399	5995	10454	1505			
1	CA	1501	Total	C	N	O	P	0	0	0
			32270	14362	5983	10424	1501			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AB	229	Total	C	N	O	S	0	0	0
			1775	1132	318	320	5			
2	CB	229	Total	C	N	O	S	0	0	0
			1775	1132	318	320	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AD	208	Total	C	N	O	S	0	0	0
			1526	963	283	274	6			
4	CD	208	Total	C	N	O	S	0	0	0
			1526	963	283	274	6			

- 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
			1105	699	204	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	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
			777	493	137	144	3			
6	CF	100	Total	C	N	O	S	0	0	0
			777	493	137	144	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
			1164	726	224	208	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1164	726	224	208	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			
8	CH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	125	Total	C	N	O	0	0	0
			852	533	163	156			
9	CI	125	Total	C	N	O	0	0	0
			852	533	163	156			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AJ	96	Total	C	N	O	0	0	0
			663	410	132	121			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	CJ	96	663	410	132	121	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AK	114	828	516	155	154	3	0	0	0
11	CK	114	828	516	155	154	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AL	122	905	567	178	159	1	0	0	0
12	CL	122	905	567	178	159	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	AM	114	804	497	164	142	1	0	0	0
13	CM	114	804	497	164	142	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	AN	60	478	303	99	72	4	0	0	0
14	CN	60	478	303	99	72	4	0	0	0

- Molecule 15 is a protein called 30S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AO	88	724	453	143	126	2	0	0	0
15	CO	88	724	453	143	126	2	0	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
			651	416	123	111	1			
16	CP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	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
			514	329	98	87			
18	CR	68	Total	C	N	O	0	0	0
			514	329	98	87			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			
19	CS	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	97	Total	C	N	O	S	0	0	0
			713	438	152	121	2			
20	CT	97	Total	C	N	O	S	0	0	0
			713	438	152	121	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 protein called Ribosome modulation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	53	Total	C	N	O	S	0	0	0
			333	204	66	61	2			
22	CV	53	Total	C	N	O	S	0	0	0
			353	218	67	66	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	56	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	57	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	58	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	59	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	60	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	61	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	56	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	57	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	58	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	59	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	60	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	61	HIS	-	EXPRESSION TAG	UNP P0AFW2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2809	Total	C	N	O	P	0	0	0
			60512	26930	11328	19446	2808			
23	DA	2814	Total	C	N	O	P	0	0	0
			60620	26978	11348	19481	2813			

- Molecule 24 is a RNA chain called 5S Ribosomal RNA.

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

Continued on next page...

Continued from previous page...

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

- Molecule 25 is a protein called 50S Ribosomal Protein L2.

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

- Molecule 26 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	BE	204	1555	982	297	270	6	0	0	0
26	DE	204	1555	982	297	270	6	0	0	0

- Molecule 27 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	BF	203	1580	1007	298	273	2	0	0	1
27	DF	203	1580	1007	298	273	2	0	0	1

- Molecule 28 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	BG	181	1368	879	242	244	3	0	0	0
28	DG	181	1368	879	242	244	3	0	0	0

- Molecule 29 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	BH	174	1317	837	243	236	1	0	0	0
29	DH	174	1317	837	243	236	1	0	0	0

- Molecule 30 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	BI	146	Total 1040	C 669	N 180	O 190	S 1	0	0	0
30	DI	146	Total 1038	C 668	N 180	O 189	S 1	0	0	0

- Molecule 31 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	BN	140	Total 1112	C 717	N 207	O 184	S 4	0	0	0
31	DN	140	Total 1112	C 717	N 207	O 184	S 4	0	0	0

- Molecule 32 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	BO	122	Total 923	C 583	N 168	O 168	S 4	0	0	0
32	DO	122	Total 923	C 583	N 168	O 168	S 4	0	0	0

- Molecule 33 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	BP	149	Total 1131	C 703	N 229	O 196	S 3	0	0	0
33	DP	149	Total 1131	C 703	N 229	O 196	S 3	0	0	0

- Molecule 34 is a protein called 50S Ribosomal Protein L16.

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

- Molecule 35 is a protein called 50S Ribosomal Protein L17.

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

- Molecule 36 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BS	110	Total	C	N	O	S	0	0	0
			865	544	172	149				
36	DS	110	Total	C	N	O	S	0	0	0
			865	544	172	149				

- Molecule 37 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			
37	DT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			

- Molecule 38 is a protein called 50S Ribosomal Protein L20.

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

- Molecule 39 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BV	100	Total	C	N	O	S	0	0	0
			760	490	136	133	1			
39	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 40 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	DW	112	881	554	172	153	2	0	0	0

- Molecule 41 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	BX	95	742	483	134	124	1	0	0	0
41	DX	95	742	483	134	124	1	0	0	0

- Molecule 42 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	BY	107	785	503	145	131	6	0	0	0
42	DY	107	785	503	145	131	6	0	0	0

- Molecule 43 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	BZ	198	1522	972	269	279	2	0	0	0
43	DZ	198	1522	972	269	279	2	0	0	0

- Molecule 44 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	B0	76	594	368	125	100	1	0	0	0
44	D0	76	594	368	125	100	1	0	0	0

- Molecule 45 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	B1	97	745	469	144	131	1	0	0	0
45	D1	97	745	469	144	131	1	0	0	0

- Molecule 46 is a protein called 50S Ribosomal Protein L29.

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

- Molecule 47 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	B3	59	Total	C	N	O	0	0	0
			458	293	87	78			
47	D3	59	Total	C	N	O	0	0	0
			458	293	87	78			

- Molecule 48 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			
48	D4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 49 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			
49	D5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			
50	D6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			

- Molecule 51 is a protein called 50S Ribosomal Protein L34.

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

- Molecule 52 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			
52	D8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 53 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			
53	D9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	618	Total	Mg	0	0
			618	618		
54	CA	69	Total	Mg	0	0
			69	69		
54	DF	2	Total	Mg	0	0
			2	2		
54	B8	3	Total	Mg	0	0
			3	3		
54	BE	6	Total	Mg	0	0
			6	6		
54	B1	1	Total	Mg	0	0
			1	1		
54	BP	1	Total	Mg	0	0
			1	1		
54	D6	1	Total	Mg	0	0
			1	1		
54	B5	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	BB	17	Total Mg 17 17	0	0
54	D8	1	Total Mg 1 1	0	0
54	B9	1	Total Mg 1 1	0	0
54	BF	2	Total Mg 2 2	0	0
54	B2	2	Total Mg 2 2	0	0
54	AA	106	Total Mg 106 106	0	0
54	BQ	3	Total Mg 3 3	0	0
54	D7	1	Total Mg 1 1	0	0
54	BU	2	Total Mg 2 2	0	0
54	AD	1	Total Mg 1 1	0	0
54	DD	1	Total Mg 1 1	0	0
54	B3	2	Total Mg 2 2	0	0
54	BR	2	Total Mg 2 2	0	0
54	DA	430	Total Mg 430 430	0	0
54	BV	1	Total Mg 1 1	0	0
54	DE	1	Total Mg 1 1	0	0
54	DP	1	Total Mg 1 1	0	0
54	BD	3	Total Mg 3 3	0	0
54	B0	2	Total Mg 2 2	0	0
54	BW	1	Total Mg 1 1	0	0
54	DB	5	Total Mg 5 5	0	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	145	Total 145	O 145	0	0
56	AF	1	Total 1	O 1	0	0
56	AK	1	Total 1	O 1	0	0
56	AQ	1	Total 1	O 1	0	0
56	BA	1422	Total 1422	O 1422	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BB	31	Total 31	O 31	0	0
56	BD	10	Total 10	O 10	0	0
56	BE	8	Total 8	O 8	0	0
56	BF	11	Total 11	O 11	0	0
56	BH	2	Total 2	O 2	0	0
56	BN	2	Total 2	O 2	0	0
56	BO	3	Total 3	O 3	0	0
56	BP	6	Total 6	O 6	0	0
56	BQ	2	Total 2	O 2	0	0
56	BR	6	Total 6	O 6	0	0
56	BT	1	Total 1	O 1	0	0
56	BU	2	Total 2	O 2	0	0
56	BV	2	Total 2	O 2	0	0
56	BW	4	Total 4	O 4	0	0
56	BX	2	Total 2	O 2	0	0
56	BY	1	Total 1	O 1	0	0
56	B0	4	Total 4	O 4	0	0
56	B3	1	Total 1	O 1	0	0
56	B4	1	Total 1	O 1	0	0
56	B5	3	Total 3	O 3	0	0
56	B7	3	Total 3	O 3	0	0

Continued on next page...

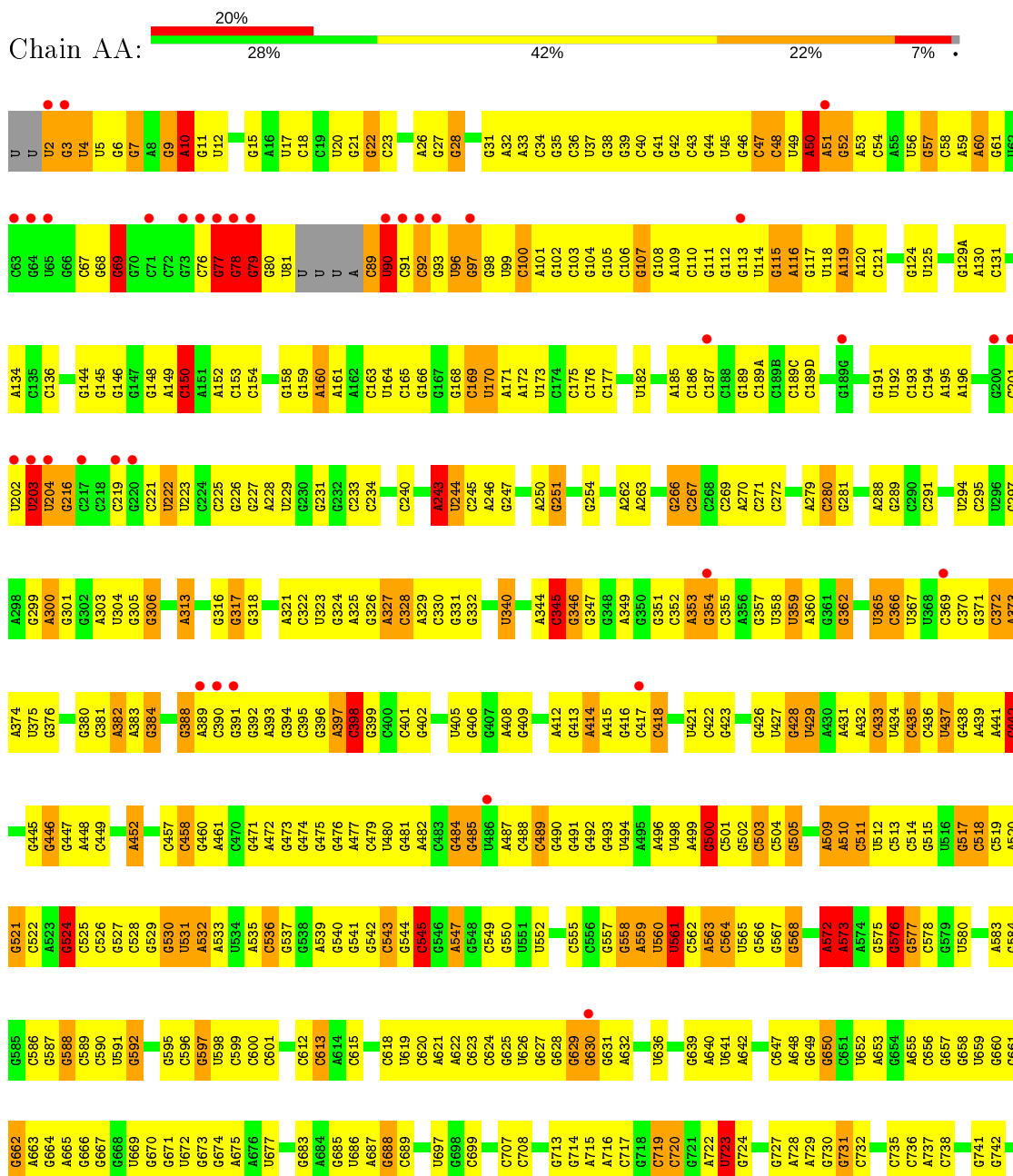
Continued from previous page...

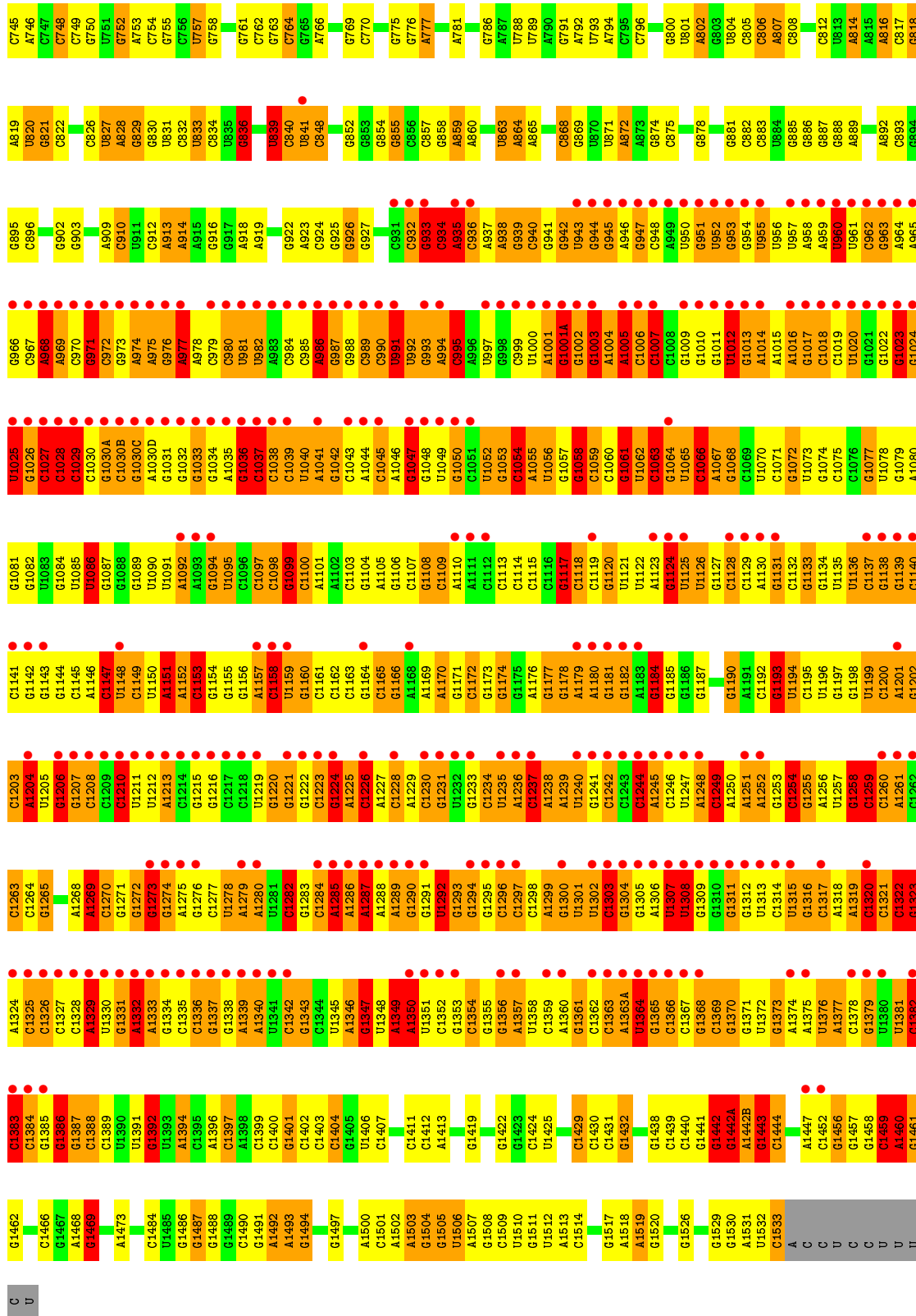
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B8	7	Total 7	O 7	0	0
56	B9	2	Total 2	O 2	0	0
56	CA	119	Total 119	O 119	0	0
56	CD	1	Total 1	O 1	0	0
56	CK	2	Total 2	O 2	0	0
56	CP	1	Total 1	O 1	0	0
56	CT	2	Total 2	O 2	0	0
56	DA	696	Total 696	O 696	0	0
56	DB	9	Total 9	O 9	0	0
56	DD	3	Total 3	O 3	0	0
56	DE	2	Total 2	O 2	0	0
56	DF	5	Total 5	O 5	0	0
56	DP	5	Total 5	O 5	0	0
56	DQ	2	Total 2	O 2	0	0
56	DR	1	Total 1	O 1	0	0
56	DV	1	Total 1	O 1	0	0
56	DX	1	Total 1	O 1	0	0
56	DY	1	Total 1	O 1	0	0
56	D0	1	Total 1	O 1	0	0
56	D1	2	Total 2	O 2	0	0

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.

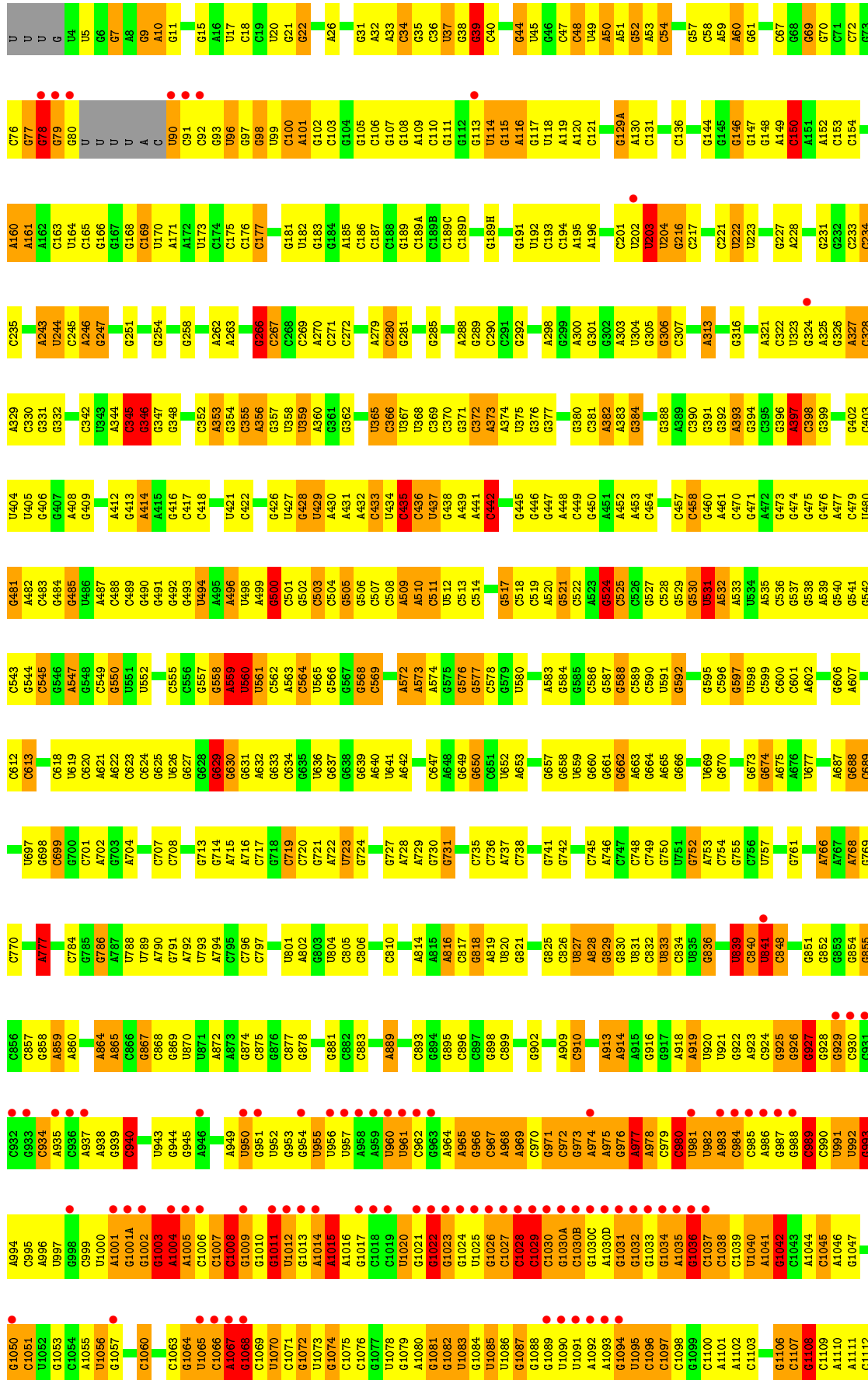
- Molecule 1: 16S Ribosomal RNA

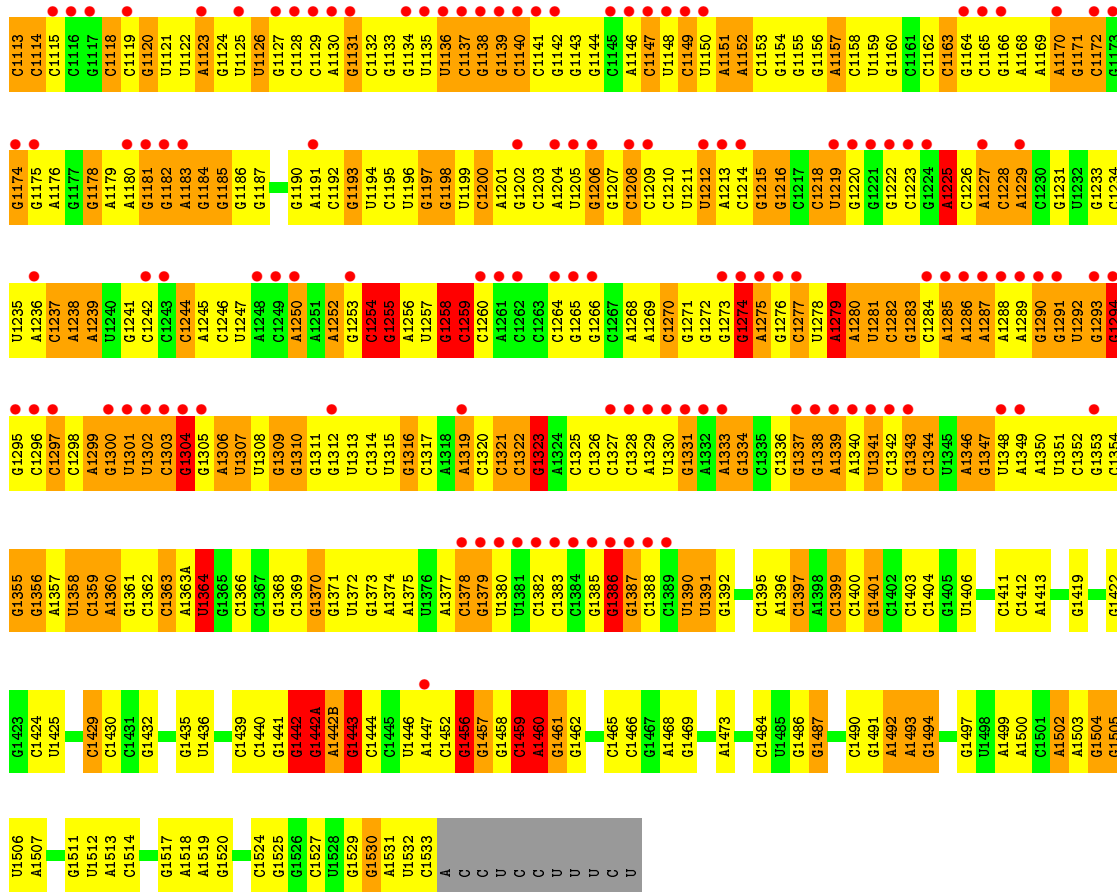




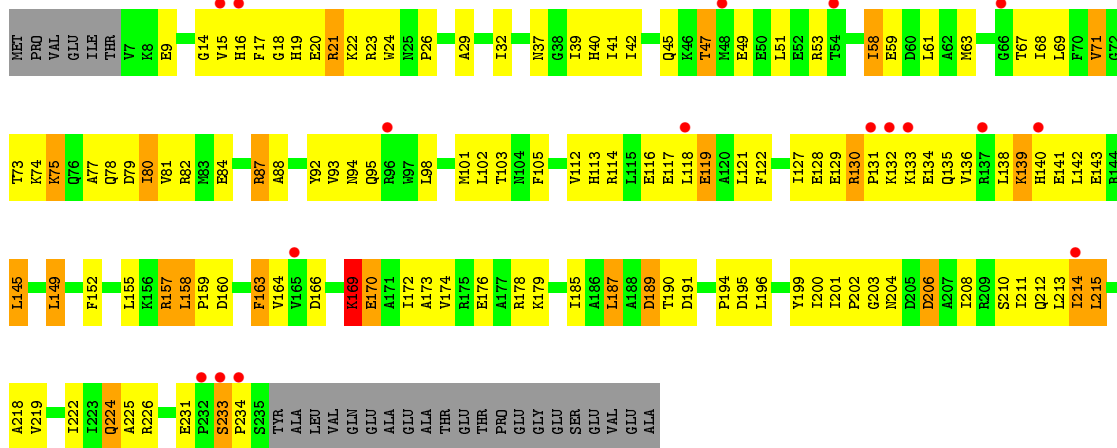
• Molecule 1: 16S Ribosomal RNA





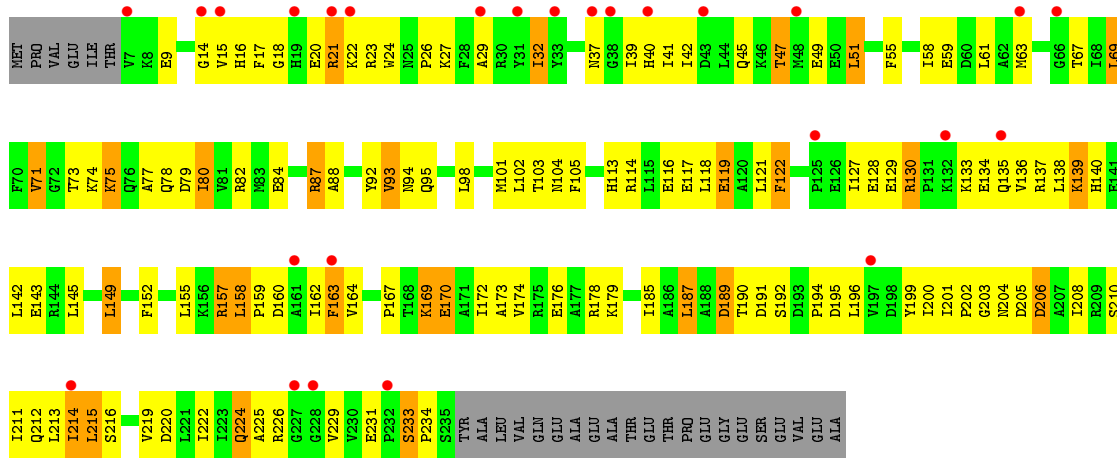


• Molecule 2: 30S Ribosomal Protein S2

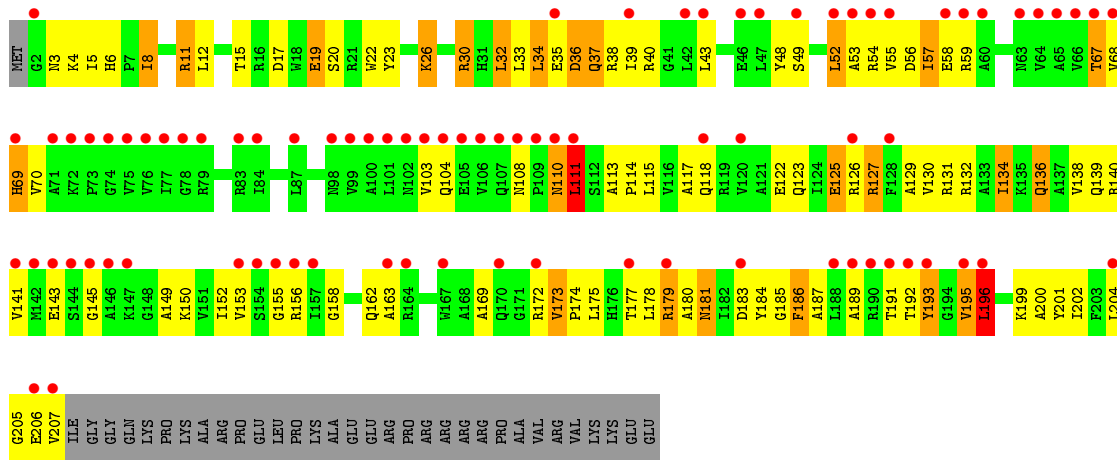


• Molecule 2: 30S Ribosomal Protein S2

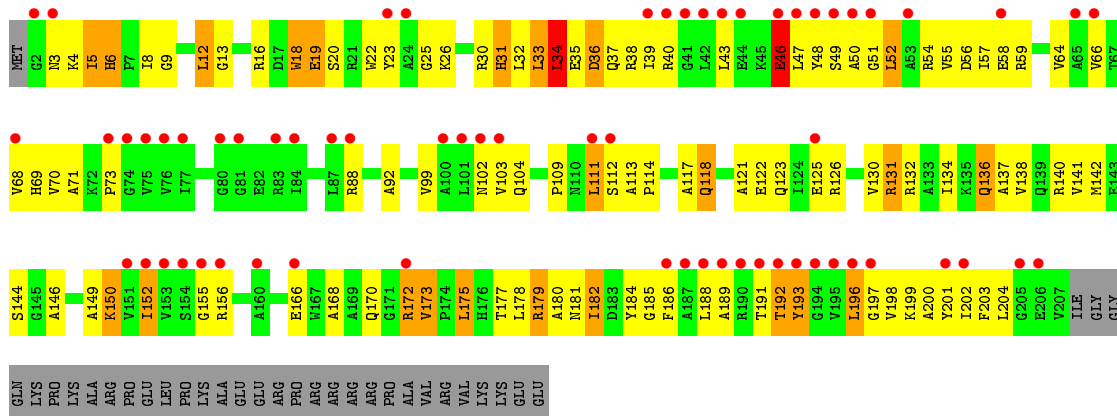




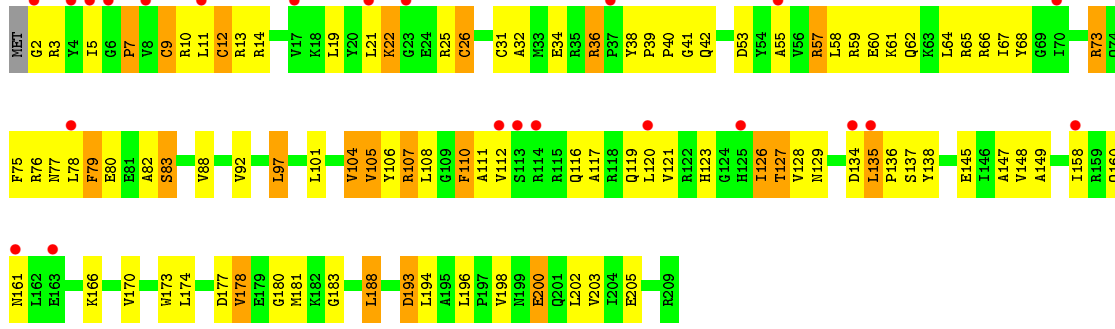
• Molecule 3: 30S Ribosomal Protein S3



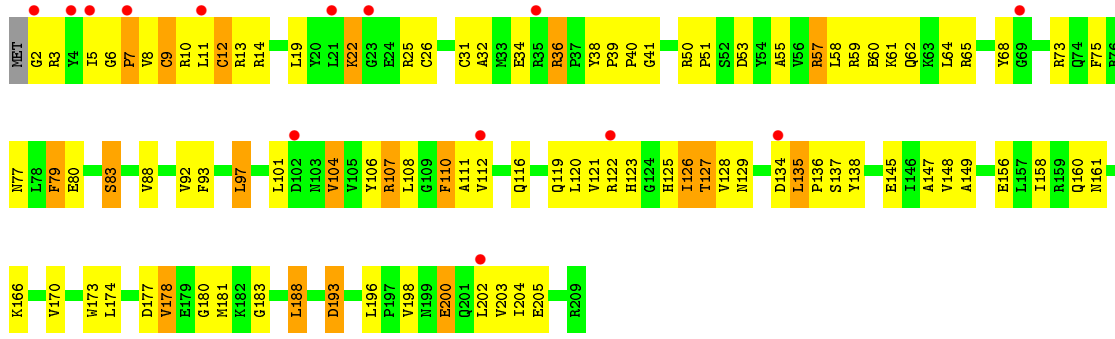
• Molecule 3: 30S Ribosomal Protein S3



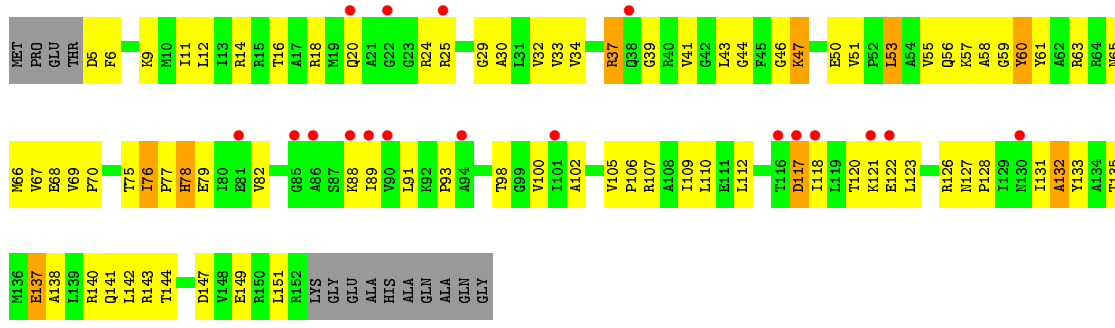
• Molecule 4: 30S Ribosomal Protein S4



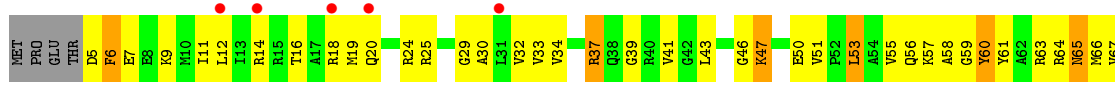
• Molecule 4: 30S Ribosomal Protein S4

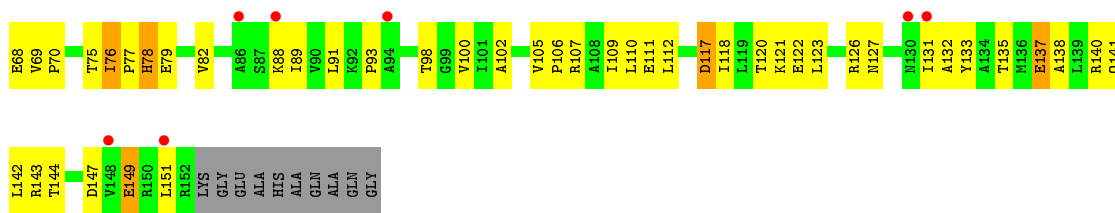


• Molecule 5: 30S Ribosomal Protein S5

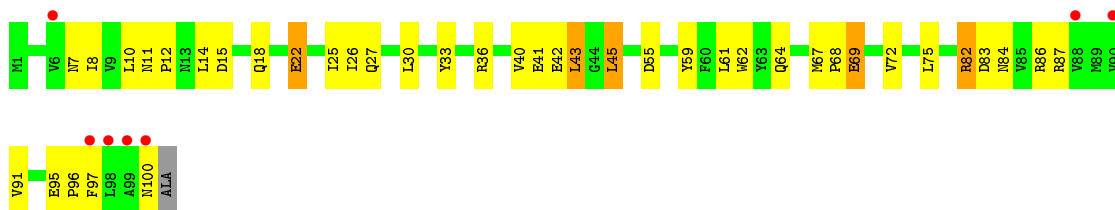


• Molecule 5: 30S Ribosomal Protein S5

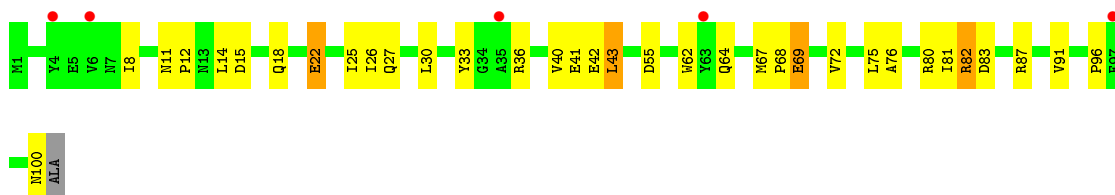




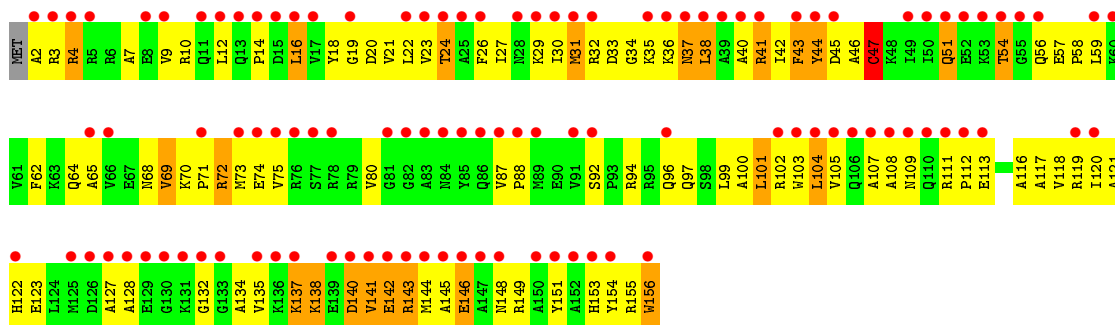
• Molecule 6: 30S Ribosomal Protein S6



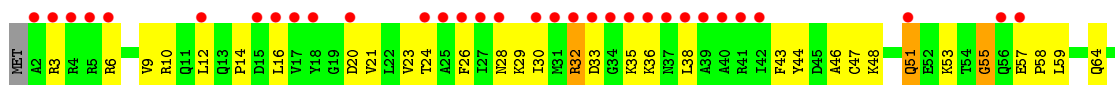
• Molecule 6: 30S Ribosomal Protein S6

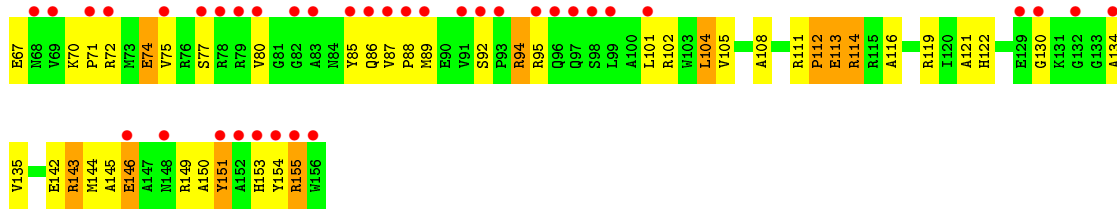


• Molecule 7: 30S Ribosomal Protein S7

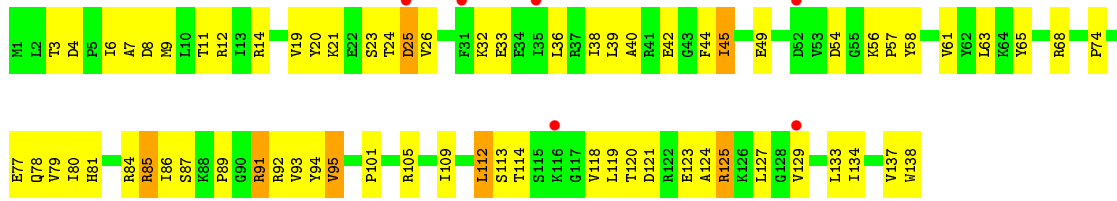


• Molecule 7: 30S Ribosomal Protein S7

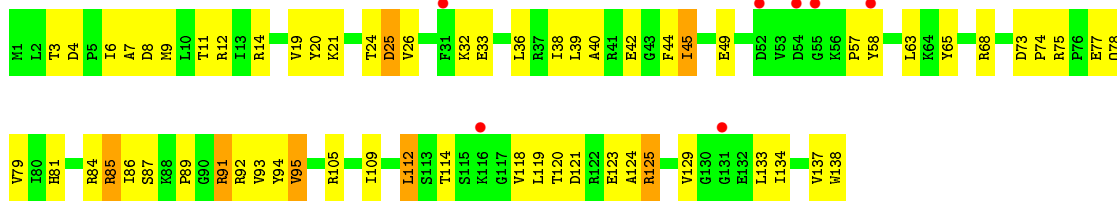




• Molecule 8: 30S Ribosomal Protein S8



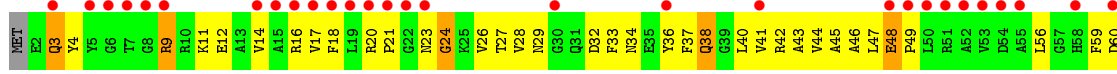
• Molecule 8: 30S Ribosomal Protein S8

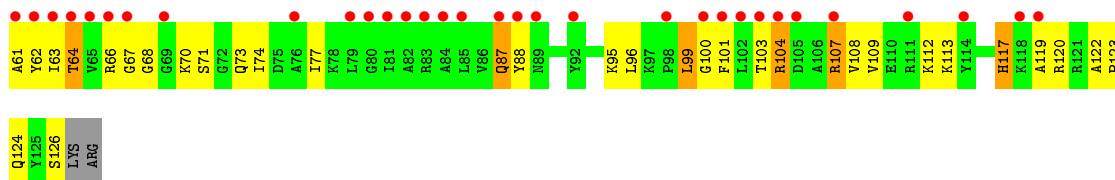


• Molecule 9: 30S Ribosomal Protein S9

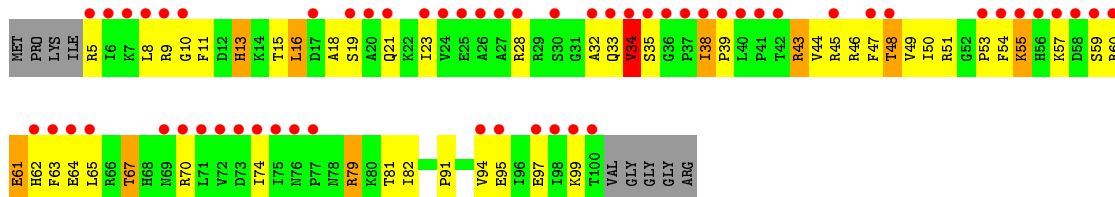
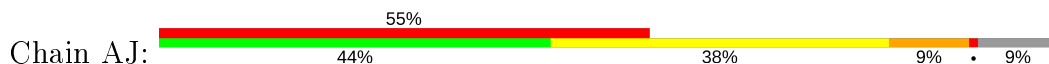


• Molecule 9: 30S Ribosomal Protein S9

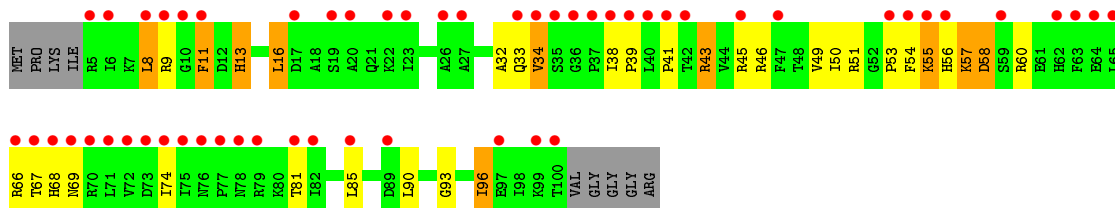




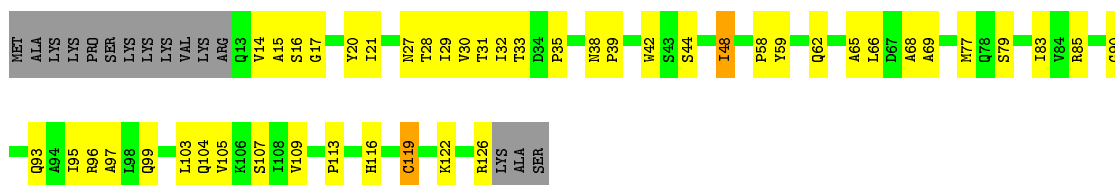
• Molecule 10: 30S Ribosomal Protein S10



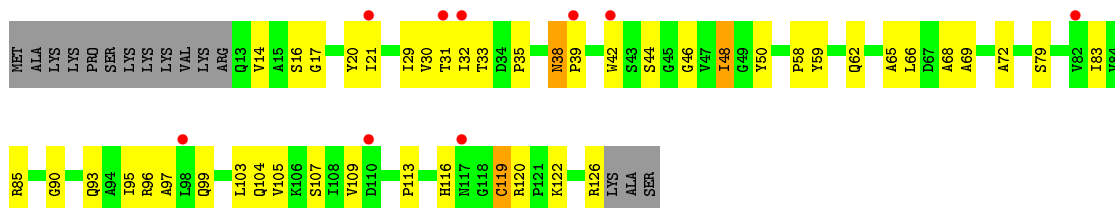
• Molecule 10: 30S Ribosomal Protein S10



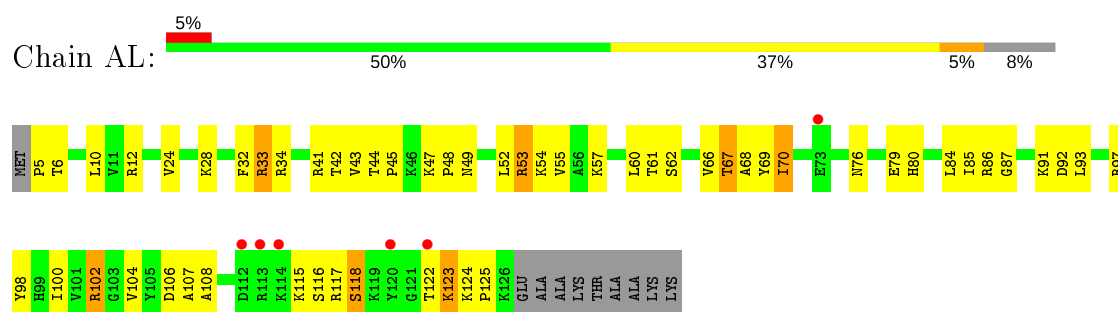
• Molecule 11: 30S Ribosomal Protein S11



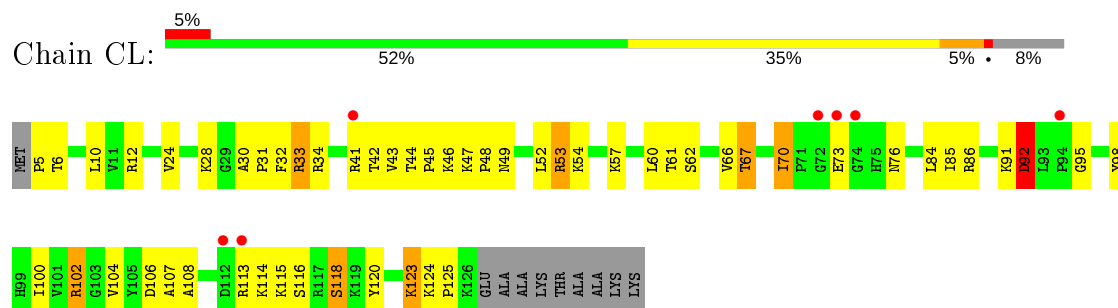
• Molecule 11: 30S Ribosomal Protein S11



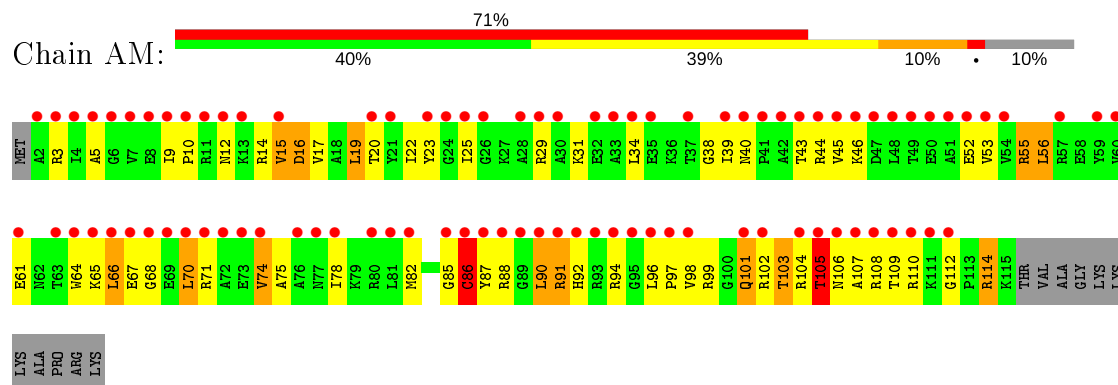
• Molecule 12: 30S Ribosomal Protein S12



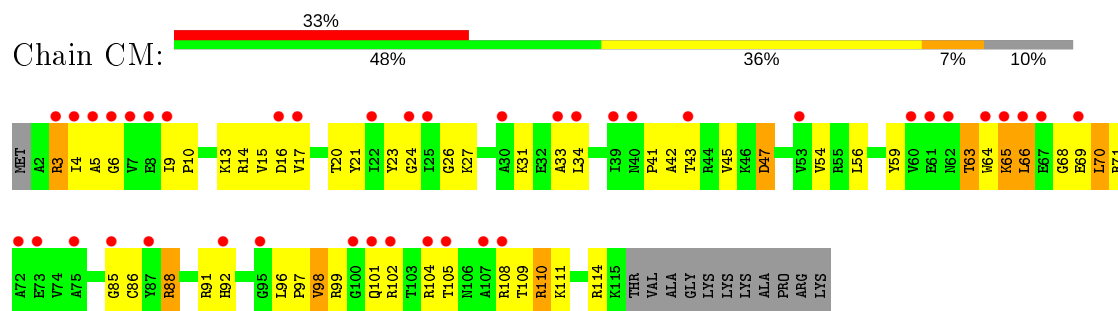
- Molecule 12: 30S Ribosomal Protein S12



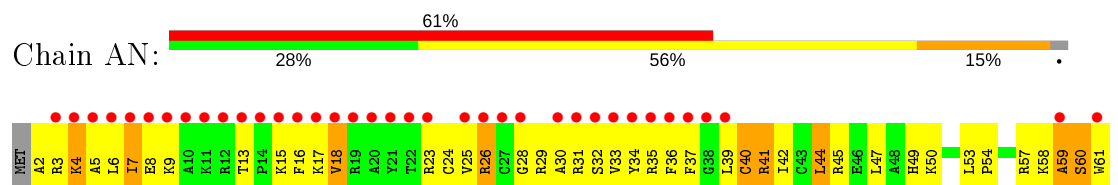
- Molecule 13: 30S Ribosomal Protein S13



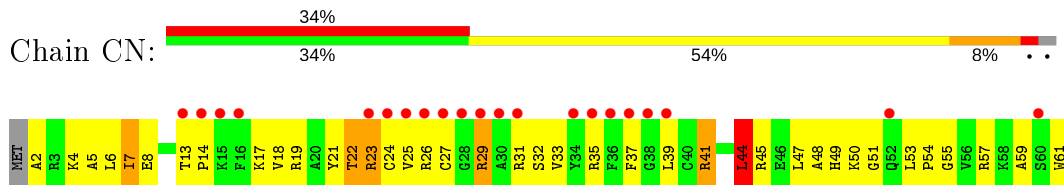
- Molecule 13: 30S Ribosomal Protein S13



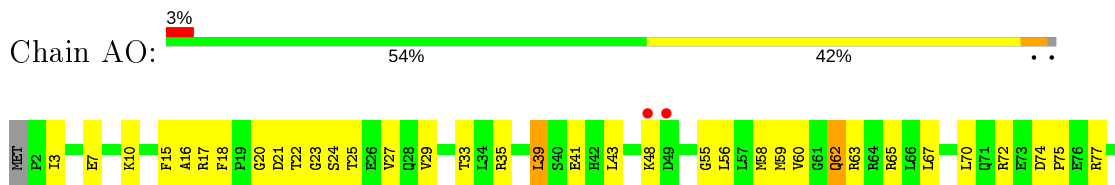
- Molecule 14: 30S Ribosomal Protein S14



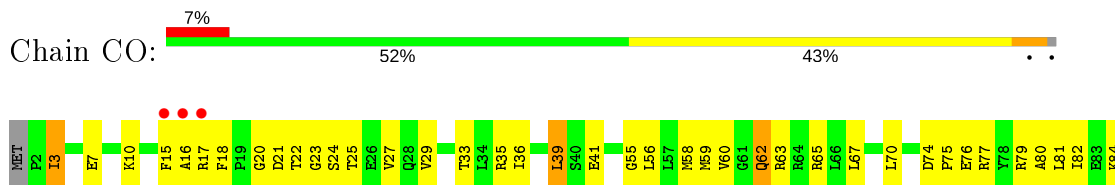
- Molecule 14: 30S Ribosomal Protein S14



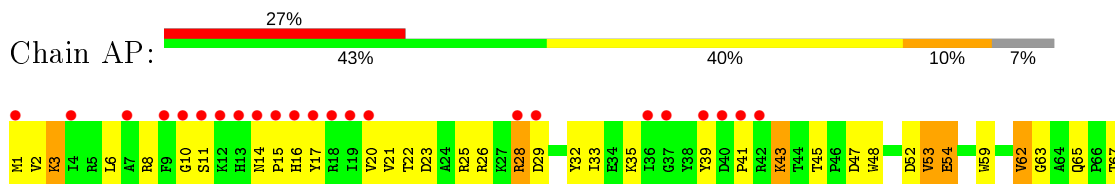
- Molecule 15: 30S Ribosomal Protein S15



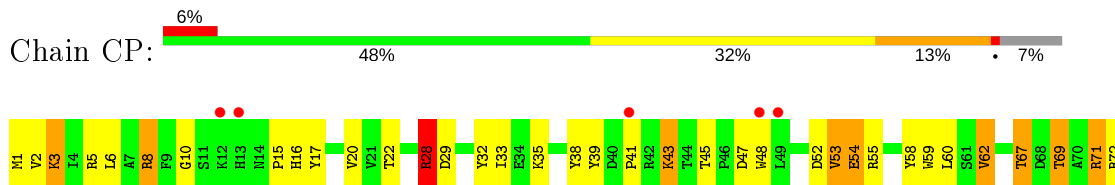
- Molecule 15: 30S Ribosomal Protein S15



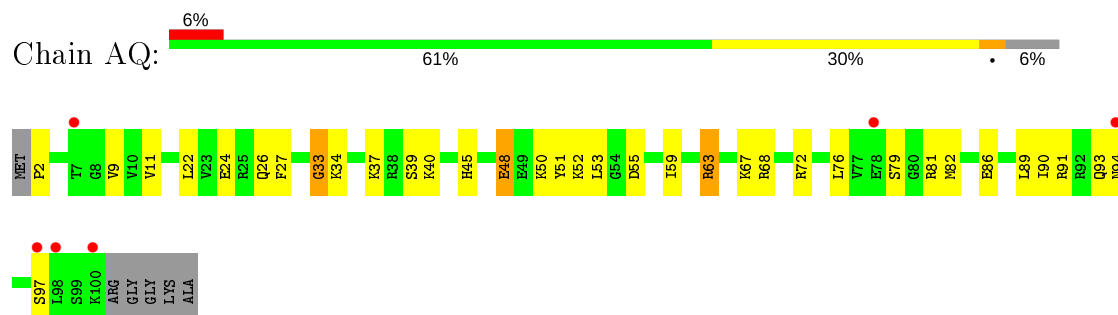
- Molecule 16: 30S Ribosomal Protein S16



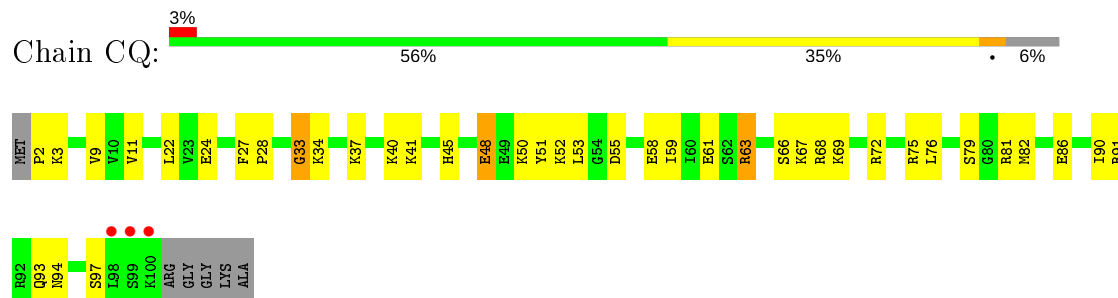
- Molecule 16: 30S Ribosomal Protein S16



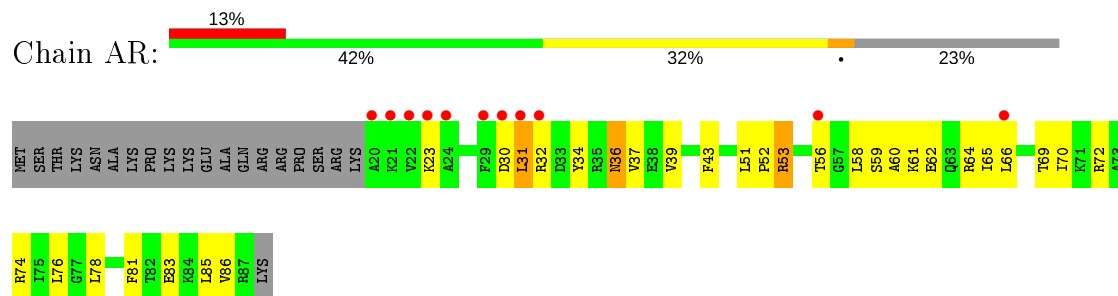
- Molecule 17: 30S Ribosomal Protein S17



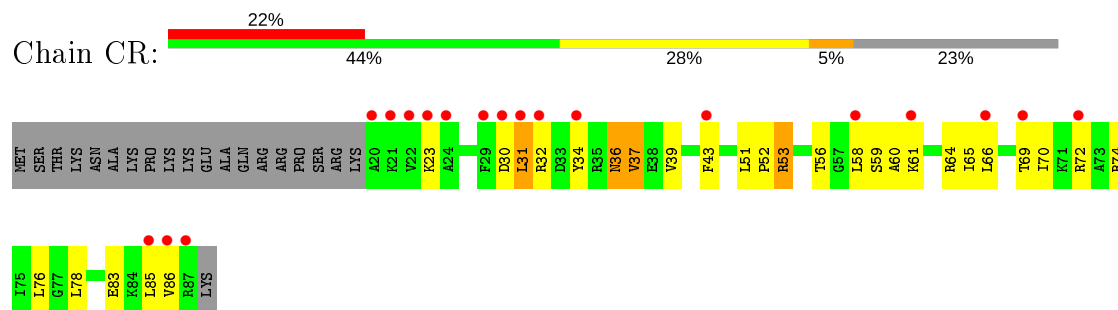
- Molecule 17: 30S Ribosomal Protein S17



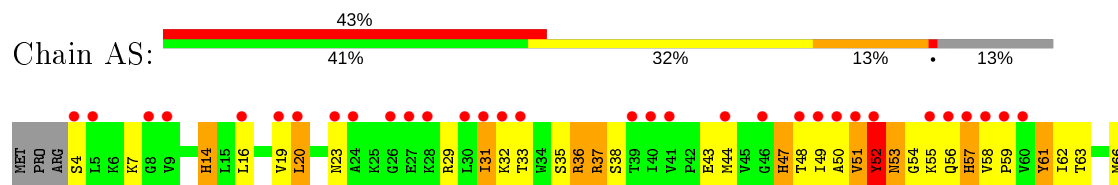
- Molecule 18: 30S Ribosomal Protein S18

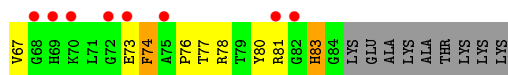


- Molecule 18: 30S Ribosomal Protein S18

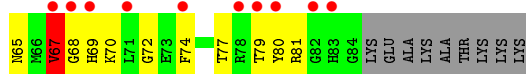
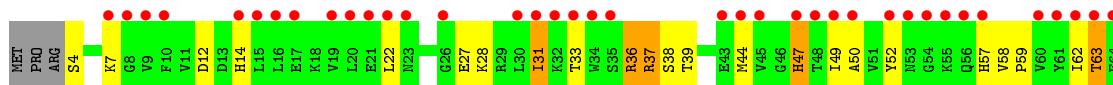


- Molecule 19: 30S Ribosomal Protein S19

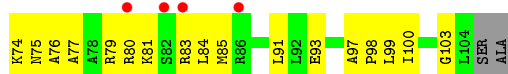
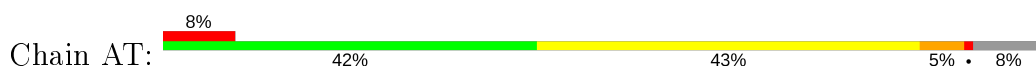




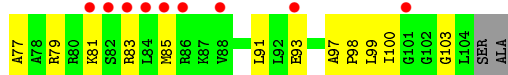
- Molecule 19: 30S Ribosomal Protein S19



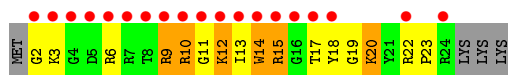
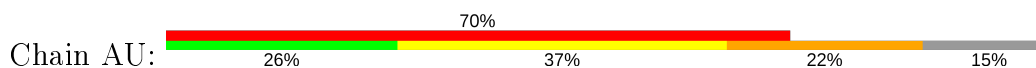
- Molecule 20: 30S Ribosomal Protein S20



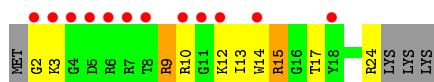
- Molecule 20: 30S Ribosomal Protein S20



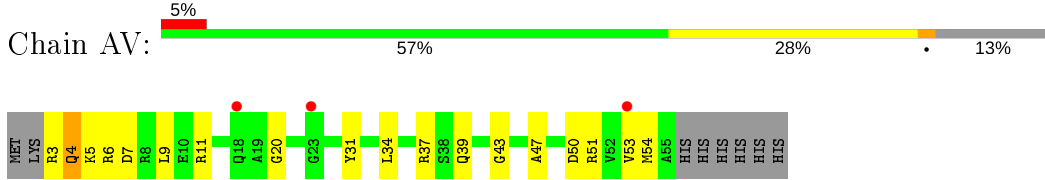
- Molecule 21: 30S Ribosomal Protein THX



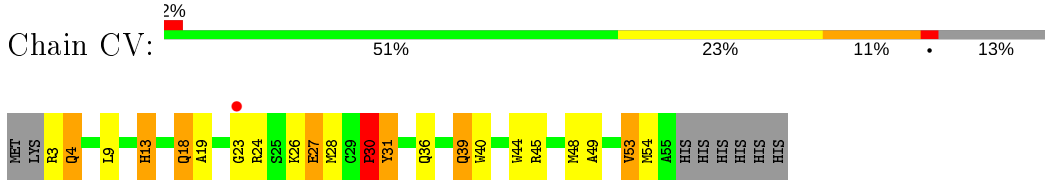
- Molecule 21: 30S Ribosomal Protein THX



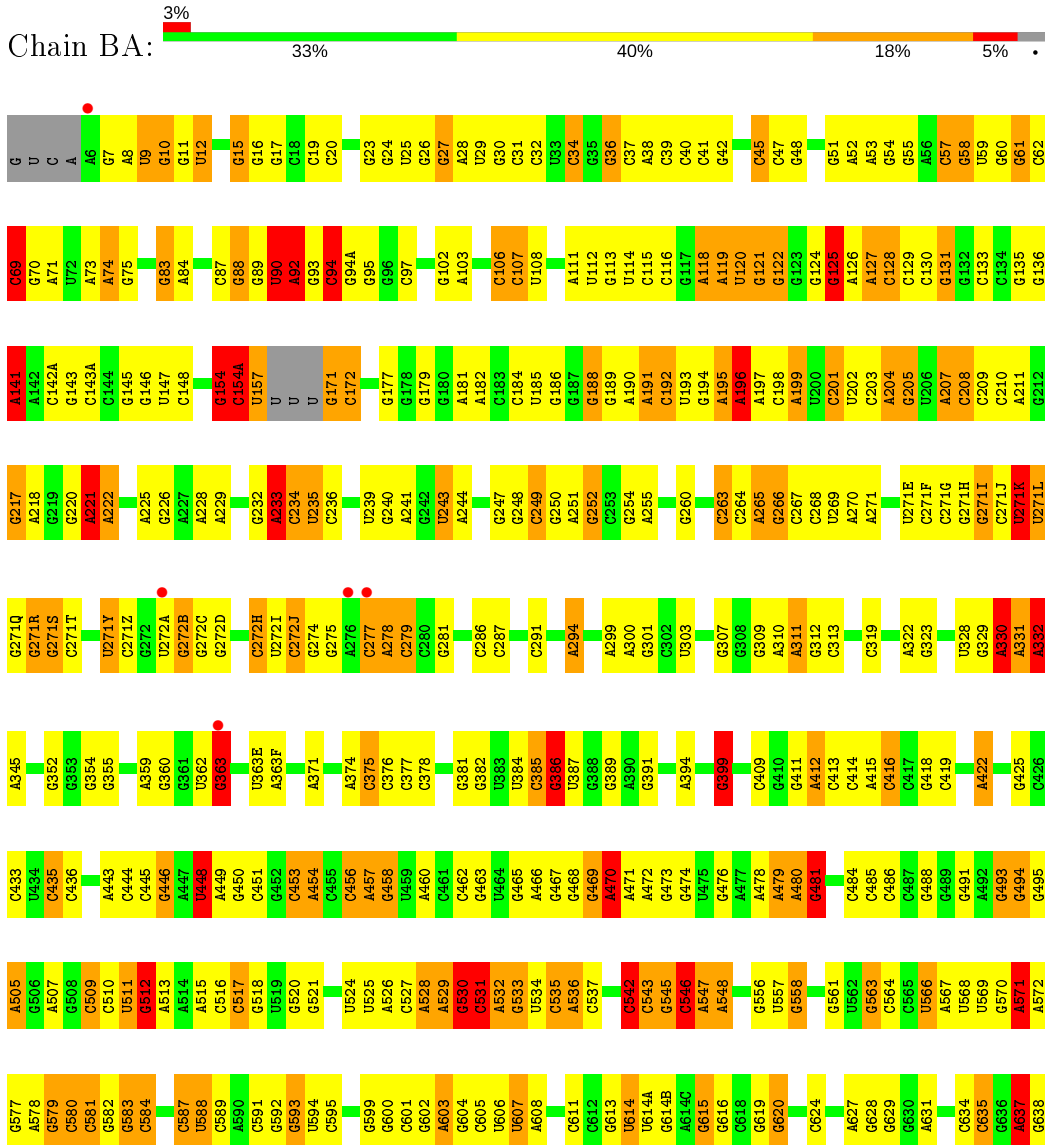
● Molecule 22: Ribosome modulation factor



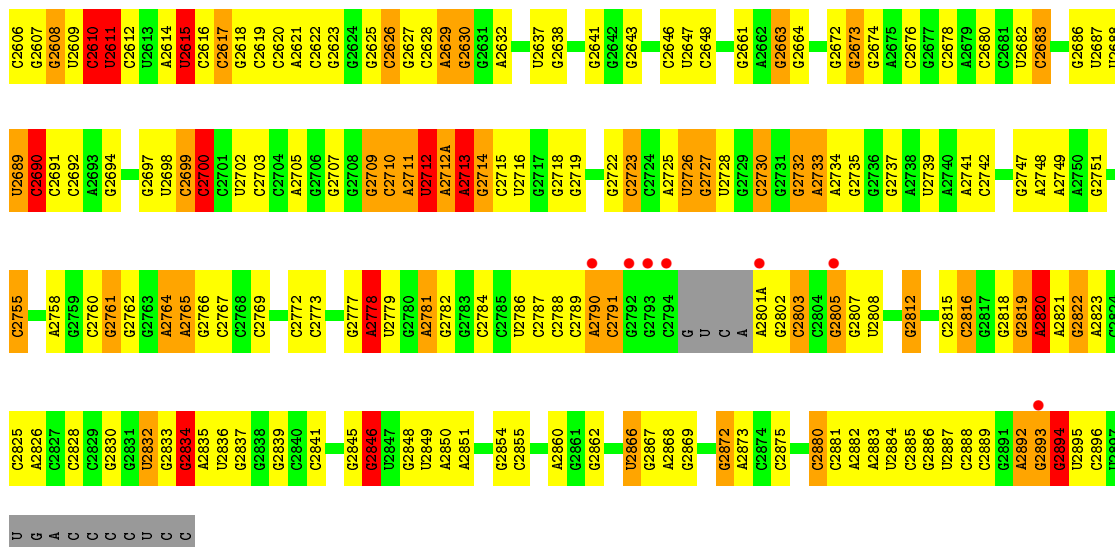
● Molecule 22: Ribosome modulation factor



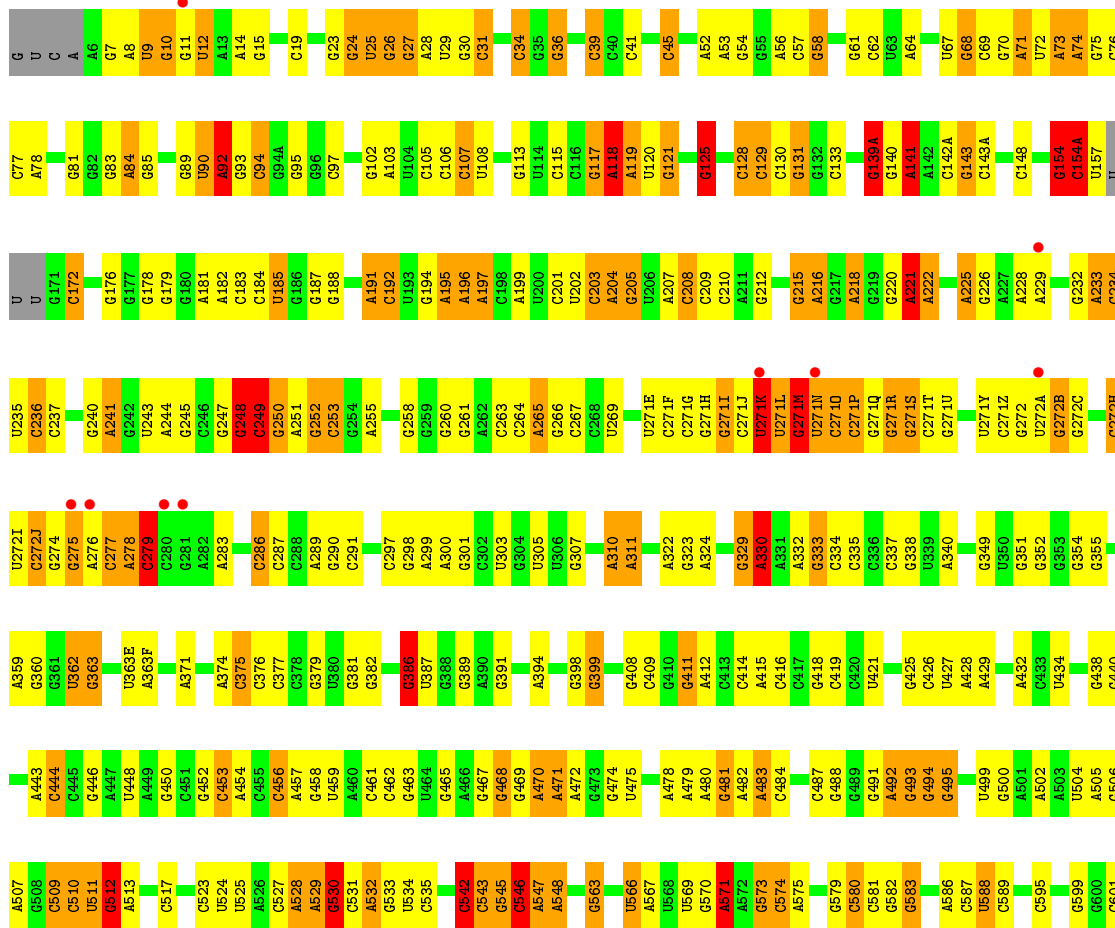
● Molecule 23: 23S Ribosomal RNA



G1526	A1449	G1377	G1306	G1286	C1188	A	U1085	C970	A899	U827	U762	G684	A643
G1527	A1450	A1378	A1307	A1297	G1164	A	G1036	C971	A900	U828	G763	A685	A644
A1528	G1379	G1238	A1308	G1238	U1165	U	G1037	G972	A901	A829	A764	G686	C645
A1529	C1450A	G1380	G1309	G1239	C1166	A	C1038	C902	C902	G830	G765	C687	A646
G1530	U1453	G1381	G1310	U1240	G1167	C	C1039	G974	C903	G831	C766	U688	G647
C1531	C1382	U1312	G1311	A1241	C	C	C1040	C975	C904	G832	U767	G649	G648
G1532	C1383	U1312	U1242	U1242	G1171	U	C1041	G975A	U905	U833	G768	G690	C650
G	A1460	C1314	G1243	G1243	A	C	G1042	C976	G906	C834	G769	C891	C651
U	G1461	C1315	U1244	U1244	G	C	A1043	G977	U907	A835	G770	C692	G652
A	U1391	G1319	G1245	A1246	U	C	A1044	G978	A910	G836	G771	C693	A652A
C	A1392	A1247	A1246	A1247	A	C	A1045	G979	A911	C837	C772	U694	G652B
G1537	A1393	G1248	C1178	U1178	G1107	G1106	A1046	A980	A911	U838	A774	C698	G652C
G1538	A1394	U1249	C1179	C1179	U1108	U1108	A1048	A982	C914	G775	A775	A699	G652D
U1539	A1395	G1250	C1180	C1180	C1109	C1109	C1049	A983	C914	G776	G776	G700	G652E
G1540	A1396	C1251	C1181	C1181	G1110	A984	G1051	G916	C915	A777	A777	G	G
G1541	U1397	G1252	A1118	G1117	C1110	A984	G1052	A917	C916	A778	A778	A706	C
A1542	C1398	U1254	C1119	G1117	A1111	C985	C	A917	C917	U847	U779	C708	C
C1543	U1326	G1260	G1120	G1120	G1119	C986	C	A917	U922	A849	G780	C709	C
A1544	C1327	U1255	C1121	C1121	G1119	A988	C	A988	C923	U852	A781	U709	C
A1545	G1328	U1256	G1116	G1116	C1116	A	A	A989	U928	G852	A782	G717	C
A1546	U1329	G1257	G1117	G1117	G1117	G	U	G989	G928	U847	A783	G717	C
C1547	U1406	C1257	C1118	C1118	C1118	A	A	A990	G931	G855	A784	C720	C
C1548	A1331	G1260	G1119	G1119	C1118	A	G	A990	G932	C856	A785	C721	C
	G1332	C1261	G1120	G1120	G1120	G	U	A991	G933	C857	G785	G722	C
	C1333	G1185	C1121	C1121	C1121	U	C	A992	A833	U858	A788	A722	G
	G1334	A1194	G1122	G1122	G1122	U	U	A993	G934	G859	G791	G723	G
	A1411	G1266	G1122	G1122	G1122	U	G	A994	G935	U860	C792	U724	C
	A1412	U1267	G1123	G1123	G1123	U	G	A995	C936	U861	G792	U725	C
	G1413	A1268	C1124	C1124	C1124	C	U	A996	G937	G862	A793	G726	C
	A1336	U1269	G1125	G1125	G1125	G	C	A997	C938	U863	A794	A727	C
	G1337	G1269	A1126	A1126	A1126	U	U	G1003	G939	G864	C795	G728	C
	G1338	C1270	U1127	U1127	U1127	U	U	C1004	G940	A865	G796	G652F	C
	U1341	G1271	A1128	A1128	A1128	U	U	C1005	G941	G866	C797	A653	C
		A1272	G1130	G1130	G1130	G	G	C1006	A941	A866	C797	C730	C
	G1344	U1273	U1130	U1130	U1130	A	A	C1007	G942	U867	G798	A654	C
		A1274	A1131	A1131	A1131	U	U	C1008	G943	G869	G799	A655	C
	G1348	A1275	G1132	G1132	G1132	G	G	A1009	U944	U870	A800	U657	C
	A1349	U1276	A1132	A1132	A1132	A	A	A1010	G945	U871	A801	C658	C
		G1278	U1133	U1133	U1133	C	C	G1011	A945	G872	G802	C659	C
	G1350	G1279	C1134	C1134	C1134	A	A	C1012	G946	A873	A802	G738	C
	G1351	U1279	G1136	G1136	G1136	G	G	U1012	C949	G873	G739	G739	C
		G1284	U1136	U1136	U1136	U	U	U1013	G950	U874	G805	U740	C
	G1352	G1285	G1137	G1137	G1137	C	C	U1014	C951	G879	C806	G663	C
	G1358	U1288	U1138	U1138	U1138	C	C	G1015	G952	U879	C807	C664	C
	A1360	C1289	G1139	G1139	G1139	A	A	G1016	C953	G881	G808	C665	C
	G1361	U1290	C1140	C1140	C1140	U	U	C	G954	G882	G809	G743	C
	A1365	C1291	U1141	U1141	U1141	C	C	U1019	A953	G	U810	G668	C
	A1366	C1292	U1142	U1142	U1142	U	U	A1020	G954	G	U811	G669	C
	A1367	C1293	A1143	A1143	A1143	U	U	A1021	C955	U812	C812	A670	C
	A1367	G1296	G1144	G1144	G1144	U	U	U1022	G956	C	C812	C671	C
	G1368	U1297	C1145	C1145	C1145	A	A	G1024	G958	A	G815	C672	C
	G1369	C1297	U1145	U1145	U1145	A	A	A	U958	C	C816	C673	C
	C1370	C1298	G1149	G1149	G1149	A	A	A	A959	C	C817	G674	C
	G1371	U1300	C1221A	C1221A	C1221A	A	A	U1026	G960	C	C817	A751	C
	A1372	A1301	C1222	C1222	C1222	G	G	A1027	C961	U896	A818	A675	C
	A1373	A1302	G1150	G1150	G1150	A	A	A1028	G964	G	A819	A676	C
	G1374	C1303	G1151	G1151	G1151	U	U	G1029	C965	C	A820	A677	C
	G1375	G1304	C1152	C1152	C1152	G	G	G1030	G966	U895	A821	C754	C
	C1376	C1305	G1153	G1153	G1153	U	U	G1031	C967	U896	U822	C755	C
			G1154	G1154	G1154	G	G	U1032	G968	A896	G823	C756	C
			A1155	A1155	A1155	C	C	A1033	C969	U897	A824	G760	C
			U1234	U1234	U1234	G	G	U1034	G969	C998	A824	A761	C
			G1157	G1157	G1157	U	U	G1034	U969				

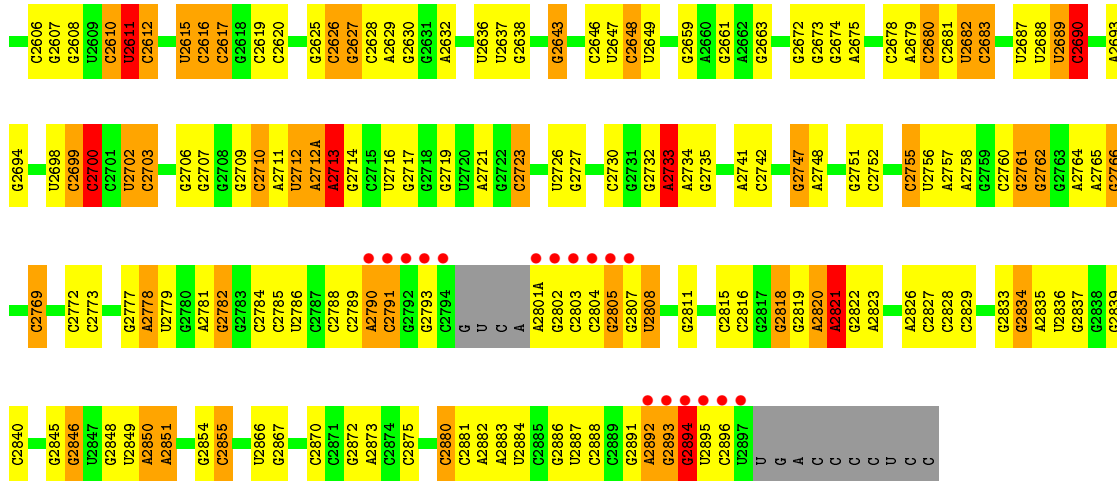


● Molecule 23: 23S Ribosomal RNA

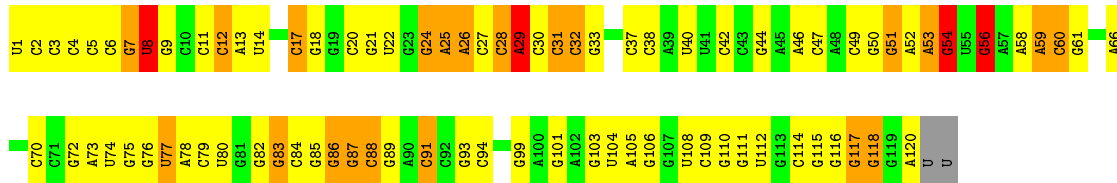


C1509	C1482	G1358	U1288	C1207	G1102	G931	U860	G797	G728	C	G682
A1509A	U1433	G1359	C1289	C1208	G1003	G932	A661	G798	G729	C652T	A603
A1509B	A1434	A1359	U1292	G1209	C1004	A933	G662	G799	C730	G652V	G604
G1510	G1435	U1292	U1292	A1210	U	A934	A663	A800	G652V	G652V	C605
G1436	G1436	C1293	U1292	A1211	G	C935	G664	G801	G733	A653	U606
C1437	C1437	A1365	U1294	G1212	C1007	C936	C665	A802	A734	A654	U607
U1514	G1441	A1366	A1295	A1213	A1009	U937	A666	U803		A655	
G1515	G1442	A1367	G1296	A1214	A1010	G938	C667	A804	C737	A656	U614
U1518	G1445	G1368	C1297	C1218	G1011	G939	U868	A805	G738	U657	U614A
G1519	A1445	C1369	C1298	G1219	U1012	C806	G669	C806	G741	G662	G614B
G1520	C1445A	C1370	G1299	U1130	C1013	U807	G669	U807	G742	G662	G614C
U1523	U1372	G1371	U1300	G1137	G1014	G808	G673	G808	G743	G663	G615
G1524	A1449	A1372	A1301	G1138	G1015	G809		G809	G744	G664	C618
G1525	G1450	A1373	A1302	G1139	G1016	U810		U810	G745	G665	G619
G1527	G1456	G1374	A1303	C1140	G1017	U811		U811	G746		
U1529	G1459	G1377	U1304	U1141	C1018	G812		G812	U747	G669	U626
C1530	A1460	A1378	C1305	U1142	U1019	U813		U813	U747	A670	A627
C1531	G1461	A1379	U1306	U1143	G1020	U814		U814	U748	A671	G628
G1532	G1466	G1380	A1307	A1143	C	C815		C815	C749	C671	G629
G1533	G1466	G1381	A1308	G1144	C	C816		C816	A750	C672	G630
G1534	G1467	G1382	A1309	G1149	C	A983		A983	A751	C673	G631
U1534	C1467	C1383	G1310	U1149	G1024	G818		G818	A752	C674	A631
C1468	C1468	C1384	G1311	U1150	G1025	A954		A954	A752	C675	A632
A1469	A1469	A1385	U1312	G1153	U1026	C955		C955	C753	A675	G632
G1470	G1470	G1388	U1313	G1154	A1027	G956		G956	C754	A676	G633
G1471	A1471	G1389	C1314	A1155	A1028	A957		A957	C755	A677	C634
C1474	C1474	U1390	A1315	A1156	G	U958		U958	C756	C678	C635
A1477	A1477	G1391	G1316	C1161	A1029	A959		A959	A756	C679	G636
G1478	G1478	U1394	U1317	G1162	G1030	A960		A960	A756	C680	G637
A1545	A1545	G1394	A1318	G1163	G1031	C961		C961	U762	G681	G638
C1546	G1480	U1396	G1319	G1164	A1032	A965		A965	U762	G682	U639
U1481	U1481	G1397	A1320	U1165	G1033	C967		C967	G763	G683	C640
C1548	C1482	U1397	U1321	U1166	U1034	G968		G968	A764	G684	C641
A1542	A1486	C1403	C1322	G1171	G1035	C971		C971	A764	A685	G642
C1543	G1487	G1404	U1327	G	U1036	G975		G975	C766	G686	A643
A1544	A1488	U1405	U1328	A	G1037	G975A		G975A	G768	C687	A644
A1545	U1489	U1406	G1329	U1041	G1038	G979		G979	U769	G690	G645
G1546	C1489	C1407	U1330	G1042	G1039	G985		G985	C772	G693	G646
C1547	A1490	C1408	G1331	G1043	U1040	U907		U907	A774	G694	G647
G1548	G1492	U1408	G1332	A	C1044	A981		A981	G775	G695	C650
A1554	A1493	U1415	C1333	U1045	A1045	C982		C982	G776	C697	A652A
A1562	A1494	G1416	U1334	A1046	A1046	A910		A910	A777	C698	A652B
G1563	A1495	C1417	C1335	G1047	G1047	A911		A911	G780	G706	G652C
C1564	A1496	C1418	G1337	G1048	C1048	C912		C912	A780	C852D	G652E
G1565	U1497	G1419	U1338	C1049	U1049	U913		U913	A781	G707	G
A1566	C1498	A1419	U1339	U1051	A1050	C914		C914	A782	C708	G
A1567	C1499	U1420	U1340	G1051	G1051	G987		G987	A783	U709	G
G1568	G1500	G1421	U1341	C1052	C	G989		G989	A784	C	C
A1569	C1501	G1422	A1342	C	A	A990		A990	G785	C	C
A1570	U1503	G1425	G1348	A	G	A918		A918	A788	C720	G
C1575	C1504	A1427	C1201	G1114	G	G919		G919	A788	C721	A
C1576	C1505	A1428	G1202	G1115	G	G993		G993	C791	A722	C
U1577	G1506	G1429	U1203	G1117	A	C994		C994	G792	C	C
U1578	A1508	A1430	G1204	C1118	G	G995		G995	A789	G724	G
		U1431	U1205	C1119	G	G996		G996	G794	G725	G
			G1206	U1120	U	G997		G997	C795	G726	G
				G1121	U	A1001		A1001	C796	A727	C
				G1122	G						

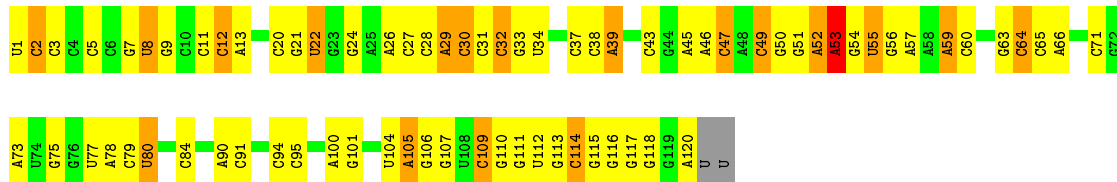
C2538	C2467	G2400	G2331	A2267	C2185	G2124	A2060	G1998	A1918	A1819	G1756	C1657	A1579
C2539	G2468	U2401	U2332	A2268	G2186	G2125	G2061	C1999	G1922	U1820	U1757	C1657	A1580
C2540	A2469	C2404	A2333	A2269	G2187	A2126	A2062	C2000	G1923	G1823	G1758	U1658	C1582
A2541	G2470	G2405	A2335	G2271	U2189	C2128	C2063	A2001	G1924	G1824	A1759	U1659	C1583
G2543	U2473	U2406	A2336	U2272	G2190	G2129	C2065	G2003	C1925	A1825	C1760	C1660	A1584
G2548	A2476	G2409	G2339	A2274	G2191	U2130	C2066	G2004	U1926	G1826	A1762	G1661	A1586
G2549	C2477	G2410	G2340	G2275	G2192	G2131	U2068	C2006	A1928	G1828	G1764	A1685	C1588
G2550	A2478	A2411	G2341	G2280	G2193	G2132	G2069	C2007	G1929	A1829	C1765	A1688	C1592
G2551	G2479	A2412	C2342	C2281	C2194	G2133	G2070	C2008	G1930	A1830	U1766	A1669	G1593
G2552	G2480	G2413	C2343	G2282	C2195	A2135	G2071	G2009	U1931	G1831	C1767	C1670	G1594
G2553	G2481	G2414	U2344	C2283	U2197	G2136	G2072	G2010	U1932	C1832	U1768	U1671	
U2554	G2482	G2415	G2345	G2284	A2198	C2137	U2074	U2011	C1934	U1833	G1769		A1597
G2555	C2483	G2416	A2346	C2285	A2199	U2138	U2074	G2012	G1935	A1834		G1674	A1598
G2556	G2484	A2417	A2347	G2286	C2200	C2139	U2075	A2013	A1936	G1835	C1675	C1598	
G2557	G2485	G2418	A2348	A2287	U2203	G2140	G2087	A2014	A1937	C1836	U1774	G1676	C1599
G2558	G2486	U2419	G2349	A2288	C2205	U2079	A2080	A2015	A1938	U1837	C1775	A1677	C1600
G2559	G2487	C2420	G2350	G2289	C2206	G2142	G2080	U2016	U1939	G1838	G1776	G1678	G1601
G2560	A2488	G2421	C2351	A2290	G2207	C2143		G2017	U1940	G1839	U1777		U1602
G2561	G2489	A2422	A2352	C2291	U2208	U2144	C2084	G2018	G1945	U1841	U1778	G1681	A1603
G2562	G2490	U2423	G2353	A2292	U2118	C2145	C2085	A2019	U1946	U1842	U1779	C1685	C1604
U2563	U2491	G2424	C2354	C2293	G2147	G2146	U2086	A2020	C1947	A1843	A1780	C1685	C1605
U2564	A2425	A2425	C2355	C2294	G2148	U2147	G2087	C2021	C1947	G1844	C1781	C1686	C1606
U2565	A2426	A2426	C2356	G2295	G2149	G2148	U2088	U2022		G1845	C1782	C1687	C1607
U2566	G2427	G2427	U2357	A2296	U2150	U2149	U2089	G2023	G1954	A1847	A1783	U1688	A1608
G2567	G2496	G2428	C2358	C2297	G2151	U2090	U2090	G2024	U1955	U1848	A1784	A1689	A1609
G2568	A2497	A2429	C2359	A2298	G2152	U2091	U2091	G2025	U1956	U1849	A1785	A1610	A1610
G2569	G2498	A2430	G2360	A2299	U2153	U2092	G2093	U2027	C1957	A1854	A1787	U1693	C1611
G2570	C2499	A2431	A2361	G2299	G2154	G2093	G2094	U2034	C1958	A1855	C1788	C1694	C1612
A2571	U2500	A2432	G2362	G2302	G2155	G2100	C2095	G2035	A1966	G1856	C1789	C1695	G1613
C2572	C2501	A2434	A2363	U2292	G2156	G2101	G2096	G2036	C1967	A1877	U1794	A1701	A1614
C2573	G2502	A2435	C2364	C2293	G2157	U2102	U2096	G2037	U1968	G1878	C1795	G1702	C1625
G2574	G2503	U2436	G2365	A2294	C2158	U2103	C2103	G2038	G1969	G1883	U1796	G1703	G1628
C2575	A2503	G2437	C2366	G2295	G2159	G2104	G2104	C2039	A1970	A1884	C1797	C1708	C1631
C2576	U2504	U2438	G2367	C2296	G2160	C2105	C2040	U2041	A1971	A1885	G1798	C1711	C1632
C2577	G2505	A2439	U2368	C2297	C2161	G2106	G2106	U2042	A1972	C1886	C1800	C1712	A1634
C2578	U2506	C2440	G2369	A2298	G2162	C2107	C2107	A2042	A1977	A1889	A1802		G1635
C2579	G2507	A2441	C2370	C2299	G2163	C2108	C2043	G2044		A1890	A1803	U1720	C1636
G2580	G2508	C2442	A2371	A2241	C2164	U2109	C2044	C2044	G1980	G1890	C1804	G1721	A1637
G2581	C2509	G2443	A2372	G2242	G2165	G2110	G2105	G2046	A1981	G1899	C1805	A1722	C1638
G2582	C2510	G2444	A2373	A2243	G2166	C2111	G2106	U2047	C1982	A1900	C1806	U1739	U1639
U2583	U2511	G2445	C2374	C2294	U2167	U2113	G2048	G2048	C1983	G1906	G1807	G1740	C1640
C2584	G2512	G2446	G2375	G2295	G2168	A2114	G2049		G1984	G1907			A1641
C2585	U2514	G2447	A2381	G2296	G2169	G2115			G1985	C1907		C1745A	G1642
G2586		A2448	G2382	C2297	A2170	G2116			A1986	C1908		G1746	G1647
A2587	C2517	U2449	G2383	G2248	A2171	A2117						G1747	C1648
A2588	A2518	G2450	A2384	U2249	U2172	U2118			G1990	U1911			
C2589	U2519	A2451	C2385	G2250	A2173	A2119			U1991	A1912			
C2590	C2520	G2452	C2386	G2252	U2174	G2120			G1992	A1913			G1651
C2591			U2387	A2253	C2175	G2121			G1985	G1907			A1652
C2592	G2521		U2388	G2254	A2176	G2122			A1986	C1908			G1653
U2593	U2522		G2389	C2255	C2177	U2116							G1654
G2594	G2523		U2390	G2256	C2178	U2118							
G2595	G2524		G2391	C2257	C2179	U2119							
A2600	G2525		G2392	G2258	U2180	G2120							
A2601	U2529		G2393	U2262	G2181	G2121							
A2602	G2530		G2330	G2263	G2182	G2123							
G2603													



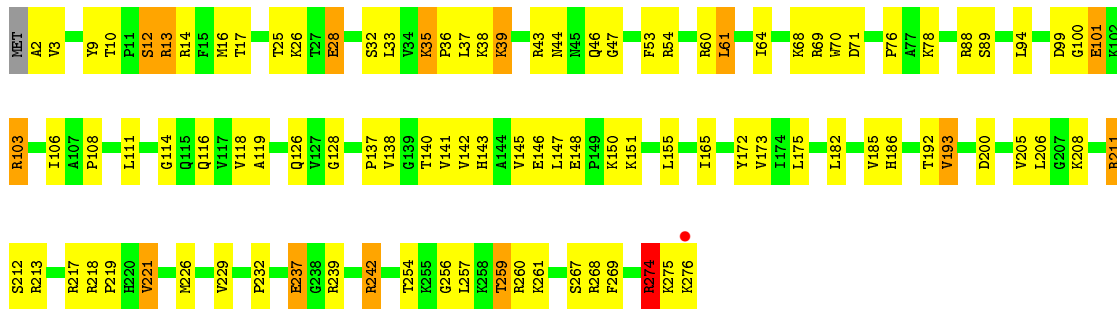
• Molecule 24: 5S Ribosomal RNA



• Molecule 24: 5S Ribosomal RNA

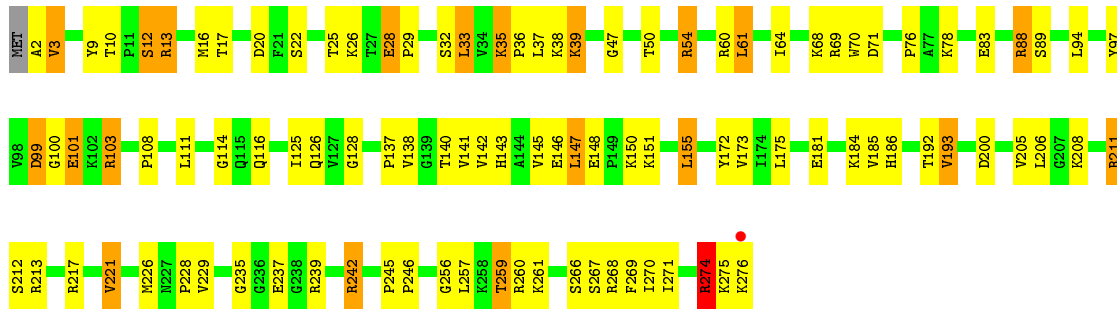


• Molecule 25: 50S Ribosomal Protein L2



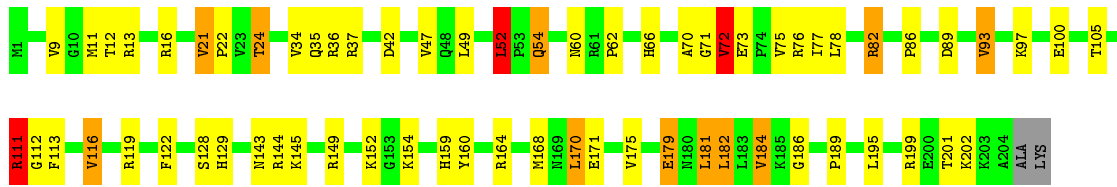
• Molecule 25: 50S Ribosomal Protein L2

Chain DD: 



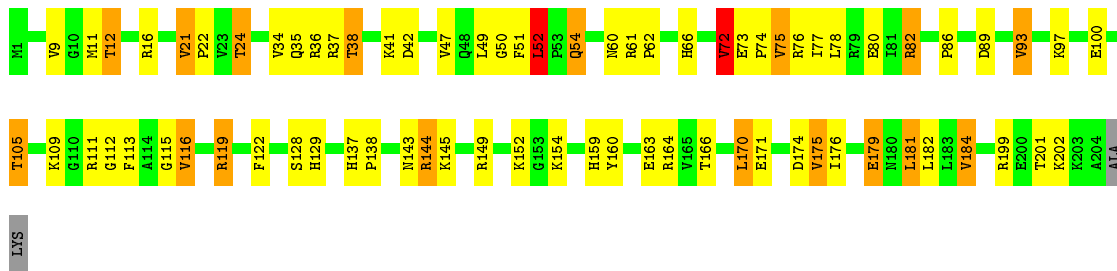
• Molecule 26: 50S Ribosomal Protein L3

Chain BE: 



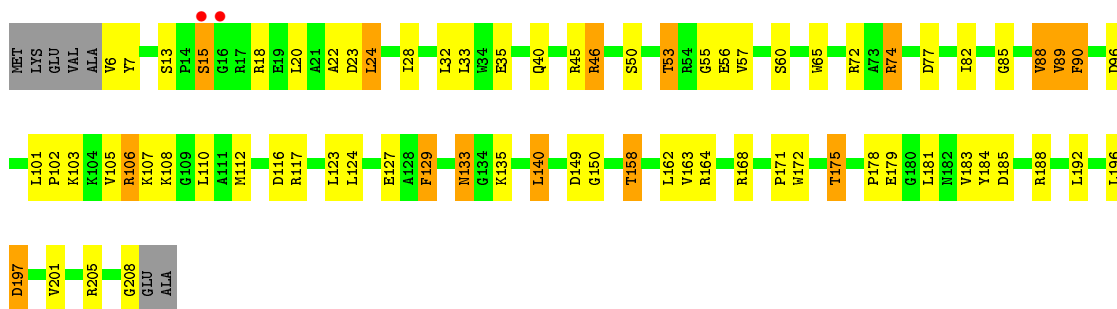
• Molecule 26: 50S Ribosomal Protein L3

Chain DE: 



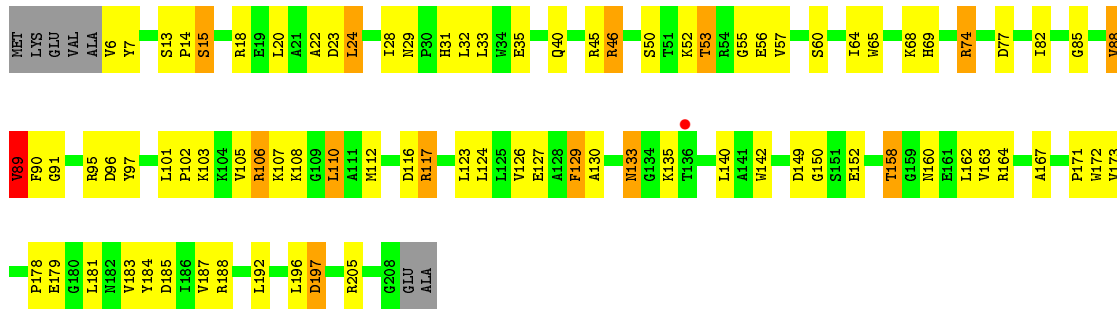
• Molecule 27: 50S Ribosomal Protein L4

Chain BF: 



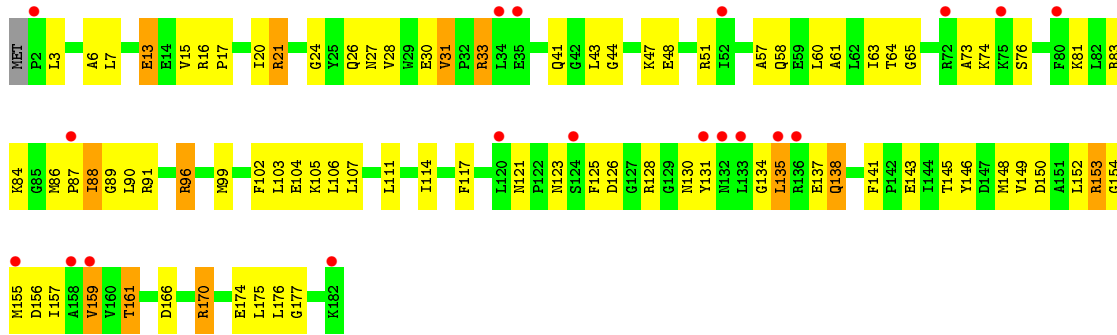
• Molecule 27: 50S Ribosomal Protein L4

Chain DF: 



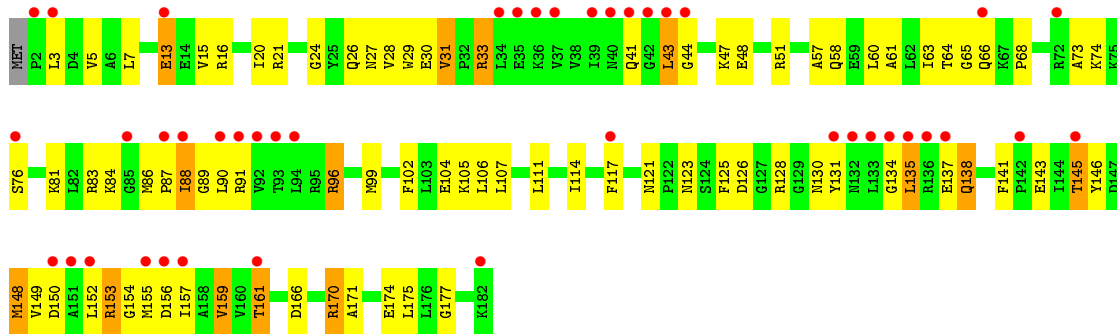
• Molecule 28: 50S Ribosomal Protein L5

Chain BG: 



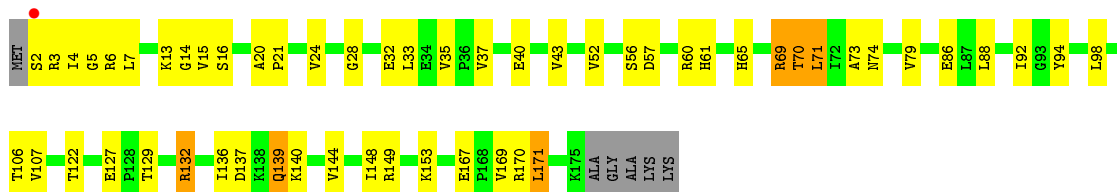
• Molecule 28: 50S Ribosomal Protein L5

Chain DG: 

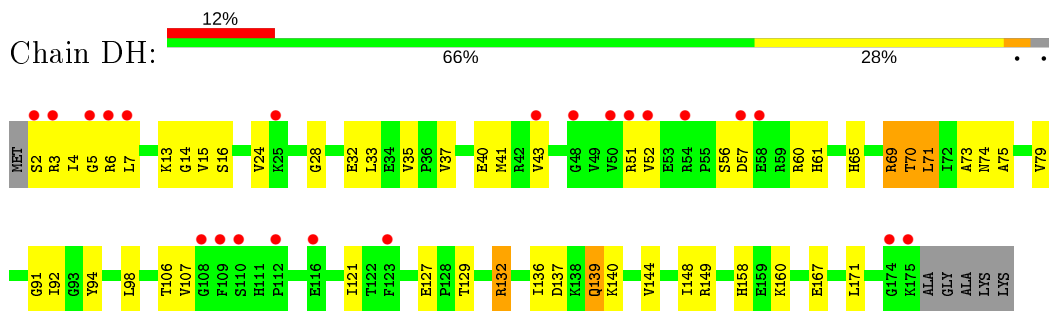


• Molecule 29: 50S Ribosomal Protein L6

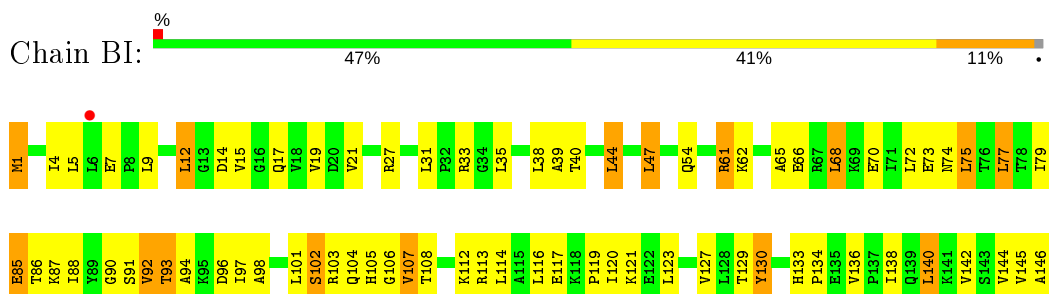
Chain BH: 



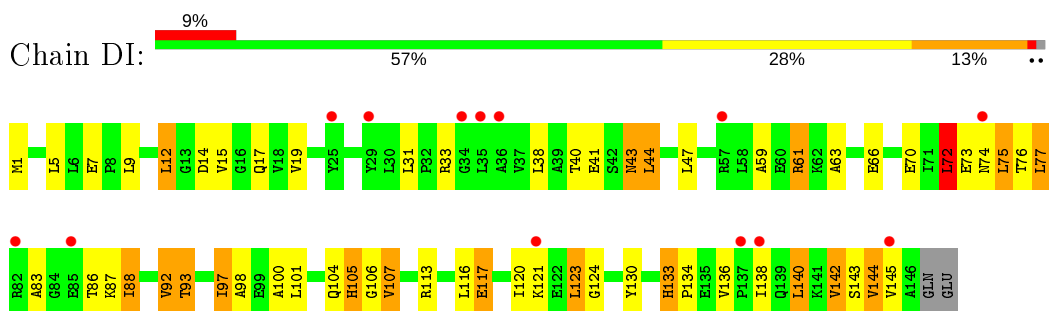
• Molecule 29: 50S Ribosomal Protein L6



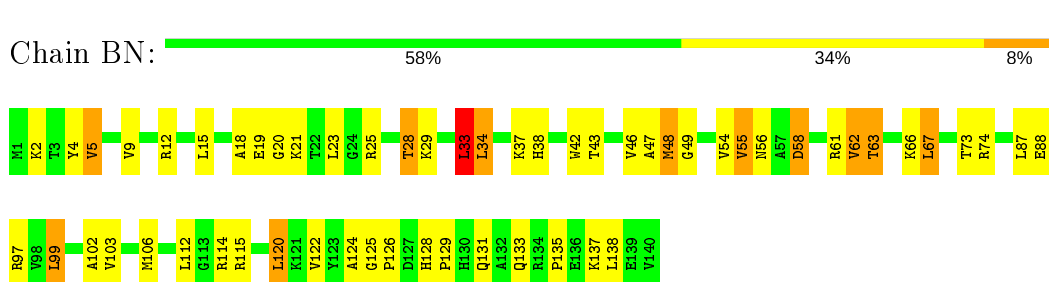
• Molecule 30: 50S Ribosomal Protein L9



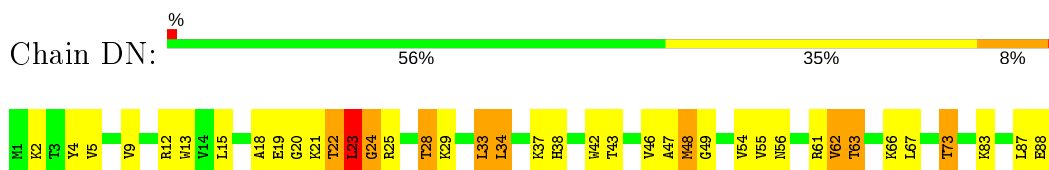
• Molecule 30: 50S Ribosomal Protein L9



• Molecule 31: 50S Ribosomal Protein L13

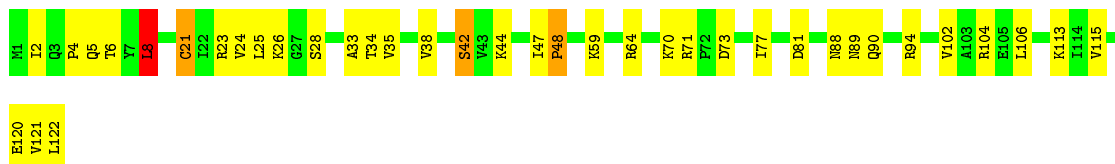


• Molecule 31: 50S Ribosomal Protein L13

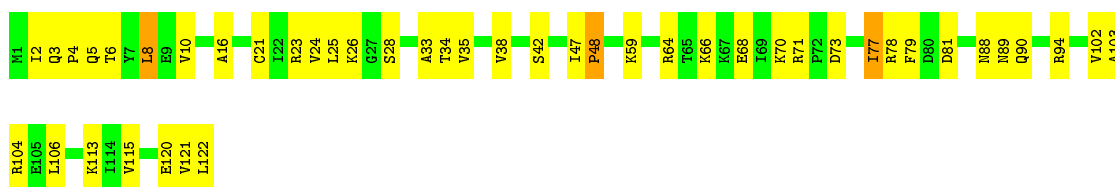




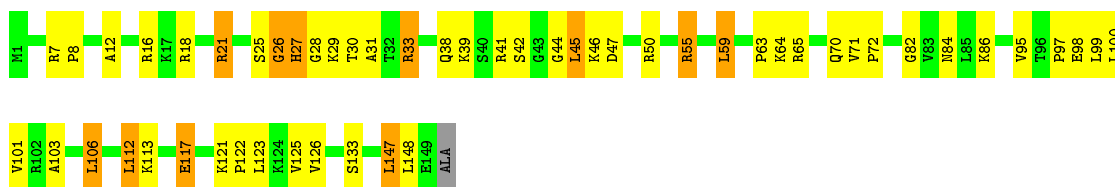
● Molecule 32: 50S Ribosomal Protein L14



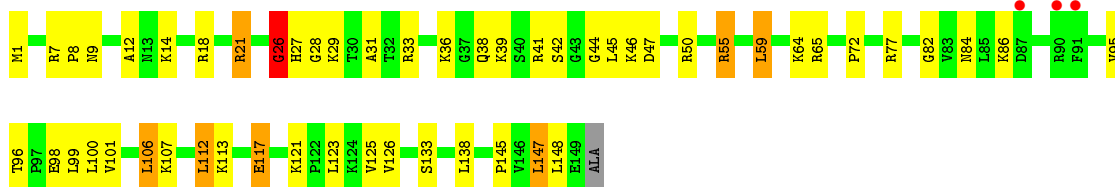
● Molecule 32: 50S Ribosomal Protein L14



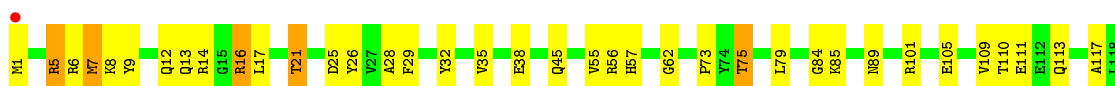
● Molecule 33: 50S Ribosomal Protein L15

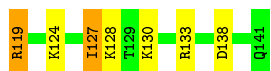


● Molecule 33: 50S Ribosomal Protein L15

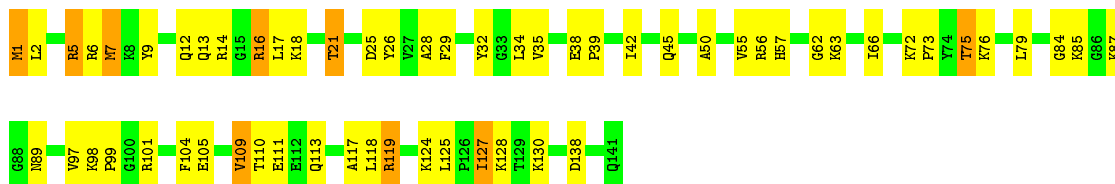


● Molecule 34: 50S Ribosomal Protein L16

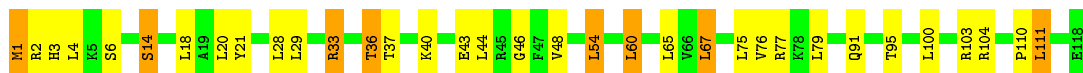




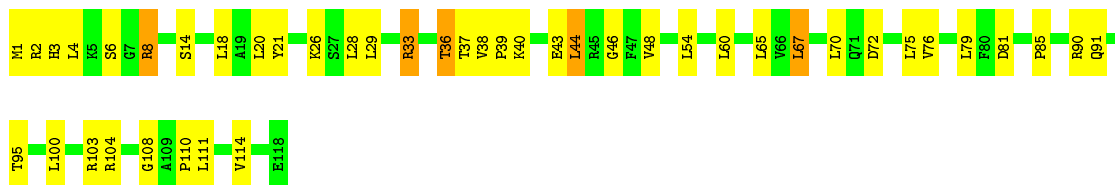
• Molecule 34: 50S Ribosomal Protein L16



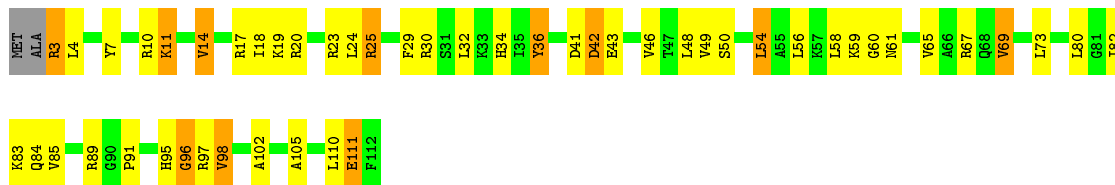
• Molecule 35: 50S Ribosomal Protein L17



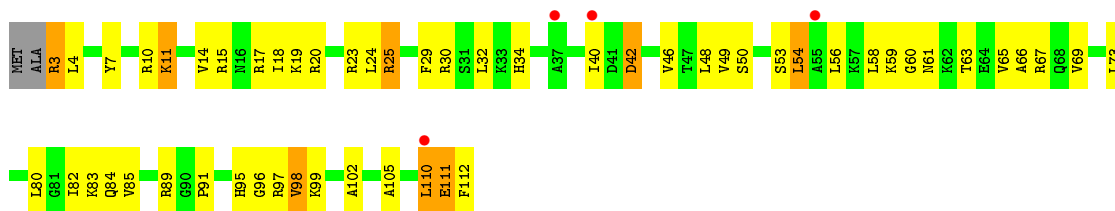
• Molecule 35: 50S Ribosomal Protein L17



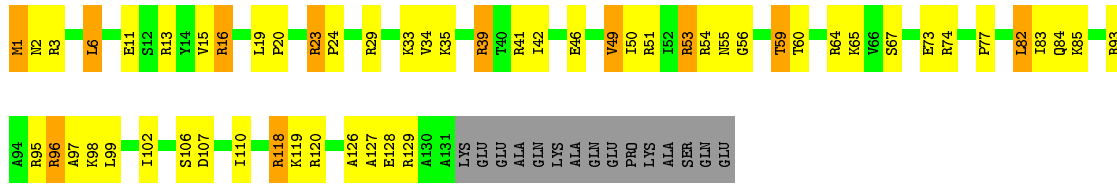
• Molecule 36: 50S Ribosomal Protein L18



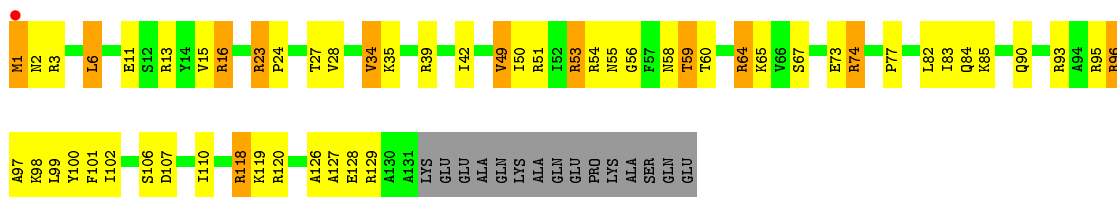
• Molecule 36: 50S Ribosomal Protein L18



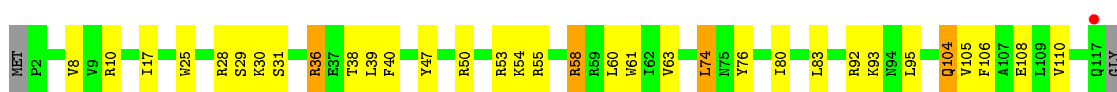
• Molecule 37: 50S Ribosomal Protein L19



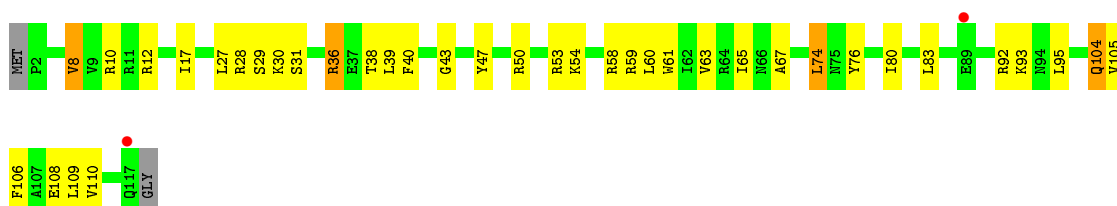
• Molecule 37: 50S Ribosomal Protein L19



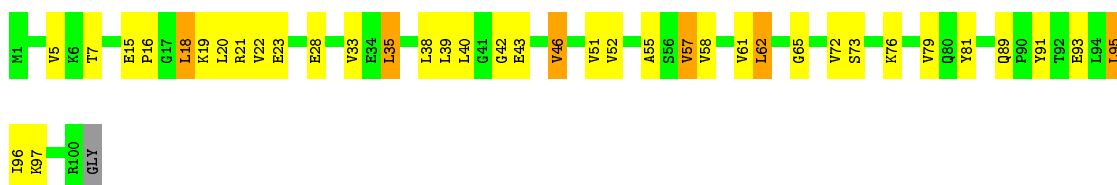
• Molecule 38: 50S Ribosomal Protein L20



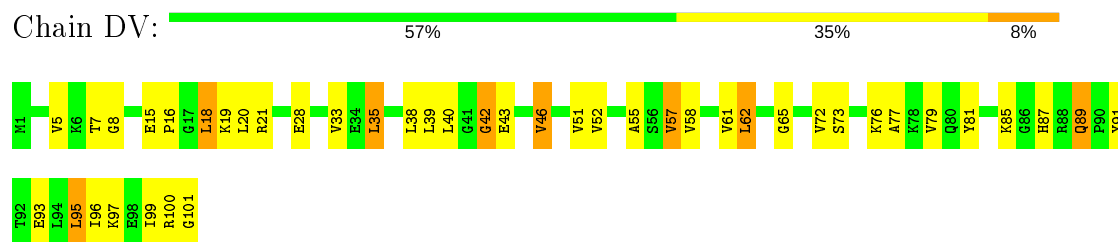
• Molecule 38: 50S Ribosomal Protein L20



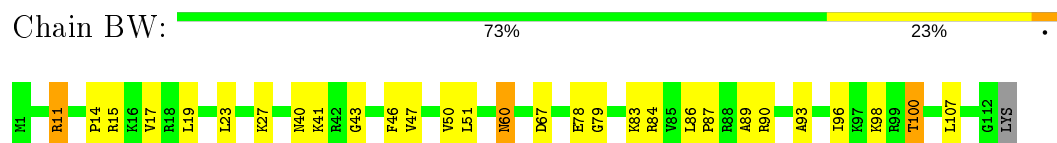
• Molecule 39: 50S Ribosomal Protein L21



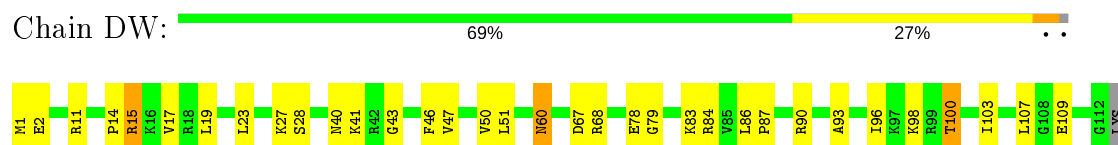
• Molecule 39: 50S Ribosomal Protein L21



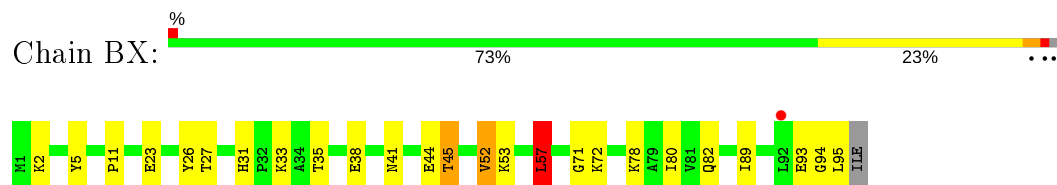
- Molecule 40: 50S Ribosomal Protein L22



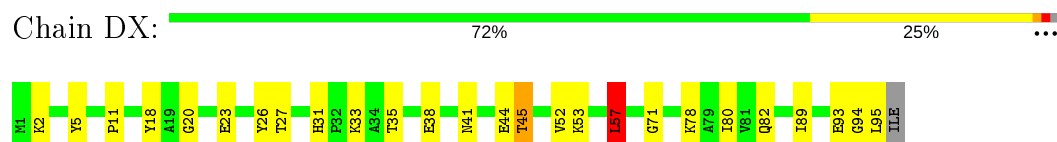
- Molecule 40: 50S Ribosomal Protein L22



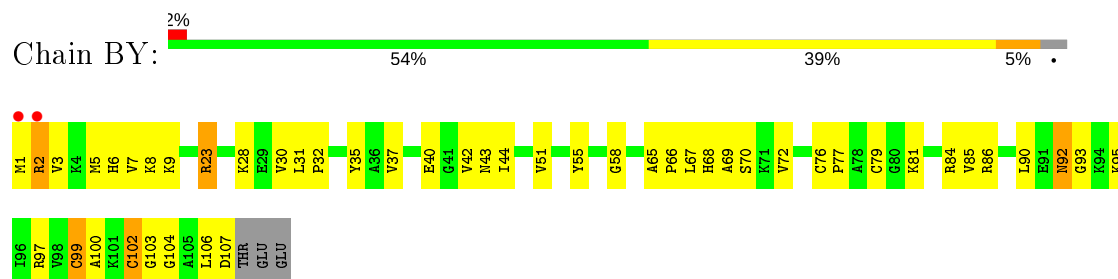
- Molecule 41: 50S Ribosomal Protein L23



- Molecule 41: 50S Ribosomal Protein L23

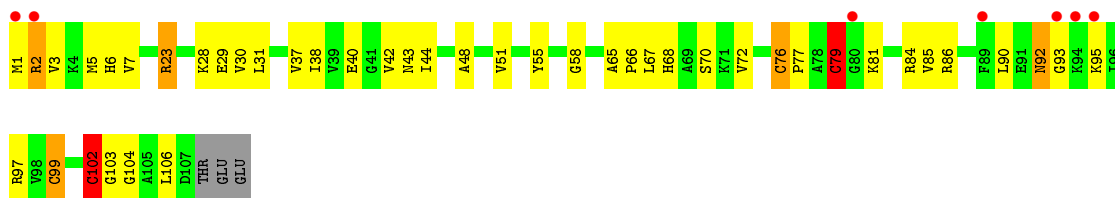


- Molecule 42: 50S Ribosomal Protein L24

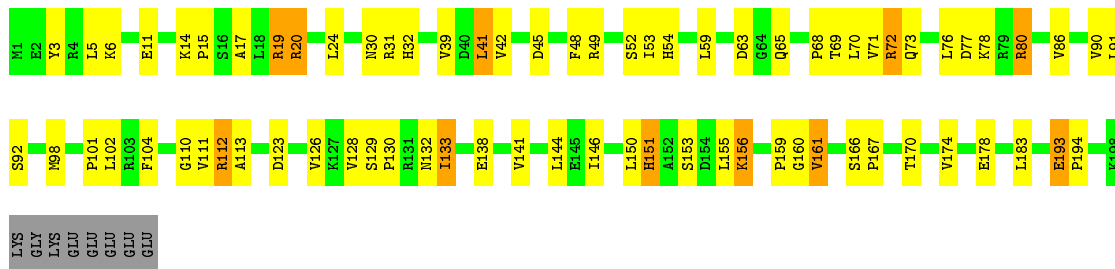


- Molecule 42: 50S Ribosomal Protein L24

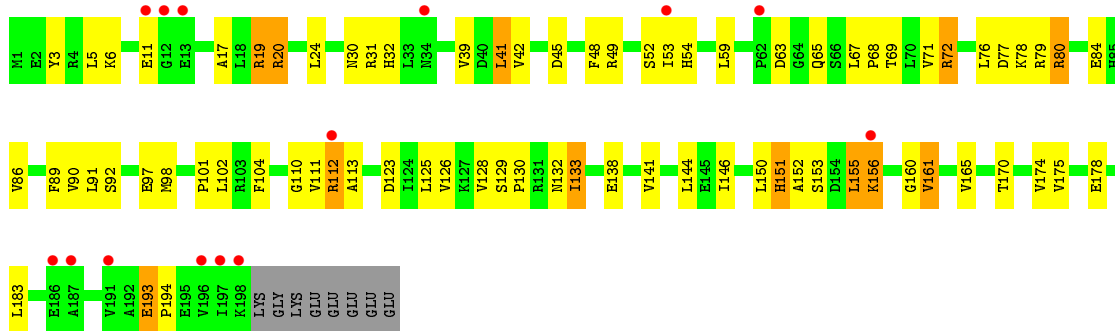




• Molecule 43: 50S Ribosomal Protein L25



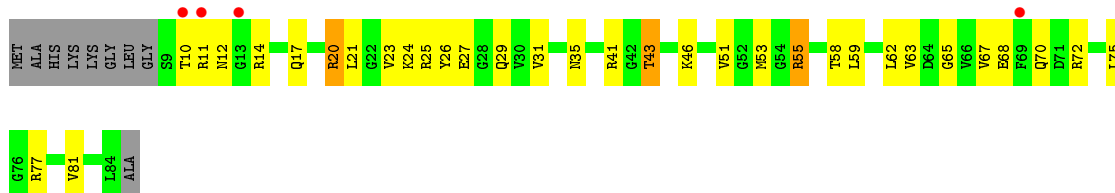
• Molecule 43: 50S Ribosomal Protein L25



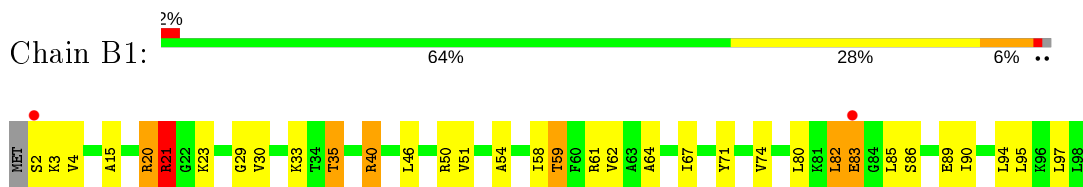
• Molecule 44: 50S Ribosomal Protein L27



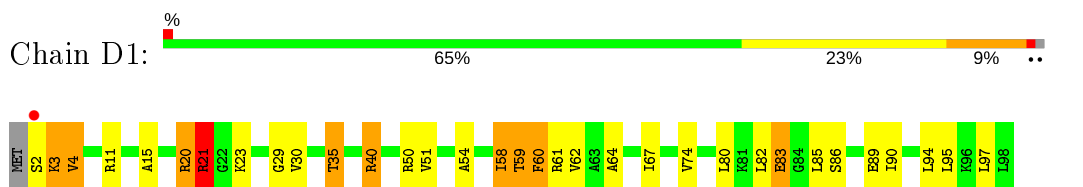
• Molecule 44: 50S Ribosomal Protein L27



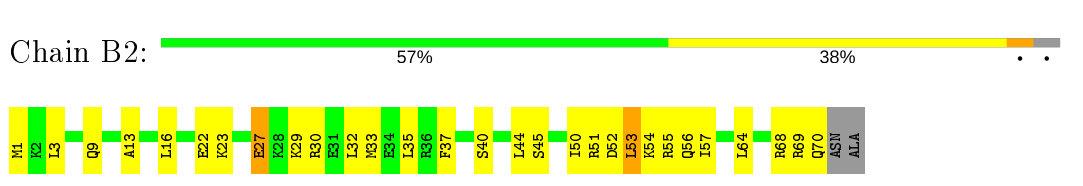
• Molecule 45: 50S Ribosomal Protein L28



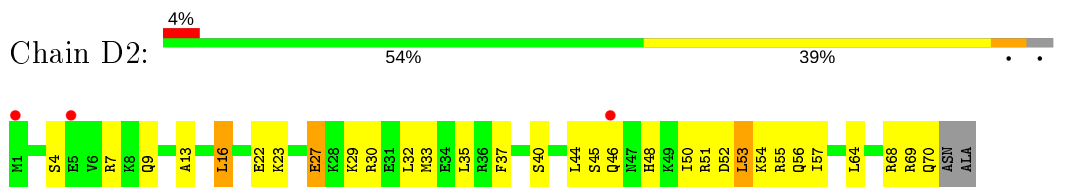
• Molecule 45: 50S Ribosomal Protein L28



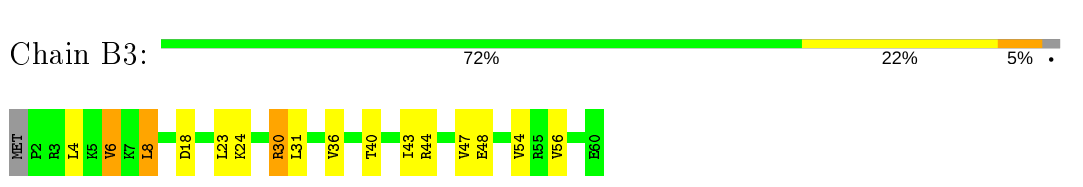
• Molecule 46: 50S Ribosomal Protein L29



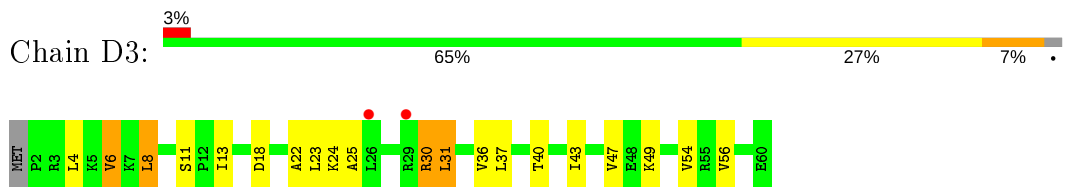
• Molecule 46: 50S Ribosomal Protein L29



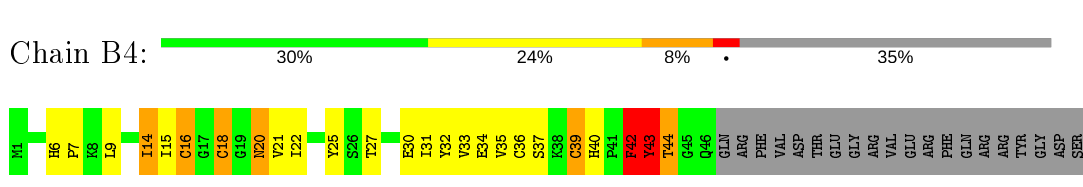
• Molecule 47: 50S Ribosomal Protein L30



• Molecule 47: 50S Ribosomal Protein L30



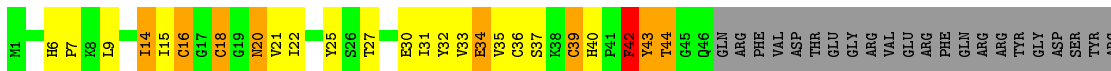
• Molecule 48: 50S Ribosomal Protein L31



LYS
GLY
ARG

- Molecule 48: 50S Ribosomal Protein L31

Chain D4: 30% 23% 11% 35%



LYS
GLY
ARG

- Molecule 49: 50S Ribosomal Protein L32

Chain B5: 70% 25%



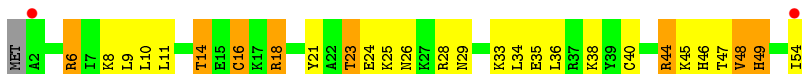
- Molecule 49: 50S Ribosomal Protein L32

Chain D5: 70% 23% 5%



- Molecule 50: 50S Ribosomal Protein L33

Chain B6: 4% 46% 37% 15%



- Molecule 50: 50S Ribosomal Protein L33

Chain D6: 9% 44% 37% 17%



- Molecule 51: 50S Ribosomal Protein L34

Chain B7: 4% 59% 31% 8%

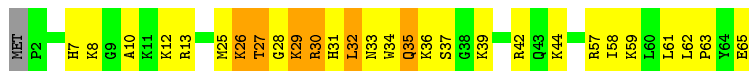


- Molecule 51: 50S Ribosomal Protein L34

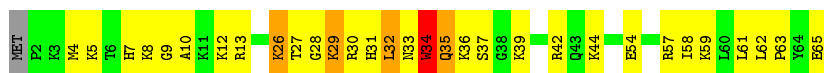
Chain D7: 59% 35%



- Molecule 52: 50S Ribosomal Protein L35



- Molecule 52: 50S Ribosomal Protein L35



- Molecule 53: 50S Ribosomal Protein L36



- Molecule 53: 50S Ribosomal Protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.24Å 451.44Å 621.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 3.00 49.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.75-3.00) 98.0 (49.75-3.00)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.218 , 0.254 0.217 , 0.253	Depositor DCC
R_{free} test set	57194 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtrriage
Anisotropy	0.254	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	283930	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.99	24/36215 (0.1%)	1.43	546/56522 (1.0%)
1	CA	0.91	21/36123 (0.1%)	1.38	452/56379 (0.8%)
2	AB	0.59	0/1809	0.73	1/2450 (0.0%)
2	CB	0.61	0/1809	0.73	1/2450 (0.0%)
3	AC	0.72	0/1474	0.82	2/2003 (0.1%)
3	CC	0.68	0/1474	0.79	2/2003 (0.1%)
4	AD	0.69	3/1556 (0.2%)	0.76	2/2113 (0.1%)
4	CD	0.64	2/1556 (0.1%)	0.74	2/2113 (0.1%)
5	AE	0.58	0/1121	0.79	0/1517
5	CE	0.58	0/1121	0.78	1/1517 (0.1%)
6	AF	0.55	0/790	0.71	0/1077
6	CF	0.54	0/790	0.70	0/1077
7	AG	0.83	0/1183	0.89	1/1599 (0.1%)
7	CG	0.72	0/1183	0.77	0/1599
8	AH	0.51	0/1065	0.67	0/1445
8	CH	0.50	0/1065	0.67	0/1445
9	AI	0.84	0/867	0.84	0/1180
9	CI	0.74	0/867	0.84	1/1180 (0.1%)
10	AJ	0.78	0/676	0.86	0/924
10	CJ	0.75	0/676	0.88	2/924 (0.2%)
11	AK	0.51	0/843	0.71	0/1144
11	CK	0.53	0/843	0.69	0/1144
12	AL	0.56	0/921	0.74	0/1247
12	CL	0.54	0/921	0.73	0/1247
13	AM	0.92	0/814	0.92	2/1107 (0.2%)
13	CM	0.72	0/814	0.83	0/1107
14	AN	0.79	0/487	0.93	0/649
14	CN	0.66	0/487	0.71	1/649 (0.2%)
15	AO	0.52	0/735	0.72	0/981
15	CO	0.52	0/735	0.72	0/981
16	AP	0.56	0/667	0.82	0/905
16	CP	0.54	0/667	0.84	1/905 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.56	0/836	0.72	0/1117
17	CQ	0.57	0/836	0.72	0/1117
18	AR	0.54	0/519	0.79	0/699
18	CR	0.56	0/519	0.79	0/699
19	AS	0.92	0/574	0.92	0/781
19	CS	0.69	0/574	0.81	0/781
20	AT	0.54	0/715	0.78	0/947
20	CT	0.52	0/715	0.77	0/947
21	AU	0.78	0/203	0.77	0/266
21	CU	0.73	0/203	0.68	0/266
22	AV	0.63	0/339	0.75	0/464
22	CV	0.65	0/360	0.85	1/492 (0.2%)
23	BA	1.60	727/67771 (1.1%)	1.72	2179/105789 (2.1%)
23	DA	1.16	149/67893 (0.2%)	1.60	1664/105982 (1.6%)
24	BB	1.11	3/2878 (0.1%)	1.57	62/4490 (1.4%)
24	DB	0.97	4/2878 (0.1%)	1.46	37/4490 (0.8%)
25	BD	0.88	3/2186 (0.1%)	0.96	0/2944
25	DD	0.80	2/2186 (0.1%)	0.91	1/2944 (0.0%)
26	BE	0.89	0/1588	0.96	3/2145 (0.1%)
26	DE	0.75	0/1588	0.92	0/2145
27	BF	0.88	1/1615 (0.1%)	0.86	0/2188
27	DF	0.70	0/1615	0.90	2/2188 (0.1%)
28	BG	0.53	0/1393	0.71	0/1892
28	DG	0.59	0/1393	0.71	0/1892
29	BH	0.68	0/1343	0.80	3/1820 (0.2%)
29	DH	0.60	0/1343	0.77	2/1820 (0.1%)
30	BI	0.64	0/1055	0.83	0/1445
30	DI	0.65	0/1053	0.84	1/1442 (0.1%)
31	BN	0.86	0/1139	0.87	2/1538 (0.1%)
31	DN	0.65	0/1139	0.87	1/1538 (0.1%)
32	BO	0.79	1/933 (0.1%)	0.86	1/1257 (0.1%)
32	DO	0.70	0/933	0.86	1/1257 (0.1%)
33	BP	0.80	0/1148	0.93	1/1529 (0.1%)
33	DP	0.67	0/1148	0.93	2/1529 (0.1%)
34	BQ	0.79	0/1143	0.89	0/1527
34	DQ	0.70	0/1143	0.86	0/1527
35	BR	0.82	0/982	0.94	2/1312 (0.2%)
35	DR	0.74	0/982	0.93	2/1312 (0.2%)
36	BS	0.65	0/875	0.88	0/1168
36	DS	0.66	0/875	0.84	0/1168
37	BT	0.74	0/1077	0.87	0/1444
37	DT	0.66	0/1077	0.85	0/1444
38	BU	1.02	0/977	0.89	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DU	0.79	0/977	0.88	0/1301
39	BV	0.89	0/771	0.84	0/1037
39	DV	0.70	0/782	0.84	1/1049 (0.1%)
40	BW	1.04	0/891	0.99	2/1197 (0.2%)
40	DW	0.87	0/891	0.91	0/1197
41	BX	0.87	0/756	0.88	1/1016 (0.1%)
41	DX	0.78	0/756	0.84	1/1016 (0.1%)
42	BY	0.81	0/798	0.88	0/1073
42	DY	0.72	1/798 (0.1%)	0.87	1/1073 (0.1%)
43	BZ	0.62	0/1555	0.82	1/2118 (0.0%)
43	DZ	0.63	0/1555	0.80	1/2118 (0.0%)
44	B0	0.83	0/602	0.86	0/804
44	D0	0.73	0/602	0.81	0/804
45	B1	0.80	0/752	1.00	3/1003 (0.3%)
45	D1	0.77	0/752	0.99	2/1003 (0.2%)
46	B2	0.81	0/590	0.82	0/781
46	D2	0.71	0/590	0.83	0/781
47	B3	0.79	0/463	0.86	1/623 (0.2%)
47	D3	0.64	0/463	0.82	0/623
48	B4	0.64	0/358	0.82	1/487 (0.2%)
48	D4	0.70	0/358	0.82	1/487 (0.2%)
49	B5	1.01	0/469	0.99	1/634 (0.2%)
49	D5	0.75	0/469	0.95	1/634 (0.2%)
50	B6	0.84	1/456 (0.2%)	0.86	0/609
50	D6	0.92	2/456 (0.4%)	0.89	2/609 (0.3%)
51	B7	1.07	0/426	1.16	2/561 (0.4%)
51	D7	0.92	0/426	1.00	0/561
52	B8	0.88	0/516	1.00	2/679 (0.3%)
52	D8	0.73	1/516 (0.2%)	0.92	1/679 (0.1%)
53	B9	0.85	0/300	0.91	0/395
53	D9	0.68	0/300	0.83	0/395
All	All	1.12	945/304490 (0.3%)	1.42	5009/455973 (1.1%)

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	3
2	CB	0	3
3	AC	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	CC	0	2
5	CE	0	1
7	AG	0	4
7	CG	0	1
9	AI	0	2
9	CI	0	1
10	AJ	0	3
12	AL	0	1
12	CL	0	1
13	AM	0	3
13	CM	0	1
14	AN	0	3
17	AQ	0	1
17	CQ	0	1
19	AS	0	1
20	AT	0	2
20	CT	0	1
22	CV	0	3
25	BD	0	1
25	DD	0	1
26	BE	0	2
26	DE	0	1
27	BF	0	2
27	DF	0	3
28	BG	0	1
28	DG	0	1
30	BI	0	1
30	DI	0	1
31	BN	0	1
31	DN	0	2
32	BO	0	1
32	DO	0	1
33	BP	0	4
33	DP	0	2
36	BS	0	2
36	DS	0	1
37	BT	0	1
37	DT	0	1
41	BX	0	1
41	DX	0	1
42	BY	0	1
42	DY	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
43	BZ	0	1
45	B1	0	1
45	D1	0	1
48	B4	0	3
48	D4	0	2
52	D8	0	2
All	All	0	83

The worst 5 of 945 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1459	C	N1-C2	17.17	1.57	1.40
1	AA	1459	C	N1-C2	16.97	1.57	1.40
1	AA	1442(A)	G	N9-C4	16.14	1.50	1.38
1	CA	1442(A)	G	N9-C4	15.91	1.50	1.38
23	DA	528	A	N9-C4	-14.88	1.28	1.37

The worst 5 of 5009 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1442(A)	G	N3-C4-C5	-27.29	114.95	128.60
1	CA	1459	C	N3-C2-O2	-27.00	103.00	121.90
1	AA	1442(A)	G	N3-C4-C5	-26.82	115.19	128.60
1	CA	1459	C	C6-N1-C2	-26.34	109.77	120.30
1	AA	1459	C	N3-C2-O2	-25.91	103.77	121.90

There are no chirality outliers.

5 of 83 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	128	GLU	Peptide
2	AB	14	GLY	Peptide
2	AB	71	VAL	Peptide
3	AC	186	PHE	Peptide
7	AG	19	GLY	Peptide

5.2 Too-close contacts [\(i\)](#)

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	32353	0	16329	1267	0
1	CA	32270	0	16287	987	1
2	AB	1775	0	1743	99	0
2	CB	1775	0	1743	93	0
3	AC	1450	0	1314	80	0
3	CC	1450	0	1314	99	0
4	AD	1526	0	1417	79	0
4	CD	1526	0	1415	91	0
5	AE	1105	0	1130	55	0
5	CE	1105	0	1130	60	0
6	AF	777	0	737	26	0
6	CF	777	0	737	24	0
7	AG	1164	0	1106	100	0
7	CG	1164	0	1106	54	0
8	AH	1045	0	1033	52	0
8	CH	1045	0	1033	52	0
9	AI	852	0	742	69	0
9	CI	852	0	742	62	0
10	AJ	663	0	558	56	0
10	CJ	663	0	558	30	0
11	AK	828	0	822	28	0
11	CK	828	0	822	31	0
12	AL	905	0	916	44	0
12	CL	905	0	916	44	0
13	AM	804	0	752	62	0
13	CM	804	0	752	48	0
14	AN	478	0	497	50	0
14	CN	478	0	497	35	0
15	AO	724	0	749	25	0
15	CO	724	0	749	29	0
16	AP	651	0	638	33	0
16	CP	651	0	638	35	0
17	AQ	823	0	891	16	0
17	CQ	823	0	891	18	0
18	AR	514	0	530	24	0
18	CR	514	0	530	24	0
19	AS	560	0	466	41	0
19	CS	560	0	466	23	0
20	AT	713	0	766	36	0
20	CT	713	0	766	30	0
21	AU	199	0	208	26	0
21	CU	199	0	208	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AV	333	0	235	14	0
22	CV	353	0	266	13	0
23	BA	60512	0	30492	877	0
23	DA	60620	0	30560	944	0
24	BB	2573	0	1304	45	0
24	DB	2573	0	1304	52	0
25	BD	2136	0	2218	67	0
25	DD	2136	0	2218	68	0
26	BE	1555	0	1607	39	0
26	DE	1555	0	1607	52	0
27	BF	1580	0	1621	51	0
27	DF	1580	0	1621	65	0
28	BG	1368	0	1324	51	0
28	DG	1368	0	1324	56	0
29	BH	1317	0	1376	30	0
29	DH	1317	0	1376	31	0
30	BI	1040	0	1045	55	1
30	DI	1038	0	1040	38	0
31	BN	1112	0	1180	37	0
31	DN	1112	0	1180	37	0
32	BO	923	0	981	24	0
32	DO	923	0	981	29	0
33	BP	1131	0	1201	38	0
33	DP	1131	0	1201	39	0
34	BQ	1122	0	1179	33	0
34	DQ	1122	0	1179	45	0
35	BR	968	0	1033	22	0
35	DR	968	0	1033	29	0
36	BS	865	0	905	46	0
36	DS	865	0	905	52	0
37	BT	1063	0	1103	41	0
37	DT	1063	0	1103	40	0
38	BU	959	0	1019	24	0
38	DU	959	0	1019	29	0
39	BV	760	0	816	20	0
39	DV	771	0	830	24	0
40	BW	881	0	935	17	0
40	DW	881	0	935	21	0
41	BX	742	0	799	17	0
41	DX	742	0	799	18	0
42	BY	785	0	828	31	0
42	DY	785	0	828	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BZ	1522	0	1511	49	0
43	DZ	1522	0	1511	52	0
44	B0	594	0	604	23	0
44	D0	594	0	604	31	0
45	B1	745	0	804	31	0
45	D1	745	0	804	31	0
46	B2	588	0	643	19	0
46	D2	588	0	643	24	0
47	B3	458	0	503	9	0
47	D3	458	0	503	13	0
48	B4	349	0	336	20	0
48	D4	349	0	336	20	0
49	B5	455	0	472	14	0
49	D5	455	0	472	17	0
50	B6	449	0	462	19	0
50	D6	449	0	462	18	0
51	B7	418	0	467	11	0
51	D7	418	0	467	15	0
52	B8	509	0	565	23	0
52	D8	509	0	565	28	0
53	B9	297	0	316	8	0
53	D9	297	0	316	10	0
54	AA	106	0	0	0	0
54	AD	1	0	0	0	0
54	B0	2	0	0	0	0
54	B1	1	0	0	0	0
54	B2	2	0	0	0	0
54	B3	2	0	0	0	0
54	B5	2	0	0	0	0
54	B8	3	0	0	0	0
54	B9	1	0	0	0	0
54	BA	618	0	0	0	0
54	BB	17	0	0	0	0
54	BD	3	0	0	0	0
54	BE	6	0	0	0	0
54	BF	2	0	0	0	0
54	BP	1	0	0	0	0
54	BQ	3	0	0	0	0
54	BR	2	0	0	0	0
54	BU	2	0	0	0	0
54	BV	1	0	0	0	0
54	BW	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	CA	69	0	0	0	0
54	D6	1	0	0	0	0
54	D7	1	0	0	0	0
54	D8	1	0	0	0	0
54	DA	430	0	0	0	0
54	DB	5	0	0	0	0
54	DD	1	0	0	0	0
54	DE	1	0	0	0	0
54	DF	2	0	0	0	0
54	DP	1	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	B4	1	0	0	0	0
55	B5	1	0	0	0	0
55	B6	1	0	0	0	0
55	B9	1	0	0	0	0
55	BY	1	0	0	0	0
55	CD	1	0	0	0	0
55	CN	1	0	0	0	0
55	D4	1	0	0	0	0
55	D5	1	0	0	0	0
55	D6	1	0	0	0	0
55	D9	1	0	0	0	0
55	DY	1	0	0	0	0
56	AA	145	0	0	23	0
56	AF	1	0	0	0	0
56	AK	1	0	0	0	0
56	AQ	1	0	0	0	0
56	B0	4	0	0	0	0
56	B3	1	0	0	0	0
56	B4	1	0	0	0	0
56	B5	3	0	0	1	0
56	B7	3	0	0	0	0
56	B8	7	0	0	0	0
56	B9	2	0	0	1	0
56	BA	1422	0	0	86	0
56	BB	31	0	0	1	0
56	BD	10	0	0	4	0
56	BE	8	0	0	0	0
56	BF	11	0	0	0	0
56	BH	2	0	0	0	0
56	BN	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BO	3	0	0	0	0
56	BP	6	0	0	0	0
56	BQ	2	0	0	0	0
56	BR	6	0	0	0	0
56	BT	1	0	0	0	0
56	BU	2	0	0	0	0
56	BV	2	0	0	0	0
56	BW	4	0	0	0	0
56	BX	2	0	0	0	0
56	BY	1	0	0	0	0
56	CA	119	0	0	13	0
56	CD	1	0	0	0	0
56	CK	2	0	0	0	0
56	CP	1	0	0	0	0
56	CT	2	0	0	0	0
56	D0	1	0	0	0	0
56	D1	2	0	0	0	0
56	DA	696	0	0	56	0
56	DB	9	0	0	0	0
56	DD	3	0	0	0	0
56	DE	2	0	0	0	0
56	DF	5	0	0	0	0
56	DP	5	0	0	0	0
56	DQ	2	0	0	0	0
56	DR	1	0	0	0	0
56	DV	1	0	0	0	0
56	DX	1	0	0	0	0
56	DY	1	0	0	0	0
All	All	283930	0	186520	7011	1

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

The worst 5 of 7011 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1303:C:N4	1:AA:1334:G:H1	1.41	1.17
23:BA:2296:U:O4	23:BA:2335:A:N6	1.76	1.15
23:DA:2296:U:O4	23:DA:2335:A:N6	1.79	1.15
1:AA:1003:G:H1	1:AA:1037:C:N4	1.46	1.14
1:AA:559:A:H4'	1:AA:560:U:H3'	1.35	1.07

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BI:91:SER:OG	1:CA:368:U:OP1[3_654]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	227/256 (89%)	188 (83%)	37 (16%)	2 (1%)	17	55
2	CB	227/256 (89%)	192 (85%)	33 (14%)	2 (1%)	17	55
3	AC	204/239 (85%)	179 (88%)	25 (12%)	0	100	100
3	CC	204/239 (85%)	177 (87%)	27 (13%)	0	100	100
4	AD	206/209 (99%)	179 (87%)	25 (12%)	2 (1%)	15	53
4	CD	206/209 (99%)	180 (87%)	24 (12%)	2 (1%)	15	53
5	AE	146/162 (90%)	125 (86%)	20 (14%)	1 (1%)	22	60
5	CE	146/162 (90%)	126 (86%)	20 (14%)	0	100	100
6	AF	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
6	CF	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
7	AG	153/156 (98%)	132 (86%)	19 (12%)	2 (1%)	12	45
7	CG	153/156 (98%)	128 (84%)	23 (15%)	2 (1%)	12	45
8	AH	136/138 (99%)	122 (90%)	14 (10%)	0	100	100
8	CH	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
9	AI	123/128 (96%)	106 (86%)	15 (12%)	2 (2%)	9	40
9	CI	123/128 (96%)	109 (89%)	12 (10%)	2 (2%)	9	40
10	AJ	94/105 (90%)	78 (83%)	14 (15%)	2 (2%)	7	33
10	CJ	94/105 (90%)	74 (79%)	18 (19%)	2 (2%)	7	33
11	AK	112/129 (87%)	100 (89%)	12 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	CK	112/129 (87%)	100 (89%)	12 (11%)	0	100	100
12	AL	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	19	57
12	CL	120/132 (91%)	107 (89%)	11 (9%)	2 (2%)	9	39
13	AM	112/126 (89%)	82 (73%)	27 (24%)	3 (3%)	5	26
13	CM	112/126 (89%)	84 (75%)	27 (24%)	1 (1%)	17	55
14	AN	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	12
14	CN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	9	39
15	AO	86/89 (97%)	71 (83%)	15 (17%)	0	100	100
15	CO	86/89 (97%)	72 (84%)	14 (16%)	0	100	100
16	AP	80/88 (91%)	69 (86%)	9 (11%)	2 (2%)	5	28
16	CP	80/88 (91%)	71 (89%)	7 (9%)	2 (2%)	5	28
17	AQ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
17	CQ	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
18	AR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
18	CR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
19	AS	79/93 (85%)	62 (78%)	16 (20%)	1 (1%)	12	45
19	CS	79/93 (85%)	60 (76%)	16 (20%)	3 (4%)	3	18
20	AT	95/106 (90%)	82 (86%)	10 (10%)	3 (3%)	4	22
20	CT	95/106 (90%)	81 (85%)	11 (12%)	3 (3%)	4	22
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
21	CU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
22	AV	51/61 (84%)	42 (82%)	9 (18%)	0	100	100
22	CV	51/61 (84%)	34 (67%)	14 (28%)	3 (6%)	1	9
25	BD	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	34	72
25	DD	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	34	72
26	BE	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	15	53
26	DE	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	15	53
27	BF	201/210 (96%)	187 (93%)	13 (6%)	1 (0%)	29	68
27	DF	201/210 (96%)	188 (94%)	12 (6%)	1 (0%)	29	68
28	BG	179/182 (98%)	151 (84%)	28 (16%)	0	100	100
28	DG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	25	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BH	172/180 (96%)	156 (91%)	14 (8%)	2 (1%)	13	48
29	DH	172/180 (96%)	158 (92%)	12 (7%)	2 (1%)	13	48
30	BI	144/148 (97%)	114 (79%)	27 (19%)	3 (2%)	7	33
30	DI	144/148 (97%)	113 (78%)	29 (20%)	2 (1%)	11	43
31	BN	138/140 (99%)	128 (93%)	6 (4%)	4 (3%)	4	24
31	DN	138/140 (99%)	126 (91%)	7 (5%)	5 (4%)	3	19
32	BO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
32	DO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
33	BP	147/150 (98%)	134 (91%)	12 (8%)	1 (1%)	22	60
33	DP	147/150 (98%)	134 (91%)	13 (9%)	0	100	100
34	BQ	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
34	DQ	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
35	BR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
35	DR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
36	BS	108/112 (96%)	96 (89%)	11 (10%)	1 (1%)	17	55
36	DS	108/112 (96%)	97 (90%)	10 (9%)	1 (1%)	17	55
37	BT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
37	DT	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
38	BU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
38	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
39	BV	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
39	DV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
40	BW	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
40	DW	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
41	BX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
41	DX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
42	BY	105/110 (96%)	94 (90%)	9 (9%)	2 (2%)	8	36
42	DY	105/110 (96%)	95 (90%)	8 (8%)	2 (2%)	8	36
43	BZ	196/206 (95%)	178 (91%)	15 (8%)	3 (2%)	10	42
43	DZ	196/206 (95%)	177 (90%)	16 (8%)	3 (2%)	10	42
44	B0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	D0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
45	B1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
45	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	50
46	B2	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
46	D2	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
47	B3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
47	D3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
48	B4	44/71 (62%)	37 (84%)	7 (16%)	0	100	100
48	D4	44/71 (62%)	38 (86%)	6 (14%)	0	100	100
49	B5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
49	D5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
50	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
50	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
51	B7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	6	31
51	D7	46/49 (94%)	45 (98%)	0	1 (2%)	6	31
52	B8	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	9	40
52	D8	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	4	22
53	B9	34/37 (92%)	34 (100%)	0	0	100	100
53	D9	34/37 (92%)	34 (100%)	0	0	100	100
All	All	11473/12250 (94%)	10289 (90%)	1089 (10%)	95 (1%)	19	57

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	AM	91	ARG
33	BP	27	HIS
12	CL	92	ASP
31	DN	23	LEU
31	DN	24	GLY

5.3.2 Protein sidechains [i](#)

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	177/220 (80%)	135 (76%)	42 (24%)	1	3
2	CB	177/220 (80%)	135 (76%)	42 (24%)	1	3
3	AC	114/188 (61%)	74 (65%)	40 (35%)	0	1
3	CC	114/188 (61%)	78 (68%)	36 (32%)	0	1
4	AD	141/181 (78%)	113 (80%)	28 (20%)	1	7
4	CD	141/181 (78%)	114 (81%)	27 (19%)	1	8
5	AE	108/123 (88%)	84 (78%)	24 (22%)	1	4
5	CE	108/123 (88%)	84 (78%)	24 (22%)	1	4
6	AF	76/90 (84%)	68 (90%)	8 (10%)	7	27
6	CF	76/90 (84%)	69 (91%)	7 (9%)	9	34
7	AG	103/127 (81%)	68 (66%)	35 (34%)	0	1
7	CG	103/127 (81%)	77 (75%)	26 (25%)	0	3
8	AH	103/119 (87%)	83 (81%)	20 (19%)	1	7
8	CH	103/119 (87%)	84 (82%)	19 (18%)	1	9
9	AI	62/99 (63%)	49 (79%)	13 (21%)	1	5
9	CI	62/99 (63%)	48 (77%)	14 (23%)	1	4
10	AJ	53/92 (58%)	41 (77%)	12 (23%)	1	4
10	CJ	53/92 (58%)	39 (74%)	14 (26%)	0	2
11	AK	81/99 (82%)	70 (86%)	11 (14%)	3	17
11	CK	81/99 (82%)	70 (86%)	11 (14%)	3	17
12	AL	91/109 (84%)	80 (88%)	11 (12%)	5	21
12	CL	91/109 (84%)	79 (87%)	12 (13%)	4	18
13	AM	64/101 (63%)	45 (70%)	19 (30%)	0	1
13	CM	64/101 (63%)	49 (77%)	15 (23%)	1	4
14	AN	46/50 (92%)	37 (80%)	9 (20%)	1	7
14	CN	46/50 (92%)	33 (72%)	13 (28%)	0	2
15	AO	77/80 (96%)	70 (91%)	7 (9%)	9	34
15	CO	77/80 (96%)	71 (92%)	6 (8%)	12	42
16	AP	63/74 (85%)	47 (75%)	16 (25%)	0	3
16	CP	63/74 (85%)	47 (75%)	16 (25%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AQ	94/97 (97%)	80 (85%)	14 (15%)	3	14
17	CQ	94/97 (97%)	80 (85%)	14 (15%)	3	14
18	AR	49/77 (64%)	43 (88%)	6 (12%)	5	21
18	CR	49/77 (64%)	42 (86%)	7 (14%)	3	15
19	AS	43/80 (54%)	24 (56%)	19 (44%)	0	0
19	CS	43/80 (54%)	32 (74%)	11 (26%)	0	3
20	AT	65/82 (79%)	56 (86%)	9 (14%)	3	17
20	CT	65/82 (79%)	55 (85%)	10 (15%)	2	13
21	AU	18/22 (82%)	11 (61%)	7 (39%)	0	0
21	CU	18/22 (82%)	13 (72%)	5 (28%)	0	2
22	AV	16/50 (32%)	13 (81%)	3 (19%)	1	8
22	CV	21/50 (42%)	14 (67%)	7 (33%)	0	1
25	BD	215/218 (99%)	181 (84%)	34 (16%)	2	12
25	DD	215/218 (99%)	180 (84%)	35 (16%)	2	11
26	BE	163/166 (98%)	138 (85%)	25 (15%)	2	13
26	DE	163/166 (98%)	135 (83%)	28 (17%)	2	10
27	BF	159/166 (96%)	133 (84%)	26 (16%)	2	11
27	DF	159/166 (96%)	133 (84%)	26 (16%)	2	11
28	BG	128/156 (82%)	106 (83%)	22 (17%)	2	10
28	DG	128/156 (82%)	106 (83%)	22 (17%)	2	10
29	BH	141/148 (95%)	127 (90%)	14 (10%)	8	30
29	DH	141/148 (95%)	127 (90%)	14 (10%)	8	30
30	BI	99/124 (80%)	75 (76%)	24 (24%)	0	3
30	DI	98/124 (79%)	67 (68%)	31 (32%)	0	1
31	BN	117/119 (98%)	92 (79%)	25 (21%)	1	5
31	DN	117/119 (98%)	93 (80%)	24 (20%)	1	6
32	BO	98/100 (98%)	90 (92%)	8 (8%)	11	39
32	DO	98/100 (98%)	90 (92%)	8 (8%)	11	39
33	BP	114/116 (98%)	98 (86%)	16 (14%)	3	16
33	DP	114/116 (98%)	100 (88%)	14 (12%)	4	21
34	BQ	111/111 (100%)	95 (86%)	16 (14%)	3	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DQ	111/111 (100%)	96 (86%)	15 (14%)	4	17
35	BR	101/101 (100%)	82 (81%)	19 (19%)	1	8
35	DR	101/101 (100%)	83 (82%)	18 (18%)	2	9
36	BS	84/88 (96%)	69 (82%)	15 (18%)	2	9
36	DS	84/88 (96%)	72 (86%)	12 (14%)	3	15
37	BT	110/127 (87%)	95 (86%)	15 (14%)	3	17
37	DT	110/127 (87%)	92 (84%)	18 (16%)	2	11
38	BU	93/94 (99%)	84 (90%)	9 (10%)	8	31
38	DU	93/94 (99%)	84 (90%)	9 (10%)	8	31
39	BV	79/82 (96%)	62 (78%)	17 (22%)	1	5
39	DV	80/82 (98%)	64 (80%)	16 (20%)	1	7
40	BW	89/92 (97%)	78 (88%)	11 (12%)	4	20
40	DW	89/92 (97%)	76 (85%)	13 (15%)	3	15
41	BX	75/78 (96%)	70 (93%)	5 (7%)	16	49
41	DX	75/78 (96%)	70 (93%)	5 (7%)	16	49
42	BY	80/91 (88%)	66 (82%)	14 (18%)	2	10
42	DY	80/91 (88%)	63 (79%)	17 (21%)	1	5
43	BZ	159/179 (89%)	141 (89%)	18 (11%)	6	24
43	DZ	159/179 (89%)	141 (89%)	18 (11%)	6	24
44	B0	59/67 (88%)	54 (92%)	5 (8%)	10	38
44	D0	59/67 (88%)	54 (92%)	5 (8%)	10	38
45	B1	78/83 (94%)	67 (86%)	11 (14%)	3	16
45	D1	78/83 (94%)	67 (86%)	11 (14%)	3	16
46	B2	65/67 (97%)	59 (91%)	6 (9%)	9	34
46	D2	65/67 (97%)	58 (89%)	7 (11%)	6	26
47	B3	49/52 (94%)	43 (88%)	6 (12%)	5	21
47	D3	49/52 (94%)	42 (86%)	7 (14%)	3	15
48	B4	39/63 (62%)	29 (74%)	10 (26%)	0	3
48	D4	39/63 (62%)	29 (74%)	10 (26%)	0	3
49	B5	50/52 (96%)	45 (90%)	5 (10%)	7	29
49	D5	50/52 (96%)	45 (90%)	5 (10%)	7	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B6	50/52 (96%)	39 (78%)	11 (22%)	1	4
50	D6	50/52 (96%)	37 (74%)	13 (26%)	0	2
51	B7	41/42 (98%)	32 (78%)	9 (22%)	1	4
51	D7	41/42 (98%)	34 (83%)	7 (17%)	2	10
52	B8	52/55 (94%)	43 (83%)	9 (17%)	2	10
52	D8	52/55 (94%)	43 (83%)	9 (17%)	2	10
53	B9	32/34 (94%)	29 (91%)	3 (9%)	8	32
53	D9	32/34 (94%)	29 (91%)	3 (9%)	8	32
All	All	8753/10166 (86%)	7236 (83%)	1517 (17%)	2	10

5 of 1517 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	B0	20	ARG
4	CD	97	LEU
41	DX	45	THR
46	B2	53	LEU
2	CB	58	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
9	CI	38	GLN
15	CO	37	ASN
42	DY	6	HIS
9	CI	73	GLN
10	CJ	33	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	425 (28%)	31 (2%)
1	CA	1499/1522 (98%)	383 (25%)	29 (1%)
23	BA	2802/2915 (96%)	556 (19%)	62 (2%)
23	DA	2808/2915 (96%)	552 (19%)	63 (2%)
24	BB	119/122 (97%)	21 (17%)	0
24	DB	119/122 (97%)	21 (17%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	8850/9118 (97%)	1958 (22%)	185 (2%)

5 of 1958 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	10	A
1	AA	22	G

5 of 185 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BA	2308	G
1	CA	484	G
23	DA	2126	A
23	BA	2439	A
1	CA	7	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1302 ligands modelled in this entry, 1302 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 i

6.1 Protein, DNA and RNA chains i

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	1505/1522 (98%)	1.08	302 (20%) 1 0	52, 116, 177, 188	0
1	CA	1501/1522 (98%)	0.62	211 (14%) 2 1	53, 112, 168, 181	0
2	AB	229/256 (89%)	0.32	17 (7%) 14 4	114, 135, 150, 160	0
2	CB	229/256 (89%)	0.60	26 (11%) 5 1	113, 135, 150, 160	0
3	AC	206/239 (86%)	1.85	83 (40%) 0 0	122, 148, 164, 172	0
3	CC	206/239 (86%)	1.47	64 (31%) 0 0	119, 140, 153, 162	0
4	AD	208/209 (99%)	0.40	23 (11%) 5 1	100, 116, 133, 143	0
4	CD	208/209 (99%)	0.19	14 (6%) 17 5	95, 111, 129, 142	0
5	AE	148/162 (91%)	0.43	18 (12%) 4 1	85, 109, 124, 129	0
5	CE	148/162 (91%)	0.42	12 (8%) 12 3	87, 108, 124, 132	0
6	AF	100/101 (99%)	-0.07	7 (7%) 16 5	88, 102, 122, 136	0
6	CF	100/101 (99%)	0.10	5 (5%) 28 10	93, 107, 123, 135	0
7	AG	155/156 (99%)	3.56	108 (69%) 0 0	134, 156, 166, 168	0
7	CG	155/156 (99%)	2.13	69 (44%) 0 0	118, 144, 151, 158	0
8	AH	138/138 (100%)	0.08	6 (4%) 35 13	93, 111, 121, 131	0
8	CH	138/138 (100%)	0.15	7 (5%) 28 10	89, 110, 120, 133	0
9	AI	125/128 (97%)	3.99	90 (72%) 0 0	131, 157, 170, 176	0
9	CI	125/128 (97%)	2.58	61 (48%) 0 0	129, 151, 161, 173	0
10	AJ	96/105 (91%)	3.61	58 (60%) 0 0	137, 155, 171, 176	0
10	CJ	96/105 (91%)	2.70	55 (57%) 0 0	130, 149, 161, 169	0
11	AK	114/129 (88%)	0.10	0 100 100	74, 109, 123, 127	0
11	CK	114/129 (88%)	0.38	9 (7%) 12 4	79, 109, 122, 124	0
12	AL	122/132 (92%)	0.17	6 (4%) 29 11	72, 95, 111, 120	0
12	CL	122/132 (92%)	0.28	7 (5%) 23 8	72, 92, 106, 116	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/126 (90%)	4.54	90 (78%) 0 0	147, 160, 171, 177	0
13	CM	114/126 (90%)	2.02	41 (35%) 0 0	124, 145, 155, 158	0
14	AN	60/61 (98%)	3.84	37 (61%) 0 0	134, 160, 169, 174	0
14	CN	60/61 (98%)	1.87	21 (35%) 0 0	136, 146, 152, 155	0
15	AO	88/89 (98%)	0.02	3 (3%) 45 19	78, 103, 120, 131	0
15	CO	88/89 (98%)	0.08	6 (6%) 17 5	79, 102, 122, 129	0
16	AP	82/88 (93%)	1.28	24 (29%) 0 0	98, 112, 132, 138	0
16	CP	82/88 (93%)	0.53	5 (6%) 21 7	89, 105, 123, 132	0
17	AQ	99/105 (94%)	0.37	6 (6%) 21 7	86, 99, 113, 118	0
17	CQ	99/105 (94%)	0.01	3 (3%) 50 22	84, 98, 113, 117	0
18	AR	68/88 (77%)	0.68	11 (16%) 1 0	93, 104, 138, 141	0
18	CR	68/88 (77%)	1.10	19 (27%) 0 0	95, 107, 138, 143	0
19	AS	81/93 (87%)	2.98	40 (49%) 0 0	131, 164, 174, 179	0
19	CS	81/93 (87%)	2.67	48 (59%) 0 0	125, 146, 153, 155	0
20	AT	97/106 (91%)	0.49	9 (9%) 8 3	90, 106, 127, 131	0
20	CT	97/106 (91%)	0.67	14 (14%) 2 1	84, 103, 125, 132	0
21	AU	23/27 (85%)	6.80	19 (82%) 0 0	147, 161, 169, 174	0
21	CU	23/27 (85%)	2.53	12 (52%) 0 0	130, 145, 153, 154	0
22	AV	53/61 (86%)	0.16	3 (5%) 23 8	93, 105, 121, 143	0
22	CV	53/61 (86%)	-0.40	1 (1%) 66 37	90, 115, 141, 151	0
23	BA	2809/2915 (96%)	0.04	85 (3%) 50 22	31, 50, 134, 186	0
23	DA	2814/2915 (96%)	-0.13	110 (3%) 39 15	34, 56, 138, 189	0
24	BB	120/122 (98%)	-0.36	0 100 100	46, 72, 94, 119	0
24	DB	120/122 (98%)	-0.24	0 100 100	63, 90, 111, 129	0
25	BD	275/276 (99%)	-0.32	1 (0%) 92 79	34, 52, 69, 117	0
25	DD	275/276 (99%)	-0.42	1 (0%) 92 79	36, 55, 72, 119	0
26	BE	204/206 (99%)	-0.19	0 100 100	32, 55, 78, 95	0
26	DE	204/206 (99%)	-0.32	0 100 100	35, 61, 84, 101	0
27	BF	203/210 (96%)	-0.28	2 (0%) 82 59	30, 60, 92, 136	0
27	DF	203/210 (96%)	-0.25	1 (0%) 91 75	34, 67, 96, 136	0
28	BG	181/182 (99%)	0.42	19 (10%) 6 2	80, 120, 143, 152	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	181/182 (99%)	1.15	42 (23%) 0 0	92, 126, 146, 156	0
29	BH	174/180 (96%)	-0.19	1 (0%) 89 72	58, 79, 97, 110	0
29	DH	174/180 (96%)	0.42	22 (12%) 3 1	70, 92, 107, 122	0
30	BI	146/148 (98%)	-0.14	1 (0%) 87 69	57, 90, 108, 120	0
30	DI	146/148 (98%)	0.48	14 (9%) 8 2	60, 108, 127, 131	0
31	BN	140/140 (100%)	-0.34	0 100 100	39, 55, 83, 98	0
31	DN	140/140 (100%)	-0.56	1 (0%) 87 69	45, 63, 89, 101	0
32	BO	122/122 (100%)	-0.26	0 100 100	43, 58, 79, 85	0
32	DO	122/122 (100%)	-0.44	0 100 100	46, 62, 82, 86	0
33	BP	149/150 (99%)	0.03	0 100 100	34, 63, 98, 109	0
33	DP	149/150 (99%)	-0.21	3 (2%) 65 36	38, 70, 102, 111	0
34	BQ	141/141 (100%)	-0.17	1 (0%) 87 69	43, 61, 77, 91	0
34	DQ	141/141 (100%)	-0.21	0 100 100	47, 67, 85, 94	0
35	BR	118/118 (100%)	-0.27	0 100 100	38, 50, 70, 78	0
35	DR	118/118 (100%)	-0.34	0 100 100	42, 55, 73, 82	0
36	BS	110/112 (98%)	0.06	0 100 100	58, 75, 93, 101	0
36	DS	110/112 (98%)	0.12	4 (3%) 42 17	64, 82, 99, 110	0
37	BT	131/146 (89%)	-0.27	0 100 100	51, 63, 98, 117	0
37	DT	131/146 (89%)	-0.39	1 (0%) 86 65	55, 67, 101, 118	0
38	BU	116/118 (98%)	-0.18	1 (0%) 84 63	35, 48, 69, 81	0
38	DU	116/118 (98%)	-0.14	2 (1%) 70 41	40, 56, 76, 86	0
39	BV	100/101 (99%)	-0.27	0 100 100	34, 62, 81, 91	0
39	DV	101/101 (100%)	-0.06	0 100 100	40, 72, 90, 98	0
40	BW	112/113 (99%)	-0.42	0 100 100	36, 43, 64, 102	0
40	DW	112/113 (99%)	-0.60	0 100 100	40, 48, 69, 95	0
41	BX	95/96 (98%)	-0.19	1 (1%) 80 56	41, 51, 74, 98	0
41	DX	95/96 (98%)	-0.46	0 100 100	47, 56, 80, 102	0
42	BY	107/110 (97%)	-0.23	2 (1%) 66 37	52, 64, 89, 107	0
42	DY	107/110 (97%)	0.13	7 (6%) 18 5	59, 72, 96, 116	0
43	BZ	198/206 (96%)	-0.17	0 100 100	65, 85, 111, 126	0
43	DZ	198/206 (96%)	0.20	14 (7%) 16 5	73, 92, 115, 132	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	B0	76/85 (89%)	-0.32	0 100 100	48, 55, 71, 87	0
44	D0	76/85 (89%)	0.25	4 (5%) 26 10	53, 61, 76, 90	0
45	B1	97/98 (98%)	-0.18	2 (2%) 63 34	37, 57, 89, 103	0
45	D1	97/98 (98%)	-0.24	1 (1%) 82 59	41, 61, 91, 108	0
46	B2	70/72 (97%)	-0.16	0 100 100	50, 66, 84, 103	0
46	D2	70/72 (97%)	0.05	3 (4%) 35 13	55, 71, 88, 112	0
47	B3	59/60 (98%)	-0.31	0 100 100	43, 57, 85, 101	0
47	D3	59/60 (98%)	0.22	2 (3%) 45 19	49, 64, 92, 112	0
48	B4	46/71 (64%)	-0.59	0 100 100	106, 141, 151, 154	0
48	D4	46/71 (64%)	0.02	0 100 100	113, 141, 152, 163	0
49	B5	59/60 (98%)	-0.37	0 100 100	33, 51, 68, 89	0
49	D5	59/60 (98%)	-0.40	0 100 100	37, 55, 73, 95	0
50	B6	53/54 (98%)	0.26	2 (3%) 40 16	53, 61, 75, 78	0
50	D6	53/54 (98%)	0.53	5 (9%) 8 3	56, 65, 79, 82	0
51	B7	48/49 (97%)	0.05	2 (4%) 36 14	32, 37, 61, 78	0
51	D7	48/49 (97%)	-0.13	0 100 100	36, 40, 64, 83	0
52	B8	64/65 (98%)	-0.10	0 100 100	42, 49, 58, 70	0
52	D8	64/65 (98%)	-0.43	0 100 100	46, 53, 62, 72	0
53	B9	36/37 (97%)	0.10	0 100 100	49, 59, 72, 83	0
53	D9	36/37 (97%)	0.59	3 (8%) 11 3	58, 68, 81, 91	0
All	All	20542/21368 (96%)	0.35	2030 (9%) 7 2	30, 80, 160, 189	0

The worst 5 of 2030 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AM	43	THR	23.7
14	AN	13	THR	22.9
9	CI	7	THR	17.6
10	AJ	72	VAL	17.0
21	AU	11	GLY	15.5

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

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

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
54	MG	BA	3145	1/1	0.26	0.48	78,78,78,78	0
55	ZN	AN	101	1/1	0.37	0.14	213,213,213,213	0
54	MG	BA	3280	1/1	0.39	0.43	89,89,89,89	0
54	MG	BA	3459	1/1	0.40	0.14	130,130,130,130	0
54	MG	BA	3183	1/1	0.46	0.29	76,76,76,76	0
54	MG	DA	3360	1/1	0.49	0.13	63,63,63,63	0
54	MG	AA	1665	1/1	0.54	0.52	86,86,86,86	0
54	MG	BA	3351	1/1	0.54	0.24	57,57,57,57	0
54	MG	AA	1604	1/1	0.55	0.31	81,81,81,81	0
54	MG	BA	3374	1/1	0.57	0.14	75,75,75,75	0
54	MG	BA	3159	1/1	0.57	0.22	66,66,66,66	0
54	MG	BA	3243	1/1	0.57	0.12	117,117,117,117	0
54	MG	BA	3314	1/1	0.58	0.16	71,71,71,71	0
54	MG	AA	1656	1/1	0.58	0.83	74,74,74,74	0
54	MG	AA	1609	1/1	0.59	0.32	91,91,91,91	0
54	MG	CA	1612	1/1	0.60	0.42	84,84,84,84	0
54	MG	BA	3608	1/1	0.60	0.12	87,87,87,87	0
54	MG	DA	3313	1/1	0.60	0.19	64,64,64,64	0
54	MG	DA	3047	1/1	0.61	0.44	65,65,65,65	0
54	MG	CA	1638	1/1	0.61	0.37	71,71,71,71	0
54	MG	CA	1619	1/1	0.61	0.45	69,69,69,69	0
54	MG	DA	3278	1/1	0.62	0.16	46,46,46,46	0
54	MG	DA	3346	1/1	0.65	0.10	89,89,89,89	0
54	MG	AA	1630	1/1	0.65	0.51	76,76,76,76	0
54	MG	BA	3205	1/1	0.65	0.41	61,61,61,61	0
54	MG	DA	3379	1/1	0.65	0.09	94,94,94,94	0
54	MG	BA	3499	1/1	0.65	0.23	107,107,107,107	0
54	MG	DA	3206	1/1	0.65	0.18	75,75,75,75	0
54	MG	CA	1668	1/1	0.65	0.22	105,105,105,105	0
55	ZN	CN	101	1/1	0.65	0.17	188,188,188,188	0
54	MG	DA	3143	1/1	0.66	0.55	62,62,62,62	0
55	ZN	B4	101	1/1	0.66	0.06	200,200,200,200	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	AA	1702	1/1	0.66	0.21	97,97,97,97	0
54	MG	DA	3098	1/1	0.66	0.29	62,62,62,62	0
54	MG	BB	207	1/1	0.67	0.60	69,69,69,69	0
54	MG	CA	1653	1/1	0.67	0.24	83,83,83,83	0
54	MG	BA	3195	1/1	0.67	0.30	84,84,84,84	0
54	MG	BA	3534	1/1	0.67	0.27	76,76,76,76	0
54	MG	AA	1675	1/1	0.67	0.40	73,73,73,73	0
54	MG	BA	3487	1/1	0.67	0.22	94,94,94,94	0
54	MG	DA	3001	1/1	0.68	0.21	62,62,62,62	0
54	MG	DA	3091	1/1	0.68	0.16	70,70,70,70	0
54	MG	BA	3593	1/1	0.68	0.10	70,70,70,70	0
54	MG	DA	3075	1/1	0.68	0.45	71,71,71,71	0
54	MG	BA	3257	1/1	0.69	0.40	64,64,64,64	0
54	MG	DA	3050	1/1	0.69	0.16	90,90,90,90	0
54	MG	DA	3400	1/1	0.69	0.33	95,95,95,95	0
54	MG	CA	1636	1/1	0.69	0.42	77,77,77,77	0
54	MG	AA	1628	1/1	0.69	0.28	84,84,84,84	0
54	MG	CA	1656	1/1	0.69	0.12	97,97,97,97	0
54	MG	AA	1697	1/1	0.69	0.16	75,75,75,75	0
54	MG	CA	1608	1/1	0.70	0.45	67,67,67,67	0
54	MG	BA	3572	1/1	0.70	0.13	49,49,49,49	0
54	MG	BA	3152	1/1	0.70	0.24	73,73,73,73	0
54	MG	BA	3217	1/1	0.71	0.40	51,51,51,51	0
54	MG	DA	3210	1/1	0.71	0.28	60,60,60,60	0
54	MG	DA	3388	1/1	0.71	0.12	72,72,72,72	0
54	MG	CA	1609	1/1	0.71	0.88	70,70,70,70	0
54	MG	DA	3102	1/1	0.71	0.47	79,79,79,79	0
54	MG	BA	3514	1/1	0.71	0.19	97,97,97,97	0
54	MG	CA	1631	1/1	0.71	0.99	88,88,88,88	0
54	MG	BA	3553	1/1	0.72	0.18	70,70,70,70	0
54	MG	AA	1616	1/1	0.72	0.44	79,79,79,79	0
54	MG	BA	3315	1/1	0.72	0.17	84,84,84,84	0
54	MG	BA	3458	1/1	0.72	0.19	45,45,45,45	0
54	MG	BA	3503	1/1	0.72	0.22	68,68,68,68	0
54	MG	DA	3393	1/1	0.73	0.11	81,81,81,81	0
54	MG	AA	1682	1/1	0.73	0.18	111,111,111,111	0
54	MG	AA	1652	1/1	0.73	0.66	82,82,82,82	0
54	MG	DA	3363	1/1	0.73	0.10	72,72,72,72	0
54	MG	BA	3363	1/1	0.73	0.26	74,74,74,74	0
54	MG	BA	3194	1/1	0.73	0.22	79,79,79,79	0
54	MG	AA	1687	1/1	0.73	0.14	70,70,70,70	0
54	MG	BB	215	1/1	0.73	0.18	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	AA	1661	1/1	0.73	0.81	77,77,77,77	0
54	MG	BA	3169	1/1	0.73	0.48	60,60,60,60	0
54	MG	DA	3103	1/1	0.74	0.30	71,71,71,71	0
54	MG	BA	3614	1/1	0.74	0.31	94,94,94,94	0
54	MG	AA	1678	1/1	0.74	0.45	75,75,75,75	0
54	MG	CA	1643	1/1	0.74	0.06	109,109,109,109	0
54	MG	DB	202	1/1	0.74	1.21	86,86,86,86	0
54	MG	DA	3190	1/1	0.74	0.34	57,57,57,57	0
54	MG	BA	3558	1/1	0.75	0.17	61,61,61,61	0
54	MG	CA	1624	1/1	0.75	0.42	82,82,82,82	0
54	MG	DA	3048	1/1	0.75	0.45	53,53,53,53	0
54	MG	DA	3089	1/1	0.75	0.39	82,82,82,82	0
54	MG	BA	3565	1/1	0.75	0.28	90,90,90,90	0
54	MG	DA	3310	1/1	0.76	0.29	56,56,56,56	0
54	MG	DA	3012	1/1	0.76	0.21	60,60,60,60	0
54	MG	AA	1620	1/1	0.76	0.93	77,77,77,77	0
54	MG	AA	1643	1/1	0.76	0.85	96,96,96,96	0
54	MG	AA	1627	1/1	0.76	0.50	70,70,70,70	0
54	MG	AA	1637	1/1	0.76	0.33	82,82,82,82	0
54	MG	BA	3220	1/1	0.76	0.24	79,79,79,79	0
54	MG	BA	3184	1/1	0.76	0.20	66,66,66,66	0
54	MG	AA	1699	1/1	0.76	0.17	69,69,69,69	0
54	MG	BA	3617	1/1	0.76	0.15	93,93,93,93	0
54	MG	BA	3034	1/1	0.77	0.29	46,46,46,46	0
54	MG	BA	3174	1/1	0.77	0.40	71,71,71,71	0
54	MG	AA	1663	1/1	0.77	0.43	70,70,70,70	0
54	MG	BA	3320	1/1	0.77	0.15	57,57,57,57	0
54	MG	BA	3469	1/1	0.77	0.24	77,77,77,77	0
54	MG	DA	3327	1/1	0.77	0.46	94,94,94,94	0
54	MG	BA	3618	1/1	0.77	0.19	85,85,85,85	0
54	MG	DA	3082	1/1	0.77	0.40	51,51,51,51	0
54	MG	BA	3076	1/1	0.77	0.13	70,70,70,70	0
54	MG	DA	3107	1/1	0.77	0.19	47,47,47,47	0
54	MG	BA	3270	1/1	0.77	0.32	74,74,74,74	0
54	MG	DA	3192	1/1	0.77	0.19	66,66,66,66	0
54	MG	AA	1622	1/1	0.77	0.73	67,67,67,67	0
54	MG	B0	101	1/1	0.77	0.16	75,75,75,75	0
54	MG	DA	3380	1/1	0.78	0.10	91,91,91,91	0
54	MG	BA	3340	1/1	0.78	0.21	65,65,65,65	0
54	MG	CA	1661	1/1	0.78	0.27	100,100,100,100	0
54	MG	DA	3033	1/1	0.78	0.29	68,68,68,68	0
54	MG	AA	1605	1/1	0.78	0.30	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3587	1/1	0.78	0.08	66,66,66,66	0
54	MG	BA	3386	1/1	0.78	0.13	77,77,77,77	0
54	MG	BA	3612	1/1	0.78	0.12	100,100,100,100	0
54	MG	BA	3509	1/1	0.78	0.22	85,85,85,85	0
54	MG	DA	3112	1/1	0.78	0.35	60,60,60,60	0
54	MG	BA	3251	1/1	0.78	0.34	63,63,63,63	0
54	MG	DA	3317	1/1	0.78	0.18	94,94,94,94	0
54	MG	DA	3037	1/1	0.78	0.45	49,49,49,49	0
54	MG	DA	3162	1/1	0.78	0.39	55,55,55,55	0
54	MG	BA	3529	1/1	0.78	0.29	86,86,86,86	0
54	MG	DA	3217	1/1	0.78	0.26	69,69,69,69	0
54	MG	BA	3216	1/1	0.79	0.23	52,52,52,52	0
54	MG	BA	3139	1/1	0.79	0.28	53,53,53,53	0
54	MG	DA	3155	1/1	0.79	0.28	57,57,57,57	0
54	MG	BA	3267	1/1	0.79	0.56	53,53,53,53	0
54	MG	AA	1655	1/1	0.79	0.19	90,90,90,90	0
54	MG	BA	3224	1/1	0.79	0.31	61,61,61,61	0
54	MG	DA	3109	1/1	0.79	0.26	70,70,70,70	0
54	MG	CA	1648	1/1	0.79	0.12	100,100,100,100	0
54	MG	AA	1691	1/1	0.79	0.10	58,58,58,58	0
54	MG	BA	3240	1/1	0.79	0.39	64,64,64,64	0
54	MG	DA	3077	1/1	0.79	0.21	66,66,66,66	0
54	MG	BA	3456	1/1	0.79	0.13	89,89,89,89	0
54	MG	BA	3594	1/1	0.79	0.15	70,70,70,70	0
54	MG	DP	201	1/1	0.79	0.78	58,58,58,58	0
54	MG	DA	3336	1/1	0.79	0.16	87,87,87,87	0
54	MG	AA	1638	1/1	0.79	0.23	78,78,78,78	0
54	MG	DA	3342	1/1	0.80	0.24	41,41,41,41	0
54	MG	BA	3118	1/1	0.80	0.87	57,57,57,57	0
54	MG	CA	1606	1/1	0.80	0.62	81,81,81,81	0
54	MG	BA	3545	1/1	0.80	0.18	79,79,79,79	0
54	MG	BA	3384	1/1	0.80	0.11	62,62,62,62	0
54	MG	BA	3274	1/1	0.80	0.14	81,81,81,81	0
54	MG	DA	3128	1/1	0.80	0.29	72,72,72,72	0
54	MG	AA	1608	1/1	0.80	0.16	90,90,90,90	0
54	MG	DA	3254	1/1	0.80	0.39	43,43,43,43	0
54	MG	AA	1667	1/1	0.80	0.28	63,63,63,63	0
54	MG	BA	3135	1/1	0.80	0.45	54,54,54,54	0
54	MG	BV	201	1/1	0.80	0.36	74,74,74,74	0
54	MG	BA	3613	1/1	0.80	0.12	109,109,109,109	0
54	MG	BA	3201	1/1	0.80	0.58	79,79,79,79	0
54	MG	DA	3299	1/1	0.80	0.14	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
54	MG	AA	1673	1/1	0.80	0.29	67,67,67,67	0
54	MG	BA	3207	1/1	0.80	0.16	59,59,59,59	0
54	MG	BA	3513	1/1	0.80	0.21	66,66,66,66	0
54	MG	BA	3196	1/1	0.80	0.79	80,80,80,80	0
54	MG	BA	3136	1/1	0.80	0.24	73,73,73,73	0
54	MG	BA	3079	1/1	0.80	0.26	68,68,68,68	0
54	MG	BA	3242	1/1	0.81	0.40	66,66,66,66	0
54	MG	DA	3200	1/1	0.81	0.19	67,67,67,67	0
54	MG	BA	3225	1/1	0.81	0.34	61,61,61,61	0
54	MG	AA	1641	1/1	0.81	0.66	93,93,93,93	0
54	MG	DA	3175	1/1	0.81	0.27	69,69,69,69	0
54	MG	BA	3093	1/1	0.81	0.18	81,81,81,81	0
54	MG	AA	1676	1/1	0.81	0.62	84,84,84,84	0
54	MG	BA	3375	1/1	0.81	0.33	46,46,46,46	0
54	MG	BU	201	1/1	0.81	0.40	51,51,51,51	0
54	MG	BA	3396	1/1	0.81	0.43	23,23,23,23	0
54	MG	CA	1660	1/1	0.81	0.15	106,106,106,106	0
54	MG	BA	3011	1/1	0.81	0.57	50,50,50,50	0
54	MG	DA	3189	1/1	0.81	0.80	66,66,66,66	0
54	MG	DA	3387	1/1	0.81	0.09	71,71,71,71	0
54	MG	DA	3141	1/1	0.81	0.52	74,74,74,74	0
54	MG	DA	3223	1/1	0.81	0.09	104,104,104,104	0
54	MG	BA	3496	1/1	0.81	0.10	79,79,79,79	0
54	MG	CA	1635	1/1	0.81	0.18	68,68,68,68	0
54	MG	DA	3130	1/1	0.81	0.24	59,59,59,59	0
54	MG	CA	1623	1/1	0.81	0.88	73,73,73,73	0
54	MG	BA	3241	1/1	0.81	0.74	62,62,62,62	0
54	MG	BA	3569	1/1	0.81	0.27	68,68,68,68	0
54	MG	DA	3126	1/1	0.81	0.12	80,80,80,80	0
54	MG	DA	3106	1/1	0.81	0.33	56,56,56,56	0
54	MG	DA	3062	1/1	0.81	0.22	65,65,65,65	0
54	MG	DA	3357	1/1	0.81	0.14	53,53,53,53	0
54	MG	DA	3252	1/1	0.81	0.36	41,41,41,41	0
54	MG	BA	3178	1/1	0.81	0.17	58,58,58,58	0
54	MG	AA	1696	1/1	0.81	0.18	74,74,74,74	0
54	MG	DA	3058	1/1	0.81	0.11	51,51,51,51	0
54	MG	AA	1625	1/1	0.82	0.24	102,102,102,102	0
54	MG	BA	3147	1/1	0.82	0.31	57,57,57,57	0
54	MG	DA	3291	1/1	0.82	0.32	43,43,43,43	0
54	MG	DA	3245	1/1	0.82	0.33	47,47,47,47	0
54	MG	BA	3567	1/1	0.82	0.09	62,62,62,62	0
54	MG	AA	1653	1/1	0.82	0.61	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	DA	3035	1/1	0.82	0.63	68,68,68,68	0
54	MG	DA	3069	1/1	0.82	0.48	61,61,61,61	0
54	MG	DA	3211	1/1	0.82	0.25	53,53,53,53	0
54	MG	BA	3562	1/1	0.82	0.32	43,43,43,43	0
54	MG	DA	3095	1/1	0.82	0.21	71,71,71,71	0
54	MG	BB	204	1/1	0.82	0.20	67,67,67,67	0
54	MG	DA	3410	1/1	0.82	0.19	72,72,72,72	0
54	MG	BA	3142	1/1	0.82	0.53	53,53,53,53	0
54	MG	BA	3237	1/1	0.82	0.40	56,56,56,56	0
54	MG	BA	3464	1/1	0.82	0.32	41,41,41,41	0
54	MG	DA	3123	1/1	0.82	0.20	56,56,56,56	0
54	MG	BA	3519	1/1	0.82	0.33	90,90,90,90	0
54	MG	DA	3172	1/1	0.82	0.27	50,50,50,50	0
54	MG	DA	3015	1/1	0.82	0.40	71,71,71,71	0
54	MG	DA	3023	1/1	0.82	0.49	61,61,61,61	0
54	MG	BA	3170	1/1	0.82	0.56	52,52,52,52	0
54	MG	AA	1700	1/1	0.82	0.35	114,114,114,114	0
54	MG	BA	3344	1/1	0.82	0.10	52,52,52,52	0
54	MG	DA	3256	1/1	0.82	0.58	59,59,59,59	0
54	MG	BA	3167	1/1	0.82	0.35	68,68,68,68	0
54	MG	DA	3084	1/1	0.82	0.30	62,62,62,62	0
54	MG	BA	3166	1/1	0.82	0.49	58,58,58,58	0
54	MG	AA	1683	1/1	0.82	0.28	139,139,139,139	0
54	MG	BA	3200	1/1	0.83	0.23	51,51,51,51	0
54	MG	DA	3326	1/1	0.83	0.10	95,95,95,95	0
54	MG	AA	1692	1/1	0.83	0.53	113,113,113,113	0
54	MG	BA	3339	1/1	0.83	0.09	91,91,91,91	0
54	MG	CA	1615	1/1	0.83	0.62	76,76,76,76	0
54	MG	BA	3055	1/1	0.83	0.32	58,58,58,58	0
54	MG	CA	1621	1/1	0.83	0.26	64,64,64,64	0
54	MG	DA	3297	1/1	0.83	0.22	66,66,66,66	0
55	ZN	D4	101	1/1	0.83	0.05	176,176,176,176	0
54	MG	BA	3063	1/1	0.83	0.20	84,84,84,84	0
54	MG	DA	3071	1/1	0.83	0.34	60,60,60,60	0
54	MG	BA	3009	1/1	0.83	0.23	59,59,59,59	0
54	MG	B2	101	1/1	0.83	0.26	75,75,75,75	0
54	MG	DA	3391	1/1	0.83	0.14	67,67,67,67	0
54	MG	BA	3039	1/1	0.83	0.30	44,44,44,44	0
54	MG	DA	3355	1/1	0.83	0.11	37,37,37,37	0
54	MG	CA	1605	1/1	0.83	0.32	74,74,74,74	0
54	MG	DA	3080	1/1	0.83	1.04	73,73,73,73	0
54	MG	BR	201	1/1	0.83	0.59	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
54	MG	DA	3390	1/1	0.83	0.17	69,69,69,69	0
54	MG	AA	1659	1/1	0.83	0.44	62,62,62,62	0
54	MG	BA	3581	1/1	0.83	0.14	47,47,47,47	0
54	MG	BA	3122	1/1	0.83	0.32	56,56,56,56	0
54	MG	BA	3297	1/1	0.83	0.17	35,35,35,35	0
54	MG	DA	3423	1/1	0.83	0.14	79,79,79,79	0
54	MG	BB	214	1/1	0.83	0.17	67,67,67,67	0
54	MG	BB	202	1/1	0.83	0.14	46,46,46,46	0
54	MG	DA	3121	1/1	0.84	0.65	53,53,53,53	0
54	MG	BB	209	1/1	0.84	0.17	79,79,79,79	0
54	MG	BA	3538	1/1	0.84	0.13	70,70,70,70	0
54	MG	BA	3517	1/1	0.84	0.26	51,51,51,51	0
54	MG	BB	213	1/1	0.84	0.21	69,69,69,69	0
54	MG	BA	3100	1/1	0.84	0.33	72,72,72,72	0
54	MG	BA	3392	1/1	0.84	0.11	55,55,55,55	0
54	MG	DA	3108	1/1	0.84	0.18	80,80,80,80	0
54	MG	AA	1606	1/1	0.84	0.89	74,74,74,74	0
54	MG	B1	101	1/1	0.84	0.28	50,50,50,50	0
54	MG	CA	1610	1/1	0.84	0.43	80,80,80,80	0
54	MG	BA	3535	1/1	0.84	0.25	70,70,70,70	0
54	MG	AA	1688	1/1	0.84	0.22	111,111,111,111	0
54	MG	DA	3129	1/1	0.84	0.35	78,78,78,78	0
54	MG	BA	3062	1/1	0.84	0.08	69,69,69,69	0
54	MG	DA	3040	1/1	0.84	0.31	50,50,50,50	0
54	MG	BA	3082	1/1	0.84	0.28	71,71,71,71	0
54	MG	DA	3127	1/1	0.84	0.29	63,63,63,63	0
54	MG	DA	3114	1/1	0.84	0.15	51,51,51,51	0
54	MG	BA	3023	1/1	0.84	0.12	52,52,52,52	0
54	MG	BA	3206	1/1	0.84	0.13	68,68,68,68	0
54	MG	CA	1669	1/1	0.84	0.10	117,117,117,117	0
54	MG	BA	3171	1/1	0.84	0.24	67,67,67,67	0
54	MG	BA	3365	1/1	0.84	0.10	84,84,84,84	0
54	MG	AA	1611	1/1	0.84	0.31	69,69,69,69	0
54	MG	BA	3559	1/1	0.84	0.27	39,39,39,39	0
55	ZN	DY	201	1/1	0.84	0.09	128,128,128,128	0
54	MG	AA	1679	1/1	0.84	0.35	64,64,64,64	0
54	MG	DA	3406	1/1	0.85	0.25	35,35,35,35	0
54	MG	BA	3536	1/1	0.85	0.09	82,82,82,82	0
54	MG	DA	3177	1/1	0.85	0.84	59,59,59,59	0
54	MG	DA	3008	1/1	0.85	0.22	48,48,48,48	0
54	MG	CA	1665	1/1	0.85	0.14	76,76,76,76	0
54	MG	BA	3031	1/1	0.85	0.38	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3362	1/1	0.85	0.11	63,63,63,63	0
54	MG	AA	1632	1/1	0.85	0.52	93,93,93,93	0
54	MG	B8	102	1/1	0.85	0.33	61,61,61,61	0
54	MG	DA	3026	1/1	0.85	0.15	49,49,49,49	0
54	MG	AA	1646	1/1	0.85	0.39	73,73,73,73	0
54	MG	CA	1634	1/1	0.85	0.35	101,101,101,101	0
54	MG	DA	3063	1/1	0.85	0.20	54,54,54,54	0
54	MG	DA	3030	1/1	0.85	0.17	52,52,52,52	0
54	MG	DA	3306	1/1	0.85	0.11	88,88,88,88	0
54	MG	AA	1694	1/1	0.85	0.19	110,110,110,110	0
54	MG	BA	3495	1/1	0.85	0.19	70,70,70,70	0
54	MG	DA	3133	1/1	0.85	0.40	78,78,78,78	0
54	MG	DA	3345	1/1	0.85	0.28	100,100,100,100	0
54	MG	DA	3221	1/1	0.85	0.47	69,69,69,69	0
54	MG	DA	3011	1/1	0.85	0.22	46,46,46,46	0
54	MG	DA	3311	1/1	0.85	0.07	65,65,65,65	0
54	MG	BA	3554	1/1	0.86	0.21	58,58,58,58	0
54	MG	DA	3376	1/1	0.86	0.13	43,43,43,43	0
54	MG	BA	3097	1/1	0.86	0.38	58,58,58,58	0
54	MG	DA	3214	1/1	0.86	0.76	74,74,74,74	0
54	MG	CA	1625	1/1	0.86	0.38	88,88,88,88	0
54	MG	BA	3334	1/1	0.86	0.16	43,43,43,43	0
54	MG	BA	3308	1/1	0.86	0.54	51,51,51,51	0
54	MG	DB	201	1/1	0.86	0.29	75,75,75,75	0
54	MG	DA	3421	1/1	0.86	0.09	69,69,69,69	0
54	MG	BA	3556	1/1	0.86	0.20	58,58,58,58	0
54	MG	BA	3068	1/1	0.86	0.18	70,70,70,70	0
54	MG	AA	1671	1/1	0.86	0.25	89,89,89,89	0
54	MG	BA	3002	1/1	0.86	0.19	98,98,98,98	0
54	MG	DA	3097	1/1	0.86	0.72	64,64,64,64	0
54	MG	DA	3424	1/1	0.86	0.15	130,130,130,130	0
54	MG	BA	3327	1/1	0.86	0.18	34,34,34,34	0
54	MG	BA	3329	1/1	0.86	0.16	45,45,45,45	0
54	MG	BA	3032	1/1	0.86	0.21	67,67,67,67	0
54	MG	BA	3500	1/1	0.86	0.21	33,33,33,33	0
54	MG	BA	3360	1/1	0.86	0.17	53,53,53,53	0
54	MG	DA	3181	1/1	0.86	0.67	51,51,51,51	0
54	MG	BA	3283	1/1	0.86	0.55	56,56,56,56	0
54	MG	BA	3584	1/1	0.86	0.15	68,68,68,68	0
54	MG	BA	3457	1/1	0.86	0.15	91,91,91,91	0
54	MG	DA	3081	1/1	0.86	0.23	52,52,52,52	0
54	MG	DA	3006	1/1	0.86	0.28	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	BB	208	1/1	0.86	0.32	70,70,70,70	0
54	MG	DA	3408	1/1	0.86	0.15	65,65,65,65	0
54	MG	DA	3043	1/1	0.86	0.18	63,63,63,63	0
54	MG	AA	1612	1/1	0.86	0.37	76,76,76,76	0
54	MG	DA	3417	1/1	0.86	0.26	81,81,81,81	0
54	MG	DA	3036	1/1	0.86	0.18	65,65,65,65	0
54	MG	BA	3590	1/1	0.86	0.16	82,82,82,82	0
54	MG	AA	1602	1/1	0.86	0.28	111,111,111,111	0
54	MG	DA	3329	1/1	0.86	0.12	47,47,47,47	0
54	MG	AA	1639	1/1	0.87	0.20	74,74,74,74	0
54	MG	BB	210	1/1	0.87	0.14	67,67,67,67	0
54	MG	BA	3176	1/1	0.87	0.50	69,69,69,69	0
54	MG	BA	3474	1/1	0.87	0.20	66,66,66,66	0
54	MG	BA	3264	1/1	0.87	0.61	38,38,38,38	0
54	MG	DA	3383	1/1	0.87	0.25	63,63,63,63	0
54	MG	AA	1623	1/1	0.87	0.48	74,74,74,74	0
54	MG	DA	3111	1/1	0.87	0.46	60,60,60,60	0
54	MG	DA	3298	1/1	0.87	0.14	71,71,71,71	0
54	MG	DA	3246	1/1	0.87	0.46	41,41,41,41	0
54	MG	CA	1667	1/1	0.87	0.14	64,64,64,64	0
54	MG	BA	3277	1/1	0.87	0.20	66,66,66,66	0
54	MG	BA	3191	1/1	0.87	0.14	45,45,45,45	0
54	MG	BA	3425	1/1	0.87	0.14	37,37,37,37	0
54	MG	DA	3161	1/1	0.87	0.47	55,55,55,55	0
54	MG	BA	3341	1/1	0.87	0.08	69,69,69,69	0
54	MG	CA	1613	1/1	0.87	1.04	71,71,71,71	0
54	MG	BA	3029	1/1	0.87	0.15	83,83,83,83	0
54	MG	DF	302	1/1	0.87	0.24	64,64,64,64	0
54	MG	BA	3024	1/1	0.87	0.29	48,48,48,48	0
54	MG	DA	3232	1/1	0.87	0.36	46,46,46,46	0
54	MG	BA	3013	1/1	0.87	0.60	103,103,103,103	0
54	MG	BA	3343	1/1	0.87	0.06	91,91,91,91	0
54	MG	CA	1629	1/1	0.87	0.23	72,72,72,72	0
54	MG	BA	3524	1/1	0.87	0.18	77,77,77,77	0
54	MG	BA	3439	1/1	0.87	0.17	53,53,53,53	0
54	MG	BA	3106	1/1	0.87	0.41	48,48,48,48	0
54	MG	BA	3422	1/1	0.87	0.23	27,27,27,27	0
54	MG	DA	3041	1/1	0.87	0.19	49,49,49,49	0
54	MG	BA	3107	1/1	0.87	0.13	49,49,49,49	0
54	MG	BA	3450	1/1	0.87	0.13	71,71,71,71	0
54	MG	DA	3104	1/1	0.88	0.11	57,57,57,57	0
54	MG	BA	3120	1/1	0.88	0.31	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	AA	1650	1/1	0.88	0.28	70,70,70,70	0
54	MG	BA	3116	1/1	0.88	0.37	56,56,56,56	0
54	MG	BA	3140	1/1	0.88	0.46	59,59,59,59	0
54	MG	DA	3049	1/1	0.88	0.30	58,58,58,58	0
54	MG	CA	1666	1/1	0.88	0.09	131,131,131,131	0
54	MG	BA	3486	1/1	0.88	0.10	48,48,48,48	0
54	MG	BA	3105	1/1	0.88	0.12	40,40,40,40	0
54	MG	DA	3024	1/1	0.88	0.41	49,49,49,49	0
54	MG	BA	3064	1/1	0.88	0.27	45,45,45,45	0
54	MG	DA	3396	1/1	0.88	0.24	37,37,37,37	0
54	MG	DA	3120	1/1	0.88	0.72	52,52,52,52	0
54	MG	BA	3157	1/1	0.88	0.15	46,46,46,46	0
54	MG	DA	3195	1/1	0.88	0.84	75,75,75,75	0
54	MG	DA	3316	1/1	0.88	0.13	75,75,75,75	0
54	MG	BA	3006	1/1	0.88	0.17	44,44,44,44	0
54	MG	BA	3371	1/1	0.88	0.10	67,67,67,67	0
54	MG	BA	3077	1/1	0.88	0.58	43,43,43,43	0
54	MG	DA	3056	1/1	0.88	0.44	61,61,61,61	0
54	MG	DA	3073	1/1	0.88	0.21	54,54,54,54	0
54	MG	DA	3066	1/1	0.88	0.18	56,56,56,56	0
54	MG	DA	3093	1/1	0.88	0.72	66,66,66,66	0
54	MG	CA	1627	1/1	0.88	0.14	79,79,79,79	0
54	MG	BA	3332	1/1	0.88	0.28	60,60,60,60	0
54	MG	BA	3244	1/1	0.88	0.45	45,45,45,45	0
54	MG	BE	301	1/1	0.88	0.53	43,43,43,43	0
54	MG	BA	3388	1/1	0.88	0.17	54,54,54,54	0
54	MG	DA	3014	1/1	0.88	0.10	52,52,52,52	0
54	MG	BA	3492	1/1	0.88	0.15	78,78,78,78	0
54	MG	BA	3269	1/1	0.88	0.26	54,54,54,54	0
54	MG	CA	1662	1/1	0.88	0.18	95,95,95,95	0
54	MG	BA	3066	1/1	0.88	0.11	43,43,43,43	0
54	MG	AA	1670	1/1	0.88	0.16	115,115,115,115	0
54	MG	BA	3030	1/1	0.88	0.25	37,37,37,37	0
54	MG	DA	3139	1/1	0.88	0.49	65,65,65,65	0
54	MG	DA	3182	1/1	0.88	0.28	59,59,59,59	0
54	MG	BA	3463	1/1	0.88	0.20	36,36,36,36	0
54	MG	BA	3420	1/1	0.88	0.28	41,41,41,41	0
54	MG	DA	3403	1/1	0.88	0.18	49,49,49,49	0
54	MG	DA	3197	1/1	0.88	0.65	66,66,66,66	0
54	MG	DA	3420	1/1	0.88	0.09	97,97,97,97	0
54	MG	BA	3330	1/1	0.88	0.28	36,36,36,36	0
54	MG	BA	3276	1/1	0.88	0.63	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	BA	3226	1/1	0.88	0.31	62,62,62,62	0
54	MG	BA	3325	1/1	0.89	0.11	47,47,47,47	0
54	MG	DA	3083	1/1	0.89	0.34	55,55,55,55	0
54	MG	BA	3180	1/1	0.89	0.25	51,51,51,51	0
54	MG	AA	1706	1/1	0.89	0.08	100,100,100,100	0
54	MG	BA	3415	1/1	0.89	0.12	49,49,49,49	0
54	MG	AA	1633	1/1	0.89	0.53	72,72,72,72	0
54	MG	BA	3022	1/1	0.89	0.09	57,57,57,57	0
54	MG	DA	3224	1/1	0.89	0.35	80,80,80,80	0
54	MG	BA	3160	1/1	0.89	0.38	46,46,46,46	0
54	MG	BA	3036	1/1	0.89	0.42	49,49,49,49	0
54	MG	BA	3153	1/1	0.89	0.32	53,53,53,53	0
54	MG	DA	3341	1/1	0.89	0.24	39,39,39,39	0
54	MG	CA	1640	1/1	0.89	0.28	62,62,62,62	0
54	MG	BA	3067	1/1	0.89	0.36	35,35,35,35	0
54	MG	DA	3239	1/1	0.89	0.29	39,39,39,39	0
54	MG	BA	3595	1/1	0.89	0.09	82,82,82,82	0
54	MG	BA	3158	1/1	0.89	0.35	51,51,51,51	0
54	MG	BA	3337	1/1	0.89	0.24	33,33,33,33	0
54	MG	BA	3273	1/1	0.89	0.22	66,66,66,66	0
54	MG	DA	3415	1/1	0.89	0.09	89,89,89,89	0
54	MG	D8	101	1/1	0.89	0.60	49,49,49,49	0
54	MG	BA	3014	1/1	0.89	0.19	57,57,57,57	0
54	MG	DA	3244	1/1	0.89	0.46	35,35,35,35	0
54	MG	DA	3053	1/1	0.89	0.36	54,54,54,54	0
54	MG	BA	3072	1/1	0.89	0.28	59,59,59,59	0
54	MG	B3	101	1/1	0.89	0.44	60,60,60,60	0
54	MG	DA	3044	1/1	0.89	0.22	51,51,51,51	0
54	MG	BA	3530	1/1	0.89	0.11	84,84,84,84	0
54	MG	BA	3114	1/1	0.89	0.25	43,43,43,43	0
54	MG	CA	1655	1/1	0.89	0.29	74,74,74,74	0
54	MG	BA	3436	1/1	0.89	0.32	38,38,38,38	0
54	MG	BA	3412	1/1	0.89	0.21	41,41,41,41	0
54	MG	DA	3205	1/1	0.89	0.07	82,82,82,82	0
54	MG	DA	3349	1/1	0.89	0.29	54,54,54,54	0
54	MG	B0	102	1/1	0.89	0.17	56,56,56,56	0
54	MG	BA	3249	1/1	0.89	0.30	70,70,70,70	0
54	MG	DA	3315	1/1	0.89	0.13	59,59,59,59	0
54	MG	BE	302	1/1	0.89	0.21	52,52,52,52	0
54	MG	BA	3475	1/1	0.89	0.23	53,53,53,53	0
54	MG	BA	3489	1/1	0.89	0.20	38,38,38,38	0
54	MG	BA	3414	1/1	0.89	0.28	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	DA	3381	1/1	0.89	0.09	79,79,79,79	0
54	MG	BA	3050	1/1	0.89	0.23	46,46,46,46	0
54	MG	BA	3549	1/1	0.89	0.12	68,68,68,68	0
54	MG	BA	3016	1/1	0.89	0.42	57,57,57,57	0
54	MG	BA	3173	1/1	0.89	0.28	65,65,65,65	0
54	MG	BA	3247	1/1	0.89	0.25	53,53,53,53	0
54	MG	BA	3037	1/1	0.89	0.22	52,52,52,52	0
54	MG	BA	3259	1/1	0.89	0.31	51,51,51,51	0
54	MG	BA	3532	1/1	0.89	0.09	35,35,35,35	0
54	MG	BA	3144	1/1	0.89	0.35	54,54,54,54	0
54	MG	BA	3335	1/1	0.89	0.15	55,55,55,55	0
54	MG	BA	3087	1/1	0.89	0.26	56,56,56,56	0
54	MG	BA	3121	1/1	0.89	0.15	38,38,38,38	0
54	MG	BA	3449	1/1	0.89	0.18	49,49,49,49	0
54	MG	BA	3130	1/1	0.89	0.38	32,32,32,32	0
54	MG	BA	3213	1/1	0.89	0.37	64,64,64,64	0
54	MG	CA	1649	1/1	0.89	0.15	92,92,92,92	0
54	MG	BA	3362	1/1	0.89	0.11	73,73,73,73	0
54	MG	DA	3125	1/1	0.89	0.43	66,66,66,66	0
54	MG	BA	3285	1/1	0.89	0.55	59,59,59,59	0
54	MG	BA	3161	1/1	0.89	0.34	54,54,54,54	0
54	MG	CA	1646	1/1	0.89	0.49	92,92,92,92	0
54	MG	BA	3465	1/1	0.89	0.20	38,38,38,38	0
54	MG	BA	3053	1/1	0.89	0.35	53,53,53,53	0
54	MG	BA	3001	1/1	0.89	0.42	56,56,56,56	0
54	MG	CA	1658	1/1	0.89	0.17	83,83,83,83	0
54	MG	AA	1651	1/1	0.89	0.86	69,69,69,69	0
54	MG	BA	3250	1/1	0.90	0.23	47,47,47,47	0
54	MG	DA	3187	1/1	0.90	0.66	47,47,47,47	0
54	MG	BA	3141	1/1	0.90	0.27	65,65,65,65	0
55	ZN	CD	301	1/1	0.90	0.32	96,96,96,96	0
54	MG	BA	3478	1/1	0.90	0.17	92,92,92,92	0
54	MG	BA	3533	1/1	0.90	0.20	48,48,48,48	0
54	MG	DA	3242	1/1	0.90	0.55	38,38,38,38	0
54	MG	BA	3197	1/1	0.90	0.32	62,62,62,62	0
54	MG	BA	3061	1/1	0.90	0.51	64,64,64,64	0
54	MG	DA	3227	1/1	0.90	0.39	65,65,65,65	0
54	MG	BA	3081	1/1	0.90	0.18	66,66,66,66	0
54	MG	BA	3527	1/1	0.90	0.15	51,51,51,51	0
54	MG	BA	3272	1/1	0.90	0.07	65,65,65,65	0
54	MG	BA	3074	1/1	0.90	0.38	55,55,55,55	0
54	MG	BA	3316	1/1	0.90	0.32	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	BA	3150	1/1	0.90	0.22	61,61,61,61	0
54	MG	AA	1677	1/1	0.90	0.90	81,81,81,81	0
54	MG	DA	3208	1/1	0.90	0.44	52,52,52,52	0
54	MG	BA	3522	1/1	0.90	0.57	68,68,68,68	0
54	MG	CA	1659	1/1	0.90	0.21	60,60,60,60	0
54	MG	BA	3356	1/1	0.90	0.28	59,59,59,59	0
54	MG	BA	3078	1/1	0.90	0.34	38,38,38,38	0
54	MG	DA	3064	1/1	0.90	0.18	53,53,53,53	0
54	MG	BA	3003	1/1	0.90	0.34	29,29,29,29	0
54	MG	DA	3034	1/1	0.90	0.28	74,74,74,74	0
54	MG	BA	3444	1/1	0.90	0.06	61,61,61,61	0
54	MG	BA	3102	1/1	0.90	0.26	59,59,59,59	0
54	MG	BA	3358	1/1	0.90	0.08	64,64,64,64	0
54	MG	BA	3254	1/1	0.90	0.20	67,67,67,67	0
54	MG	BA	3154	1/1	0.90	0.15	49,49,49,49	0
54	MG	DA	3186	1/1	0.90	0.24	42,42,42,42	0
54	MG	BA	3204	1/1	0.90	0.18	47,47,47,47	0
54	MG	BA	3004	1/1	0.90	0.22	41,41,41,41	0
54	MG	BA	3124	1/1	0.90	0.23	68,68,68,68	0
54	MG	BA	3448	1/1	0.90	0.26	33,33,33,33	0
54	MG	DA	3219	1/1	0.90	0.30	38,38,38,38	0
54	MG	DA	3411	1/1	0.90	0.15	90,90,90,90	0
54	MG	DA	3378	1/1	0.90	0.14	98,98,98,98	0
54	MG	BA	3073	1/1	0.90	0.11	67,67,67,67	0
54	MG	AA	1615	1/1	0.90	0.37	56,56,56,56	0
54	MG	DA	3213	1/1	0.90	0.13	64,64,64,64	0
54	MG	DA	3374	1/1	0.90	0.26	44,44,44,44	0
54	MG	BA	3511	1/1	0.90	0.16	33,33,33,33	0
54	MG	BD	301	1/1	0.90	0.20	41,41,41,41	0
54	MG	AA	1669	1/1	0.90	0.39	96,96,96,96	0
54	MG	DA	3199	1/1	0.90	0.06	74,74,74,74	0
54	MG	CA	1622	1/1	0.90	0.32	74,74,74,74	0
54	MG	BA	3138	1/1	0.90	0.20	54,54,54,54	0
54	MG	DA	3386	1/1	0.90	0.11	63,63,63,63	0
54	MG	BA	3616	1/1	0.90	0.08	82,82,82,82	0
54	MG	BA	3357	1/1	0.90	0.15	47,47,47,47	0
54	MG	AA	1654	1/1	0.90	0.07	87,87,87,87	0
54	MG	BA	3111	1/1	0.90	0.30	57,57,57,57	0
54	MG	CA	1641	1/1	0.90	0.19	74,74,74,74	0
54	MG	CA	1637	1/1	0.90	0.65	67,67,67,67	0
54	MG	DA	3057	1/1	0.90	0.14	67,67,67,67	0
54	MG	CA	1663	1/1	0.90	0.18	91,91,91,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	BA	3046	1/1	0.90	0.27	49,49,49,49	0
54	MG	BA	3155	1/1	0.90	0.36	64,64,64,64	0
54	MG	BA	3175	1/1	0.90	0.35	70,70,70,70	0
54	MG	DA	3134	1/1	0.90	0.22	64,64,64,64	0
54	MG	BA	3026	1/1	0.90	0.18	68,68,68,68	0
54	MG	BA	3546	1/1	0.90	0.09	57,57,57,57	0
54	MG	BA	3187	1/1	0.91	0.27	30,30,30,30	0
54	MG	AA	1601	1/1	0.91	0.29	68,68,68,68	0
54	MG	BA	3338	1/1	0.91	0.15	30,30,30,30	0
54	MG	BA	3101	1/1	0.91	0.28	51,51,51,51	0
54	MG	BA	3041	1/1	0.91	0.12	56,56,56,56	0
54	MG	DA	3138	1/1	0.91	0.74	60,60,60,60	0
54	MG	DA	3262	1/1	0.91	0.16	46,46,46,46	0
54	MG	BA	3051	1/1	0.91	0.15	52,52,52,52	0
54	MG	DA	3296	1/1	0.91	0.12	50,50,50,50	0
54	MG	BA	3181	1/1	0.91	0.21	48,48,48,48	0
54	MG	BA	3347	1/1	0.91	0.22	55,55,55,55	0
54	MG	B5	101	1/1	0.91	0.28	51,51,51,51	0
54	MG	BA	3369	1/1	0.91	0.32	74,74,74,74	0
54	MG	BA	3232	1/1	0.91	0.14	54,54,54,54	0
54	MG	BE	304	1/1	0.91	0.17	32,32,32,32	0
54	MG	BA	3137	1/1	0.91	0.17	38,38,38,38	0
54	MG	BA	3098	1/1	0.91	0.40	54,54,54,54	0
54	MG	D7	101	1/1	0.91	0.30	52,52,52,52	0
54	MG	BA	3148	1/1	0.91	0.28	54,54,54,54	0
54	MG	DA	3259	1/1	0.91	0.58	64,64,64,64	0
54	MG	AA	1703	1/1	0.91	0.20	89,89,89,89	0
54	MG	BP	201	1/1	0.91	0.28	43,43,43,43	0
54	MG	BA	3289	1/1	0.91	0.67	50,50,50,50	0
54	MG	BA	3186	1/1	0.91	0.39	64,64,64,64	0
54	MG	DA	3261	1/1	0.91	0.41	56,56,56,56	0
54	MG	BA	3040	1/1	0.91	0.23	33,33,33,33	0
54	MG	DA	3174	1/1	0.91	0.46	60,60,60,60	0
54	MG	DA	3079	1/1	0.91	0.20	60,60,60,60	0
54	MG	BF	301	1/1	0.91	0.38	56,56,56,56	0
54	MG	BA	3480	1/1	0.91	0.13	70,70,70,70	0
54	MG	DA	3198	1/1	0.91	0.17	55,55,55,55	0
54	MG	BA	3219	1/1	0.91	0.33	62,62,62,62	0
54	MG	BA	3295	1/1	0.91	0.11	44,44,44,44	0
54	MG	DA	3339	1/1	0.91	0.11	48,48,48,48	0
54	MG	BA	3501	1/1	0.91	0.11	61,61,61,61	0
54	MG	CA	1611	1/1	0.91	0.18	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3142	1/1	0.91	0.24	46,46,46,46	0
54	MG	CA	1657	1/1	0.91	0.23	86,86,86,86	0
54	MG	AA	1634	1/1	0.91	0.75	95,95,95,95	0
54	MG	BA	3070	1/1	0.91	0.17	61,61,61,61	0
54	MG	CA	1664	1/1	0.91	0.15	94,94,94,94	0
54	MG	AA	1631	1/1	0.91	0.42	64,64,64,64	0
54	MG	DA	3328	1/1	0.91	0.09	34,34,34,34	0
54	MG	AA	1618	1/1	0.91	0.12	69,69,69,69	0
54	MG	DA	3260	1/1	0.91	0.50	44,44,44,44	0
54	MG	DA	3293	1/1	0.91	0.29	50,50,50,50	0
54	MG	BA	3361	1/1	0.91	0.20	53,53,53,53	0
54	MG	DA	3060	1/1	0.91	0.21	60,60,60,60	0
54	MG	BA	3555	1/1	0.91	0.31	49,49,49,49	0
54	MG	AA	1695	1/1	0.91	0.12	93,93,93,93	0
54	MG	DA	3158	1/1	0.91	0.41	72,72,72,72	0
54	MG	BA	3498	1/1	0.91	0.14	69,69,69,69	0
54	MG	DA	3409	1/1	0.91	0.06	79,79,79,79	0
54	MG	BA	3239	1/1	0.91	0.27	38,38,38,38	0
54	MG	BA	3592	1/1	0.91	0.08	51,51,51,51	0
54	MG	AA	1624	1/1	0.91	0.88	66,66,66,66	0
54	MG	AA	1666	1/1	0.91	0.53	62,62,62,62	0
54	MG	DA	3216	1/1	0.91	0.19	53,53,53,53	0
54	MG	BA	3091	1/1	0.91	0.34	47,47,47,47	0
54	MG	DA	3203	1/1	0.91	0.75	48,48,48,48	0
54	MG	DA	3231	1/1	0.91	0.48	54,54,54,54	0
54	MG	BA	3103	1/1	0.91	0.46	67,67,67,67	0
54	MG	AA	1698	1/1	0.91	0.44	68,68,68,68	0
54	MG	DA	3314	1/1	0.91	0.23	54,54,54,54	0
54	MG	AA	1603	1/1	0.91	0.11	68,68,68,68	0
54	MG	DA	3401	1/1	0.91	0.07	85,85,85,85	0
54	MG	DA	3367	1/1	0.91	0.14	68,68,68,68	0
54	MG	AA	1613	1/1	0.91	0.25	74,74,74,74	0
54	MG	AA	1686	1/1	0.91	0.19	115,115,115,115	0
54	MG	BA	3095	1/1	0.91	0.37	45,45,45,45	0
54	MG	BA	3185	1/1	0.91	0.23	44,44,44,44	0
54	MG	DA	3269	1/1	0.91	0.14	54,54,54,54	0
54	MG	BA	3435	1/1	0.92	0.28	36,36,36,36	0
54	MG	BA	3279	1/1	0.92	0.17	54,54,54,54	0
54	MG	BA	3542	1/1	0.92	0.23	60,60,60,60	0
54	MG	BA	3467	1/1	0.92	0.13	73,73,73,73	0
54	MG	BA	3231	1/1	0.92	0.41	45,45,45,45	0
54	MG	DA	3017	1/1	0.92	0.29	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
54	MG	CA	1607	1/1	0.92	0.24	72,72,72,72	0
54	MG	AA	1619	1/1	0.92	0.34	68,68,68,68	0
54	MG	DA	3215	1/1	0.92	0.23	58,58,58,58	0
54	MG	DA	3382	1/1	0.92	0.10	53,53,53,53	0
54	MG	DA	3295	1/1	0.92	0.17	42,42,42,42	0
54	MG	BU	202	1/1	0.92	0.53	62,62,62,62	0
54	MG	BA	3089	1/1	0.92	0.40	46,46,46,46	0
54	MG	DA	3180	1/1	0.92	0.24	78,78,78,78	0
54	MG	BA	3505	1/1	0.92	0.07	76,76,76,76	0
54	MG	BA	3069	1/1	0.92	0.52	53,53,53,53	0
54	MG	BA	3044	1/1	0.92	0.16	49,49,49,49	0
54	MG	DA	3146	1/1	0.92	0.44	35,35,35,35	0
54	MG	DA	3105	1/1	0.92	0.55	33,33,33,33	0
54	MG	DA	3240	1/1	0.92	0.21	67,67,67,67	0
54	MG	DA	3301	1/1	0.92	0.17	55,55,55,55	0
54	MG	DA	3369	1/1	0.92	0.17	57,57,57,57	0
54	MG	DA	3257	1/1	0.92	0.61	59,59,59,59	0
54	MG	DA	3324	1/1	0.92	0.20	64,64,64,64	0
54	MG	DA	3070	1/1	0.92	0.32	53,53,53,53	0
54	MG	CA	1626	1/1	0.92	0.27	86,86,86,86	0
54	MG	BA	3015	1/1	0.92	0.37	42,42,42,42	0
54	MG	DA	3018	1/1	0.92	0.17	42,42,42,42	0
54	MG	BA	3018	1/1	0.92	0.11	72,72,72,72	0
54	MG	BA	3402	1/1	0.92	0.08	47,47,47,47	0
54	MG	BA	3052	1/1	0.92	0.26	61,61,61,61	0
54	MG	BA	3271	1/1	0.92	0.15	60,60,60,60	0
54	MG	DA	3286	1/1	0.92	0.16	50,50,50,50	0
54	MG	AD	302	1/1	0.92	0.17	120,120,120,120	0
54	MG	DA	3019	1/1	0.92	0.20	41,41,41,41	0
54	MG	BA	3085	1/1	0.92	0.31	63,63,63,63	0
54	MG	BA	3092	1/1	0.92	0.42	55,55,55,55	0
54	MG	DA	3312	1/1	0.92	0.09	67,67,67,67	0
54	MG	DA	3046	1/1	0.92	0.70	43,43,43,43	0
54	MG	CA	1630	1/1	0.92	0.47	72,72,72,72	0
54	MG	DA	3002	1/1	0.92	0.69	67,67,67,67	0
54	MG	BA	3407	1/1	0.92	0.22	35,35,35,35	0
54	MG	DA	3397	1/1	0.92	0.05	65,65,65,65	0
54	MG	DA	3135	1/1	0.92	0.26	44,44,44,44	0
54	MG	BA	3071	1/1	0.92	0.20	49,49,49,49	0
54	MG	BQ	202	1/1	0.92	0.36	53,53,53,53	0
54	MG	B8	101	1/1	0.92	0.40	64,64,64,64	0
54	MG	DA	3003	1/1	0.92	0.36	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	CA	1645	1/1	0.92	0.29	63,63,63,63	0
54	MG	AA	1680	1/1	0.92	0.17	83,83,83,83	0
54	MG	BA	3298	1/1	0.92	0.11	53,53,53,53	0
54	MG	BA	3399	1/1	0.92	0.23	41,41,41,41	0
54	MG	CA	1616	1/1	0.92	0.41	72,72,72,72	0
54	MG	BA	3318	1/1	0.92	0.23	73,73,73,73	0
54	MG	DA	3258	1/1	0.92	0.10	56,56,56,56	0
54	MG	BA	3127	1/1	0.92	0.23	51,51,51,51	0
54	MG	DA	3207	1/1	0.92	0.42	53,53,53,53	0
54	MG	BA	3027	1/1	0.92	0.15	56,56,56,56	0
54	MG	BA	3571	1/1	0.92	0.14	76,76,76,76	0
54	MG	DA	3119	1/1	0.92	0.61	57,57,57,57	0
54	MG	BA	3151	1/1	0.92	0.21	62,62,62,62	0
54	MG	DA	3330	1/1	0.92	0.25	44,44,44,44	0
54	MG	DA	3347	1/1	0.92	0.07	76,76,76,76	0
54	MG	DA	3065	1/1	0.92	0.19	58,58,58,58	0
54	MG	DA	3157	1/1	0.92	0.32	69,69,69,69	0
54	MG	AA	1681	1/1	0.92	0.12	65,65,65,65	0
54	MG	DA	3375	1/1	0.92	0.14	50,50,50,50	0
54	MG	DA	3358	1/1	0.92	0.15	68,68,68,68	0
54	MG	DA	3148	1/1	0.92	0.41	70,70,70,70	0
54	MG	DA	3072	1/1	0.92	0.36	50,50,50,50	0
54	MG	DA	3042	1/1	0.92	0.58	46,46,46,46	0
54	MG	BA	3389	1/1	0.92	0.20	33,33,33,33	0
54	MG	AA	1657	1/1	0.92	0.53	81,81,81,81	0
54	MG	B2	102	1/1	0.92	0.26	60,60,60,60	0
54	MG	BA	3525	1/1	0.92	0.07	112,112,112,112	0
54	MG	DA	3173	1/1	0.92	0.40	49,49,49,49	0
54	MG	DA	3209	1/1	0.92	0.24	79,79,79,79	0
54	MG	AA	1660	1/1	0.92	0.96	91,91,91,91	0
54	MG	BA	3589	1/1	0.92	0.06	70,70,70,70	0
54	MG	D6	102	1/1	0.92	0.50	64,64,64,64	0
54	MG	BA	3086	1/1	0.92	0.26	57,57,57,57	0
54	MG	BA	3286	1/1	0.92	0.24	52,52,52,52	0
54	MG	DA	3229	1/1	0.92	0.37	55,55,55,55	0
54	MG	BA	3521	1/1	0.92	0.19	41,41,41,41	0
54	MG	DA	3159	1/1	0.92	0.61	59,59,59,59	0
54	MG	DA	3028	1/1	0.92	0.20	53,53,53,53	0
54	MG	CA	1650	1/1	0.92	0.21	100,100,100,100	0
54	MG	BA	3615	1/1	0.93	0.06	91,91,91,91	0
54	MG	BA	3090	1/1	0.93	0.15	45,45,45,45	0
54	MG	BA	3045	1/1	0.93	0.21	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	DA	3226	1/1	0.93	0.22	53,53,53,53	0
54	MG	BB	212	1/1	0.93	0.06	68,68,68,68	0
54	MG	AA	1607	1/1	0.93	0.40	69,69,69,69	0
54	MG	DA	3101	1/1	0.93	0.19	62,62,62,62	0
54	MG	DA	3292	1/1	0.93	0.18	39,39,39,39	0
54	MG	BA	3165	1/1	0.93	0.13	56,56,56,56	0
54	MG	BQ	201	1/1	0.93	0.20	49,49,49,49	0
54	MG	DA	3359	1/1	0.93	0.37	49,49,49,49	0
54	MG	AA	1649	1/1	0.93	0.20	66,66,66,66	0
54	MG	DA	3371	1/1	0.93	0.19	50,50,50,50	0
54	MG	BA	3188	1/1	0.93	0.27	43,43,43,43	0
54	MG	DA	3318	1/1	0.93	0.07	66,66,66,66	0
54	MG	BA	3208	1/1	0.93	0.29	54,54,54,54	0
54	MG	BA	3294	1/1	0.93	0.20	37,37,37,37	0
54	MG	BA	3218	1/1	0.93	0.38	54,54,54,54	0
55	ZN	AD	301	1/1	0.93	0.24	107,107,107,107	0
54	MG	DA	3354	1/1	0.93	0.27	41,41,41,41	0
54	MG	BA	3520	1/1	0.93	0.23	67,67,67,67	0
54	MG	AA	1690	1/1	0.93	0.12	59,59,59,59	0
54	MG	BA	3096	1/1	0.93	0.52	63,63,63,63	0
54	MG	DA	3007	1/1	0.93	0.18	36,36,36,36	0
54	MG	BA	3445	1/1	0.93	0.09	56,56,56,56	0
54	MG	BA	3227	1/1	0.93	0.19	42,42,42,42	0
54	MG	DA	3099	1/1	0.93	0.26	40,40,40,40	0
54	MG	AA	1693	1/1	0.93	0.10	78,78,78,78	0
54	MG	AA	1701	1/1	0.93	0.13	96,96,96,96	0
54	MG	DA	3061	1/1	0.93	0.38	52,52,52,52	0
54	MG	DA	3096	1/1	0.93	0.42	46,46,46,46	0
54	MG	BA	3418	1/1	0.93	0.09	54,54,54,54	0
54	MG	DA	3021	1/1	0.93	0.25	53,53,53,53	0
54	MG	DA	3364	1/1	0.93	0.12	67,67,67,67	0
54	MG	DA	3059	1/1	0.93	0.26	55,55,55,55	0
54	MG	DB	203	1/1	0.93	0.48	61,61,61,61	0
54	MG	BA	3537	1/1	0.93	0.17	38,38,38,38	0
54	MG	DA	3027	1/1	0.93	0.42	51,51,51,51	0
54	MG	AA	1704	1/1	0.93	0.11	90,90,90,90	0
54	MG	DA	3113	1/1	0.93	0.37	42,42,42,42	0
54	MG	AA	1674	1/1	0.93	0.20	73,73,73,73	0
54	MG	BA	3588	1/1	0.93	0.26	86,86,86,86	0
54	MG	DA	3152	1/1	0.93	0.46	58,58,58,58	0
54	MG	BW	201	1/1	0.93	0.17	51,51,51,51	0
54	MG	AA	1621	1/1	0.93	0.98	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	DA	3201	1/1	0.93	0.36	69,69,69,69	0
54	MG	DA	3348	1/1	0.93	0.11	85,85,85,85	0
54	MG	BA	3428	1/1	0.93	0.24	35,35,35,35	0
54	MG	BF	302	1/1	0.93	0.21	62,62,62,62	0
54	MG	BA	3193	1/1	0.93	0.19	50,50,50,50	0
54	MG	AA	1629	1/1	0.93	0.15	63,63,63,63	0
54	MG	DA	3140	1/1	0.93	0.53	70,70,70,70	0
54	MG	BA	3526	1/1	0.93	0.30	28,28,28,28	0
54	MG	BE	306	1/1	0.93	0.09	56,56,56,56	0
54	MG	BA	3132	1/1	0.93	0.31	31,31,31,31	0
54	MG	BA	3611	1/1	0.93	0.07	70,70,70,70	0
54	MG	DA	3085	1/1	0.93	0.45	51,51,51,51	0
54	MG	DA	3412	1/1	0.93	0.16	45,45,45,45	0
54	MG	BA	3377	1/1	0.93	0.12	69,69,69,69	0
54	MG	BA	3397	1/1	0.93	0.18	31,31,31,31	0
54	MG	CA	1617	1/1	0.93	0.89	70,70,70,70	0
54	MG	AA	1664	1/1	0.93	0.15	85,85,85,85	0
54	MG	BA	3172	1/1	0.93	0.23	71,71,71,71	0
54	MG	BA	3350	1/1	0.93	0.18	60,60,60,60	0
54	MG	BA	3146	1/1	0.93	0.51	52,52,52,52	0
54	MG	DA	3384	1/1	0.93	0.21	57,57,57,57	0
54	MG	BA	3577	1/1	0.93	0.23	58,58,58,58	0
54	MG	BA	3300	1/1	0.93	0.15	37,37,37,37	0
54	MG	BA	3017	1/1	0.93	0.14	47,47,47,47	0
54	MG	BA	3481	1/1	0.93	0.10	76,76,76,76	0
54	MG	DA	3193	1/1	0.93	0.32	63,63,63,63	0
54	MG	CA	1618	1/1	0.93	0.37	75,75,75,75	0
54	MG	BB	206	1/1	0.93	0.15	62,62,62,62	0
54	MG	DA	3334	1/1	0.93	0.16	56,56,56,56	0
54	MG	DA	3250	1/1	0.93	0.43	41,41,41,41	0
54	MG	BA	3266	1/1	0.93	0.77	48,48,48,48	0
54	MG	DA	3294	1/1	0.93	0.16	52,52,52,52	0
54	MG	BA	3468	1/1	0.93	0.15	38,38,38,38	0
54	MG	BA	3088	1/1	0.93	0.35	46,46,46,46	0
54	MG	DA	3194	1/1	0.93	0.54	77,77,77,77	0
54	MG	BA	3479	1/1	0.93	0.17	35,35,35,35	0
54	MG	AA	1617	1/1	0.93	0.11	82,82,82,82	0
54	MG	BA	3531	1/1	0.93	0.15	49,49,49,49	0
54	MG	BA	3209	1/1	0.93	0.37	67,67,67,67	0
54	MG	DA	3078	1/1	0.93	0.45	53,53,53,53	0
54	MG	BA	3210	1/1	0.93	0.25	57,57,57,57	0
54	MG	BA	3117	1/1	0.93	0.26	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3446	1/1	0.94	0.10	40,40,40,40	0
54	MG	AA	1648	1/1	0.94	0.20	62,62,62,62	0
54	MG	BA	3198	1/1	0.94	0.25	29,29,29,29	0
54	MG	CA	1639	1/1	0.94	0.64	61,61,61,61	0
54	MG	BA	3491	1/1	0.94	0.14	65,65,65,65	0
54	MG	BA	3189	1/1	0.94	0.28	46,46,46,46	0
54	MG	DA	3045	1/1	0.94	0.34	72,72,72,72	0
54	MG	DA	3343	1/1	0.94	0.17	35,35,35,35	0
54	MG	DA	3225	1/1	0.94	0.26	64,64,64,64	0
54	MG	BA	3447	1/1	0.94	0.28	37,37,37,37	0
54	MG	DA	3335	1/1	0.94	0.24	72,72,72,72	0
54	MG	DA	3372	1/1	0.94	0.33	40,40,40,40	0
54	MG	BA	3359	1/1	0.94	0.13	49,49,49,49	0
54	MG	BA	3065	1/1	0.94	0.13	47,47,47,47	0
54	MG	BA	3547	1/1	0.94	0.24	31,31,31,31	0
54	MG	BR	202	1/1	0.94	0.38	49,49,49,49	0
54	MG	BA	3282	1/1	0.94	0.28	43,43,43,43	0
54	MG	BA	3007	1/1	0.94	0.21	36,36,36,36	0
54	MG	BA	3214	1/1	0.94	0.56	34,34,34,34	0
54	MG	BA	3306	1/1	0.94	0.16	51,51,51,51	0
54	MG	DA	3248	1/1	0.94	0.56	44,44,44,44	0
54	MG	BA	3028	1/1	0.94	0.24	46,46,46,46	0
54	MG	DA	3090	1/1	0.94	0.24	53,53,53,53	0
54	MG	AA	1642	1/1	0.94	0.15	64,64,64,64	0
54	MG	CA	1603	1/1	0.94	0.28	73,73,73,73	0
54	MG	DA	3222	1/1	0.94	0.26	47,47,47,47	0
54	MG	DA	3303	1/1	0.94	0.19	37,37,37,37	0
54	MG	BA	3203	1/1	0.94	0.32	69,69,69,69	0
54	MG	BA	3510	1/1	0.94	0.17	33,33,33,33	0
54	MG	BB	203	1/1	0.94	0.20	80,80,80,80	0
54	MG	CA	1628	1/1	0.94	0.27	55,55,55,55	0
54	MG	BA	3563	1/1	0.94	0.11	67,67,67,67	0
54	MG	BA	3328	1/1	0.94	0.20	27,27,27,27	0
54	MG	DA	3052	1/1	0.94	0.29	71,71,71,71	0
54	MG	DA	3368	1/1	0.94	0.17	78,78,78,78	0
54	MG	BA	3049	1/1	0.94	0.19	54,54,54,54	0
54	MG	DA	3086	1/1	0.94	0.63	54,54,54,54	0
54	MG	BA	3255	1/1	0.94	0.58	65,65,65,65	0
54	MG	AA	1636	1/1	0.94	0.17	86,86,86,86	0
54	MG	DA	3428	1/1	0.94	0.12	81,81,81,81	0
54	MG	DA	3425	1/1	0.94	0.07	60,60,60,60	0
54	MG	AA	1644	1/1	0.94	0.34	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3543	1/1	0.94	0.19	59,59,59,59	0
54	MG	DA	3151	1/1	0.94	0.37	58,58,58,58	0
54	MG	BA	3460	1/1	0.94	0.09	58,58,58,58	0
54	MG	BA	3515	1/1	0.94	0.12	46,46,46,46	0
54	MG	DA	3167	1/1	0.94	0.10	59,59,59,59	0
54	MG	DE	301	1/1	0.94	0.51	37,37,37,37	0
54	MG	AA	1640	1/1	0.94	0.51	80,80,80,80	0
54	MG	BA	3108	1/1	0.94	0.26	56,56,56,56	0
54	MG	BA	3059	1/1	0.94	0.31	49,49,49,49	0
54	MG	BA	3301	1/1	0.94	0.05	62,62,62,62	0
54	MG	BA	3233	1/1	0.94	0.13	59,59,59,59	0
54	MG	BA	3453	1/1	0.94	0.17	74,74,74,74	0
54	MG	DA	3179	1/1	0.94	0.27	62,62,62,62	0
54	MG	DA	3337	1/1	0.94	0.10	42,42,42,42	0
54	MG	BA	3404	1/1	0.94	0.11	46,46,46,46	0
54	MG	BA	3382	1/1	0.94	0.08	58,58,58,58	0
54	MG	BA	3405	1/1	0.94	0.19	38,38,38,38	0
54	MG	DA	3183	1/1	0.94	0.12	50,50,50,50	0
54	MG	BA	3275	1/1	0.94	0.19	41,41,41,41	0
54	MG	BA	3113	1/1	0.94	0.40	35,35,35,35	0
54	MG	DA	3399	1/1	0.94	0.41	60,60,60,60	0
54	MG	BA	3265	1/1	0.94	0.39	30,30,30,30	0
54	MG	BA	3400	1/1	0.94	0.19	34,34,34,34	0
54	MG	BA	3342	1/1	0.94	0.08	57,57,57,57	0
54	MG	BA	3235	1/1	0.94	0.12	45,45,45,45	0
54	MG	DA	3405	1/1	0.94	0.17	70,70,70,70	0
54	MG	DA	3165	1/1	0.94	0.17	58,58,58,58	0
54	MG	BA	3125	1/1	0.94	0.23	50,50,50,50	0
54	MG	BA	3156	1/1	0.94	0.15	57,57,57,57	0
54	MG	BA	3260	1/1	0.94	0.61	50,50,50,50	0
54	MG	DA	3353	1/1	0.94	0.20	40,40,40,40	0
54	MG	B3	102	1/1	0.94	0.27	54,54,54,54	0
54	MG	DA	3087	1/1	0.94	0.32	58,58,58,58	0
54	MG	BA	3054	1/1	0.94	0.15	52,52,52,52	0
54	MG	DA	3407	1/1	0.94	0.25	59,59,59,59	0
54	MG	DA	3168	1/1	0.94	0.29	42,42,42,42	0
54	MG	BA	3302	1/1	0.94	0.28	45,45,45,45	0
54	MG	BA	3128	1/1	0.94	0.20	53,53,53,53	0
54	MG	BA	3494	1/1	0.94	0.47	44,44,44,44	0
54	MG	BA	3580	1/1	0.94	0.07	61,61,61,61	0
54	MG	DA	3051	1/1	0.94	0.15	43,43,43,43	0
54	MG	BA	3143	1/1	0.94	0.39	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
54	MG	BA	3012	1/1	0.94	0.21	34,34,34,34	0
54	MG	DA	3184	1/1	0.94	0.44	39,39,39,39	0
54	MG	BA	3119	1/1	0.94	0.22	39,39,39,39	0
54	MG	BA	3109	1/1	0.94	0.25	57,57,57,57	0
54	MG	DA	3302	1/1	0.94	0.26	36,36,36,36	0
54	MG	DA	3282	1/1	0.94	0.08	42,42,42,42	0
54	MG	AA	1658	1/1	0.94	0.16	60,60,60,60	0
54	MG	DA	3029	1/1	0.94	0.15	72,72,72,72	0
54	MG	DA	3237	1/1	0.94	0.51	39,39,39,39	0
54	MG	BA	3355	1/1	0.94	0.16	54,54,54,54	0
54	MG	DA	3370	1/1	0.94	0.19	51,51,51,51	0
54	MG	BA	3019	1/1	0.94	0.10	39,39,39,39	0
54	MG	DA	3013	1/1	0.94	0.15	41,41,41,41	0
54	MG	BA	3585	1/1	0.94	0.24	54,54,54,54	0
54	MG	CA	1602	1/1	0.94	0.57	82,82,82,82	0
54	MG	DA	3212	1/1	0.94	0.25	38,38,38,38	0
54	MG	DA	3005	1/1	0.94	0.19	64,64,64,64	0
54	MG	DA	3271	1/1	0.94	0.10	57,57,57,57	0
54	MG	BA	3561	1/1	0.94	0.27	49,49,49,49	0
54	MG	BA	3410	1/1	0.94	0.20	34,34,34,34	0
54	MG	BA	3099	1/1	0.94	0.28	52,52,52,52	0
54	MG	BA	3586	1/1	0.94	0.09	58,58,58,58	0
54	MG	BA	3043	1/1	0.94	0.34	54,54,54,54	0
54	MG	AA	1662	1/1	0.94	0.21	83,83,83,83	0
54	MG	BA	3497	1/1	0.94	0.17	55,55,55,55	0
54	MG	DA	3176	1/1	0.94	0.32	61,61,61,61	0
54	MG	BA	3094	1/1	0.94	0.17	41,41,41,41	0
54	MG	DA	3009	1/1	0.94	0.26	54,54,54,54	0
54	MG	DA	3394	1/1	0.94	0.33	56,56,56,56	0
54	MG	BA	3394	1/1	0.94	0.10	29,29,29,29	0
54	MG	BA	3333	1/1	0.94	0.30	36,36,36,36	0
54	MG	BA	3433	1/1	0.94	0.14	35,35,35,35	0
54	MG	DA	3188	1/1	0.95	0.23	54,54,54,54	0
54	MG	DA	3340	1/1	0.95	0.38	44,44,44,44	0
54	MG	BA	3376	1/1	0.95	0.11	55,55,55,55	0
54	MG	BA	3345	1/1	0.95	0.16	45,45,45,45	0
54	MG	BA	3042	1/1	0.95	0.50	47,47,47,47	0
54	MG	AA	1685	1/1	0.95	0.11	77,77,77,77	0
54	MG	DA	3389	1/1	0.95	0.14	58,58,58,58	0
54	MG	BA	3311	1/1	0.95	0.27	60,60,60,60	0
54	MG	DA	3429	1/1	0.95	0.16	44,44,44,44	0
54	MG	BA	3434	1/1	0.95	0.38	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
54	MG	BA	3222	1/1	0.95	0.19	51,51,51,51	0
54	MG	DA	3228	1/1	0.95	0.54	51,51,51,51	0
54	MG	BA	3452	1/1	0.95	0.12	62,62,62,62	0
54	MG	BA	3134	1/1	0.95	0.45	44,44,44,44	0
54	MG	DA	3266	1/1	0.95	0.09	58,58,58,58	0
54	MG	BB	201	1/1	0.95	0.21	61,61,61,61	0
54	MG	DA	3284	1/1	0.95	0.17	61,61,61,61	0
54	MG	CA	1604	1/1	0.95	0.19	110,110,110,110	0
54	MG	DA	3416	1/1	0.95	0.13	32,32,32,32	0
54	MG	DA	3230	1/1	0.95	0.17	67,67,67,67	0
54	MG	BA	3566	1/1	0.95	0.21	40,40,40,40	0
54	MG	DA	3038	1/1	0.95	0.33	39,39,39,39	0
54	MG	BA	3606	1/1	0.95	0.11	29,29,29,29	0
54	MG	DA	3147	1/1	0.95	0.68	78,78,78,78	0
54	MG	BA	3508	1/1	0.95	0.11	40,40,40,40	0
54	MG	BA	3319	1/1	0.95	0.05	68,68,68,68	0
54	MG	BA	3387	1/1	0.95	0.26	33,33,33,33	0
54	MG	BA	3211	1/1	0.95	0.19	53,53,53,53	0
54	MG	DA	3016	1/1	0.95	0.10	41,41,41,41	0
54	MG	BA	3413	1/1	0.95	0.28	31,31,31,31	0
54	MG	DA	3249	1/1	0.95	0.36	67,67,67,67	0
54	MG	BA	3322	1/1	0.95	0.13	45,45,45,45	0
54	MG	BA	3416	1/1	0.95	0.17	46,46,46,46	0
54	MG	BA	3401	1/1	0.95	0.17	45,45,45,45	0
54	MG	BA	3129	1/1	0.95	0.40	49,49,49,49	0
54	MG	CA	1651	1/1	0.95	0.18	61,61,61,61	0
54	MG	BA	3437	1/1	0.95	0.21	28,28,28,28	0
54	MG	BA	3551	1/1	0.95	0.26	40,40,40,40	0
54	MG	DA	3321	1/1	0.95	0.21	53,53,53,53	0
54	MG	CA	1632	1/1	0.95	0.29	65,65,65,65	0
54	MG	DA	3238	1/1	0.95	0.61	52,52,52,52	0
54	MG	BA	3304	1/1	0.95	0.17	27,27,27,27	0
54	MG	AA	1672	1/1	0.95	0.66	82,82,82,82	0
54	MG	BA	3493	1/1	0.95	0.19	52,52,52,52	0
54	MG	DA	3395	1/1	0.95	0.26	37,37,37,37	0
54	MG	BA	3133	1/1	0.95	0.30	31,31,31,31	0
54	MG	BA	3263	1/1	0.95	0.62	41,41,41,41	0
54	MG	DA	3290	1/1	0.95	0.24	42,42,42,42	0
54	MG	DA	3422	1/1	0.95	0.10	75,75,75,75	0
54	MG	AA	1645	1/1	0.95	0.86	77,77,77,77	0
54	MG	BA	3598	1/1	0.95	0.13	39,39,39,39	0
54	MG	BA	3149	1/1	0.95	0.14	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
54	MG	B9	102	1/1	0.95	0.31	45,45,45,45	0
54	MG	BA	3182	1/1	0.95	0.09	69,69,69,69	0
54	MG	DA	3350	1/1	0.95	0.14	50,50,50,50	0
54	MG	BA	3199	1/1	0.95	0.23	31,31,31,31	0
54	MG	BA	3429	1/1	0.95	0.17	29,29,29,29	0
54	MG	DA	3054	1/1	0.95	0.71	75,75,75,75	0
54	MG	BA	3607	1/1	0.95	0.13	38,38,38,38	0
54	MG	DA	3031	1/1	0.95	0.45	43,43,43,43	0
54	MG	DA	3265	1/1	0.95	0.21	39,39,39,39	0
54	MG	DA	3131	1/1	0.95	0.28	39,39,39,39	0
54	MG	BA	3336	1/1	0.95	0.12	46,46,46,46	0
54	MG	BA	3472	1/1	0.95	0.21	29,29,29,29	0
54	MG	BA	3010	1/1	0.95	0.20	48,48,48,48	0
54	MG	DA	3122	1/1	0.95	0.52	47,47,47,47	0
54	MG	DA	3055	1/1	0.95	0.46	43,43,43,43	0
55	ZN	BY	201	1/1	0.95	0.14	74,74,74,74	0
54	MG	BA	3291	1/1	0.95	0.12	59,59,59,59	0
54	MG	BD	303	1/1	0.95	0.35	58,58,58,58	0
54	MG	BA	3168	1/1	0.95	0.39	52,52,52,52	0
54	MG	BA	3523	1/1	0.95	0.06	79,79,79,79	0
54	MG	BA	3353	1/1	0.95	0.13	28,28,28,28	0
54	MG	BA	3084	1/1	0.95	0.16	56,56,56,56	0
54	MG	BA	3473	1/1	0.95	0.44	59,59,59,59	0
54	MG	BA	3373	1/1	0.95	0.09	55,55,55,55	0
54	MG	DA	3191	1/1	0.95	0.26	50,50,50,50	0
54	MG	DA	3233	1/1	0.95	0.32	43,43,43,43	0
54	MG	BA	3236	1/1	0.95	0.21	50,50,50,50	0
54	MG	BA	3123	1/1	0.95	0.20	43,43,43,43	0
54	MG	BA	3281	1/1	0.95	0.29	56,56,56,56	0
54	MG	BA	3056	1/1	0.95	0.39	48,48,48,48	0
54	MG	BA	3284	1/1	0.95	0.13	40,40,40,40	0
54	MG	BA	3112	1/1	0.95	0.40	47,47,47,47	0
54	MG	BA	3252	1/1	0.95	0.25	44,44,44,44	0
54	MG	DA	3247	1/1	0.95	0.37	52,52,52,52	0
54	MG	DA	3170	1/1	0.95	0.25	52,52,52,52	0
54	MG	AA	1635	1/1	0.95	0.21	71,71,71,71	0
54	MG	BA	3383	1/1	0.95	0.17	71,71,71,71	0
54	MG	DA	3115	1/1	0.95	0.41	39,39,39,39	0
54	MG	BA	3179	1/1	0.95	0.44	48,48,48,48	0
54	MG	BA	3126	1/1	0.95	0.41	57,57,57,57	0
54	MG	BA	3417	1/1	0.95	0.21	37,37,37,37	0
54	MG	BA	3230	1/1	0.95	0.37	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
54	MG	DA	3153	1/1	0.95	0.47	38,38,38,38	0
54	MG	BA	3485	1/1	0.95	0.15	60,60,60,60	0
54	MG	DA	3338	1/1	0.95	0.19	50,50,50,50	0
54	MG	DA	3402	1/1	0.95	0.21	59,59,59,59	0
54	MG	CA	1601	1/1	0.95	0.37	50,50,50,50	0
54	MG	DA	3365	1/1	0.95	0.08	50,50,50,50	0
54	MG	DA	3163	1/1	0.95	0.38	56,56,56,56	0
54	MG	DA	3251	1/1	0.95	0.48	39,39,39,39	0
54	MG	BA	3005	1/1	0.95	0.14	42,42,42,42	0
54	MG	DA	3185	1/1	0.95	0.45	47,47,47,47	0
54	MG	BA	3057	1/1	0.95	0.21	46,46,46,46	0
54	MG	DA	3234	1/1	0.95	0.48	56,56,56,56	0
54	MG	DA	3100	1/1	0.95	0.31	61,61,61,61	0
54	MG	DA	3092	1/1	0.95	0.22	63,63,63,63	0
54	MG	DA	3289	1/1	0.95	0.20	52,52,52,52	0
54	MG	BA	3212	1/1	0.95	0.16	47,47,47,47	0
54	MG	BA	3258	1/1	0.95	0.44	56,56,56,56	0
54	MG	DA	3068	1/1	0.95	0.23	48,48,48,48	0
54	MG	BA	3083	1/1	0.95	0.46	56,56,56,56	0
54	MG	BA	3290	1/1	0.95	0.37	47,47,47,47	0
54	MG	BA	3287	1/1	0.95	0.45	65,65,65,65	0
54	MG	BA	3223	1/1	0.95	0.18	57,57,57,57	0
54	MG	DA	3331	1/1	0.95	0.17	69,69,69,69	0
54	MG	BA	3610	1/1	0.95	0.06	56,56,56,56	0
54	MG	DA	3413	1/1	0.95	0.18	37,37,37,37	0
54	MG	BA	3583	1/1	0.95	0.05	50,50,50,50	0
54	MG	DA	3144	1/1	0.95	0.30	42,42,42,42	0
54	MG	DA	3067	1/1	0.95	0.33	32,32,32,32	0
54	MG	DA	3272	1/1	0.96	0.18	47,47,47,47	0
54	MG	BA	3321	1/1	0.96	0.11	65,65,65,65	0
54	MG	BA	3075	1/1	0.96	0.31	53,53,53,53	0
54	MG	DA	3218	1/1	0.96	0.71	53,53,53,53	0
54	MG	BA	3326	1/1	0.96	0.14	30,30,30,30	0
54	MG	DA	3150	1/1	0.96	0.38	41,41,41,41	0
54	MG	BA	3229	1/1	0.96	0.37	51,51,51,51	0
54	MG	DA	3196	1/1	0.96	0.48	63,63,63,63	0
54	MG	BA	3541	1/1	0.96	0.30	54,54,54,54	0
54	MG	CA	1642	1/1	0.96	0.07	87,87,87,87	0
54	MG	DA	3305	1/1	0.96	0.09	55,55,55,55	0
54	MG	DA	3235	1/1	0.96	0.34	36,36,36,36	0
54	MG	BA	3426	1/1	0.96	0.22	28,28,28,28	0
54	MG	DA	3322	1/1	0.96	0.15	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
54	MG	BQ	203	1/1	0.96	0.23	44,44,44,44	0
54	MG	DA	3323	1/1	0.96	0.20	36,36,36,36	0
54	MG	BA	3432	1/1	0.96	0.18	31,31,31,31	0
54	MG	BA	3568	1/1	0.96	0.14	60,60,60,60	0
54	MG	BA	3564	1/1	0.96	0.28	36,36,36,36	0
54	MG	AA	1626	1/1	0.96	0.52	67,67,67,67	0
54	MG	BA	3391	1/1	0.96	0.28	38,38,38,38	0
54	MG	DA	3377	1/1	0.96	0.10	61,61,61,61	0
54	MG	BA	3379	1/1	0.96	0.06	56,56,56,56	0
54	MG	DA	3304	1/1	0.96	0.18	38,38,38,38	0
54	MG	DA	3032	1/1	0.96	0.30	43,43,43,43	0
54	MG	BA	3048	1/1	0.96	0.20	42,42,42,42	0
54	MG	BA	3346	1/1	0.96	0.07	45,45,45,45	0
54	MG	DA	3427	1/1	0.96	0.16	40,40,40,40	0
54	MG	DA	3117	1/1	0.96	0.35	34,34,34,34	0
54	MG	BA	3548	1/1	0.96	0.20	41,41,41,41	0
54	MG	AA	1610	1/1	0.96	0.28	75,75,75,75	0
54	MG	DA	3241	1/1	0.96	0.24	63,63,63,63	0
54	MG	BA	3035	1/1	0.96	0.24	45,45,45,45	0
54	MG	DA	3136	1/1	0.96	0.52	42,42,42,42	0
54	MG	BA	3573	1/1	0.96	0.09	55,55,55,55	0
54	MG	BA	3288	1/1	0.96	0.51	33,33,33,33	0
54	MG	BB	211	1/1	0.96	0.09	51,51,51,51	0
54	MG	DA	3361	1/1	0.96	0.06	67,67,67,67	0
54	MG	BA	3131	1/1	0.96	0.19	44,44,44,44	0
54	MG	AA	1705	1/1	0.96	0.14	68,68,68,68	0
54	MG	BA	3215	1/1	0.96	0.14	61,61,61,61	0
54	MG	DA	3255	1/1	0.96	0.37	63,63,63,63	0
54	MG	BA	3058	1/1	0.96	0.10	56,56,56,56	0
54	MG	BA	3021	1/1	0.96	0.27	33,33,33,33	0
54	MG	BA	3490	1/1	0.96	0.26	53,53,53,53	0
54	MG	DA	3277	1/1	0.96	0.12	42,42,42,42	0
54	MG	BA	3253	1/1	0.96	0.23	38,38,38,38	0
54	MG	DA	3137	1/1	0.96	0.58	64,64,64,64	0
54	MG	DA	3160	1/1	0.96	0.50	48,48,48,48	0
54	MG	DA	3333	1/1	0.96	0.07	53,53,53,53	0
54	MG	DA	3166	1/1	0.96	0.21	55,55,55,55	0
54	MG	DA	3124	1/1	0.96	0.47	35,35,35,35	0
54	MG	DA	3274	1/1	0.96	0.10	35,35,35,35	0
54	MG	BA	3349	1/1	0.96	0.13	39,39,39,39	0
54	MG	BA	3544	1/1	0.96	0.20	91,91,91,91	0
54	MG	DA	3074	1/1	0.96	0.50	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
54	MG	BA	3190	1/1	0.96	0.30	46,46,46,46	0
54	MG	BA	3324	1/1	0.96	0.10	82,82,82,82	0
54	MG	BA	3512	1/1	0.96	0.33	45,45,45,45	0
54	MG	DA	3164	1/1	0.96	0.23	46,46,46,46	0
54	MG	CA	1614	1/1	0.96	0.26	69,69,69,69	0
54	MG	BA	3025	1/1	0.96	0.11	52,52,52,52	0
54	MG	BA	3033	1/1	0.96	0.37	40,40,40,40	0
55	ZN	D6	101	1/1	0.96	0.10	86,86,86,86	0
54	MG	DA	3116	1/1	0.96	0.40	46,46,46,46	0
54	MG	BA	3427	1/1	0.96	0.22	32,32,32,32	0
54	MG	DA	3088	1/1	0.96	0.26	65,65,65,65	0
54	MG	DA	3156	1/1	0.96	0.25	52,52,52,52	0
54	MG	AA	1647	1/1	0.96	0.32	61,61,61,61	0
54	MG	BA	3192	1/1	0.96	0.33	43,43,43,43	0
54	MG	DA	3275	1/1	0.96	0.12	48,48,48,48	0
54	MG	AA	1684	1/1	0.96	0.05	76,76,76,76	0
54	MG	BA	3162	1/1	0.96	0.48	62,62,62,62	0
54	MG	BA	3312	1/1	0.96	0.09	50,50,50,50	0
54	MG	BA	3008	1/1	0.96	0.28	32,32,32,32	0
54	MG	BA	3278	1/1	0.96	0.25	43,43,43,43	0
54	MG	BA	3115	1/1	0.96	0.36	43,43,43,43	0
54	MG	DA	3253	1/1	0.96	0.30	42,42,42,42	0
54	MG	BE	303	1/1	0.96	0.14	54,54,54,54	0
54	MG	BA	3038	1/1	0.96	0.10	36,36,36,36	0
54	MG	DA	3243	1/1	0.96	0.35	53,53,53,53	0
54	MG	DA	3178	1/1	0.96	0.47	58,58,58,58	0
54	MG	BA	3261	1/1	0.96	0.29	59,59,59,59	0
54	MG	CA	1620	1/1	0.96	0.32	57,57,57,57	0
54	MG	BA	3164	1/1	0.96	0.17	39,39,39,39	0
54	MG	DA	3010	1/1	0.96	0.15	43,43,43,43	0
54	MG	BA	3438	1/1	0.96	0.17	38,38,38,38	0
54	MG	BA	3256	1/1	0.96	0.67	69,69,69,69	0
54	MG	CA	1633	1/1	0.96	0.25	71,71,71,71	0
54	MG	BA	3364	1/1	0.96	0.12	46,46,46,46	0
54	MG	BA	3528	1/1	0.96	0.12	43,43,43,43	0
54	MG	BA	3582	1/1	0.96	0.12	54,54,54,54	0
54	MG	DB	205	1/1	0.96	0.14	70,70,70,70	0
54	MG	DA	3025	1/1	0.97	0.17	57,57,57,57	0
54	MG	BA	3292	1/1	0.97	0.20	44,44,44,44	0
54	MG	DA	3325	1/1	0.97	0.26	36,36,36,36	0
54	MG	BA	3488	1/1	0.97	0.15	34,34,34,34	0
54	MG	DA	3288	1/1	0.97	0.11	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	BA	3047	1/1	0.97	0.29	50,50,50,50	0
54	MG	BA	3462	1/1	0.97	0.12	25,25,25,25	0
54	MG	BA	3317	1/1	0.97	0.09	51,51,51,51	0
54	MG	BA	3385	1/1	0.97	0.10	73,73,73,73	0
54	MG	DA	3283	1/1	0.97	0.14	48,48,48,48	0
54	MG	DA	3366	1/1	0.97	0.14	35,35,35,35	0
54	MG	BA	3502	1/1	0.97	0.17	41,41,41,41	0
54	MG	BA	3221	1/1	0.97	0.17	51,51,51,51	0
54	MG	DA	3309	1/1	0.97	0.47	48,48,48,48	0
54	MG	DA	3022	1/1	0.97	0.36	52,52,52,52	0
54	MG	BA	3238	1/1	0.97	0.16	32,32,32,32	0
54	MG	BA	3309	1/1	0.97	0.16	38,38,38,38	0
54	MG	BA	3455	1/1	0.97	0.34	42,42,42,42	0
54	MG	BA	3293	1/1	0.97	0.21	29,29,29,29	0
54	MG	BA	3507	1/1	0.97	0.14	53,53,53,53	0
54	MG	DA	3154	1/1	0.97	0.83	62,62,62,62	0
54	MG	DA	3287	1/1	0.97	0.06	46,46,46,46	0
54	MG	DA	3020	1/1	0.97	0.20	39,39,39,39	0
54	MG	BA	3352	1/1	0.97	0.09	53,53,53,53	0
54	MG	BA	3552	1/1	0.97	0.18	38,38,38,38	0
54	MG	DA	3356	1/1	0.97	0.19	42,42,42,42	0
54	MG	BA	3163	1/1	0.97	0.43	42,42,42,42	0
54	MG	DA	3132	1/1	0.97	0.41	49,49,49,49	0
54	MG	DD	301	1/1	0.97	0.16	40,40,40,40	0
54	MG	BA	3367	1/1	0.97	0.21	33,33,33,33	0
54	MG	DA	3319	1/1	0.97	0.10	59,59,59,59	0
54	MG	DA	3414	1/1	0.97	0.12	68,68,68,68	0
54	MG	DA	3263	1/1	0.97	0.08	70,70,70,70	0
54	MG	DA	3276	1/1	0.97	0.12	51,51,51,51	0
54	MG	BA	3518	1/1	0.97	0.36	59,59,59,59	0
54	MG	BA	3441	1/1	0.97	0.25	35,35,35,35	0
54	MG	BA	3483	1/1	0.97	0.16	57,57,57,57	0
54	MG	BA	3419	1/1	0.97	0.25	35,35,35,35	0
54	MG	DA	3430	1/1	0.97	0.05	72,72,72,72	0
54	MG	BA	3020	1/1	0.97	0.10	34,34,34,34	0
54	MG	BA	3591	1/1	0.97	0.13	56,56,56,56	0
54	MG	BA	3228	1/1	0.97	0.38	26,26,26,26	0
54	MG	BA	3409	1/1	0.97	0.18	26,26,26,26	0
54	MG	DA	3320	1/1	0.97	0.13	57,57,57,57	0
54	MG	BA	3354	1/1	0.97	0.06	49,49,49,49	0
54	MG	DA	3039	1/1	0.97	0.28	41,41,41,41	0
54	MG	BA	3604	1/1	0.97	0.07	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
54	MG	DA	3398	1/1	0.97	0.12	52,52,52,52	0
54	MG	BA	3398	1/1	0.97	0.17	36,36,36,36	0
54	MG	DA	3385	1/1	0.97	0.36	49,49,49,49	0
54	MG	BA	3599	1/1	0.97	0.09	50,50,50,50	0
54	MG	BA	3268	1/1	0.97	0.29	44,44,44,44	0
54	MG	BA	3423	1/1	0.97	0.22	30,30,30,30	0
54	MG	BA	3516	1/1	0.97	0.14	39,39,39,39	0
54	MG	BA	3576	1/1	0.97	0.12	41,41,41,41	0
54	MG	BA	3380	1/1	0.97	0.07	50,50,50,50	0
54	MG	DA	3169	1/1	0.97	0.25	39,39,39,39	0
54	MG	DF	301	1/1	0.97	0.37	58,58,58,58	0
54	MG	DA	3094	1/1	0.97	0.12	39,39,39,39	0
55	ZN	D9	101	1/1	0.97	0.05	87,87,87,87	0
54	MG	DA	3351	1/1	0.97	0.14	78,78,78,78	0
54	MG	BA	3470	1/1	0.97	0.23	35,35,35,35	0
54	MG	DA	3171	1/1	0.97	0.31	53,53,53,53	0
54	MG	BA	3440	1/1	0.97	0.09	63,63,63,63	0
54	MG	DA	3076	1/1	0.97	0.17	70,70,70,70	0
54	MG	DA	3204	1/1	0.97	0.31	37,37,37,37	0
54	MG	DA	3308	1/1	0.97	0.42	49,49,49,49	0
54	MG	BA	3262	1/1	0.97	0.38	32,32,32,32	0
54	MG	BA	3406	1/1	0.97	0.18	40,40,40,40	0
54	MG	BA	3408	1/1	0.97	0.32	34,34,34,34	0
54	MG	BA	3305	1/1	0.97	0.09	37,37,37,37	0
54	MG	DA	3267	1/1	0.97	0.19	59,59,59,59	0
54	MG	BA	3110	1/1	0.97	0.37	23,23,23,23	0
54	MG	BE	305	1/1	0.97	0.22	32,32,32,32	0
54	MG	DA	3145	1/1	0.97	0.45	47,47,47,47	0
54	MG	BA	3506	1/1	0.97	0.16	61,61,61,61	0
54	MG	BA	3539	1/1	0.97	0.06	61,61,61,61	0
54	MG	BA	3454	1/1	0.97	0.17	34,34,34,34	0
54	MG	BA	3442	1/1	0.97	0.15	31,31,31,31	0
54	MG	BB	216	1/1	0.98	0.33	46,46,46,46	0
54	MG	DA	3307	1/1	0.98	0.22	39,39,39,39	0
54	MG	CA	1652	1/1	0.98	0.09	65,65,65,65	0
54	MG	AA	1689	1/1	0.98	0.09	55,55,55,55	0
54	MG	DA	3332	1/1	0.98	0.05	62,62,62,62	0
54	MG	BA	3578	1/1	0.98	0.21	60,60,60,60	0
54	MG	BA	3477	1/1	0.98	0.08	45,45,45,45	0
54	MG	BA	3550	1/1	0.98	0.28	37,37,37,37	0
54	MG	DA	3344	1/1	0.98	0.09	51,51,51,51	0
54	MG	BA	3299	1/1	0.98	0.22	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
55	ZN	D5	101	1/1	0.98	0.07	65,65,65,65	0
54	MG	DA	3220	1/1	0.98	0.25	48,48,48,48	0
54	MG	BA	3303	1/1	0.98	0.20	36,36,36,36	0
54	MG	BA	3390	1/1	0.98	0.22	29,29,29,29	0
54	MG	BA	3060	1/1	0.98	0.30	45,45,45,45	0
54	MG	B8	103	1/1	0.98	0.14	51,51,51,51	0
54	MG	DA	3280	1/1	0.98	0.26	40,40,40,40	0
54	MG	BA	3246	1/1	0.98	0.21	49,49,49,49	0
54	MG	BA	3570	1/1	0.98	0.17	36,36,36,36	0
54	MG	DA	3118	1/1	0.98	0.45	44,44,44,44	0
54	MG	CA	1654	1/1	0.98	0.11	95,95,95,95	0
54	MG	DA	3202	1/1	0.98	0.22	37,37,37,37	0
54	MG	BA	3609	1/1	0.98	0.18	51,51,51,51	0
54	MG	DA	3279	1/1	0.98	0.33	40,40,40,40	0
54	MG	DA	3270	1/1	0.98	0.11	34,34,34,34	0
54	MG	BA	3451	1/1	0.98	0.24	34,34,34,34	0
54	MG	DA	3392	1/1	0.98	0.09	56,56,56,56	0
54	MG	BD	302	1/1	0.98	0.29	38,38,38,38	0
54	MG	BA	3378	1/1	0.98	0.12	38,38,38,38	0
54	MG	BA	3430	1/1	0.98	0.22	30,30,30,30	0
54	MG	BA	3461	1/1	0.98	0.23	38,38,38,38	0
54	MG	BA	3381	1/1	0.98	0.08	49,49,49,49	0
54	MG	BA	3466	1/1	0.98	0.07	67,67,67,67	0
54	MG	BA	3575	1/1	0.98	0.07	54,54,54,54	0
54	MG	DA	3419	1/1	0.98	0.08	50,50,50,50	0
55	ZN	B9	101	1/1	0.98	0.13	69,69,69,69	0
54	MG	BA	3348	1/1	0.98	0.22	37,37,37,37	0
54	MG	DA	3149	1/1	0.98	0.38	36,36,36,36	0
54	MG	BA	3177	1/1	0.98	0.10	45,45,45,45	0
54	MG	BA	3431	1/1	0.98	0.26	34,34,34,34	0
54	MG	BA	3482	1/1	0.98	0.18	58,58,58,58	0
54	MG	BA	3372	1/1	0.98	0.13	50,50,50,50	0
54	MG	BA	3403	1/1	0.98	0.13	44,44,44,44	0
54	MG	BA	3104	1/1	0.98	0.21	48,48,48,48	0
54	MG	DA	3110	1/1	0.98	0.08	46,46,46,46	0
54	MG	BA	3202	1/1	0.98	0.52	65,65,65,65	0
54	MG	BA	3331	1/1	0.98	0.16	51,51,51,51	0
54	MG	BB	205	1/1	0.98	0.29	57,57,57,57	0
54	MG	BA	3313	1/1	0.98	0.12	42,42,42,42	0
54	MG	BA	3596	1/1	0.98	0.13	46,46,46,46	0
54	MG	BA	3579	1/1	0.98	0.12	53,53,53,53	0
54	MG	BA	3540	1/1	0.98	0.06	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
54	MG	BA	3421	1/1	0.98	0.13	36,36,36,36	0
54	MG	DA	3236	1/1	0.98	0.55	44,44,44,44	0
54	MG	DA	3273	1/1	0.98	0.11	37,37,37,37	0
54	MG	BA	3307	1/1	0.98	0.20	29,29,29,29	0
54	MG	BA	3557	1/1	0.98	0.49	42,42,42,42	0
54	MG	BA	3234	1/1	0.98	0.33	34,34,34,34	0
54	MG	BA	3574	1/1	0.98	0.06	41,41,41,41	0
54	MG	BA	3605	1/1	0.98	0.12	30,30,30,30	0
54	MG	BA	3395	1/1	0.98	0.14	32,32,32,32	0
54	MG	CA	1644	1/1	0.98	0.15	74,74,74,74	0
54	MG	BA	3080	1/1	0.98	0.51	42,42,42,42	0
54	MG	DB	204	1/1	0.98	0.14	74,74,74,74	0
54	MG	DA	3426	1/1	0.98	0.10	94,94,94,94	0
54	MG	BA	3602	1/1	0.98	0.09	24,24,24,24	0
54	MG	DA	3300	1/1	0.98	0.20	62,62,62,62	0
54	MG	BA	3484	1/1	0.98	0.12	40,40,40,40	0
54	MG	DA	3264	1/1	0.98	0.21	46,46,46,46	0
54	MG	BA	3601	1/1	0.98	0.06	33,33,33,33	0
54	MG	BA	3248	1/1	0.98	0.18	50,50,50,50	0
54	MG	BA	3411	1/1	0.98	0.27	43,43,43,43	0
54	MG	DA	3285	1/1	0.98	0.14	52,52,52,52	0
54	MG	DA	3268	1/1	0.98	0.16	43,43,43,43	0
54	MG	BA	3476	1/1	0.98	0.23	44,44,44,44	0
54	MG	BA	3370	1/1	0.98	0.10	66,66,66,66	0
54	MG	CA	1647	1/1	0.98	0.13	78,78,78,78	0
54	MG	BA	3603	1/1	0.98	0.19	30,30,30,30	0
54	MG	AA	1668	1/1	0.98	0.11	83,83,83,83	0
54	MG	AA	1614	1/1	0.98	0.23	62,62,62,62	0
54	MG	BA	3296	1/1	0.98	0.07	48,48,48,48	0
54	MG	BA	3597	1/1	0.99	0.09	26,26,26,26	0
54	MG	BA	3471	1/1	0.99	0.21	38,38,38,38	0
54	MG	DA	3404	1/1	0.99	0.07	53,53,53,53	0
54	MG	BB	217	1/1	0.99	0.25	42,42,42,42	0
54	MG	BA	3310	1/1	0.99	0.21	44,44,44,44	0
54	MG	BA	3424	1/1	0.99	0.22	32,32,32,32	0
54	MG	DA	3352	1/1	0.99	0.10	61,61,61,61	0
54	MG	BA	3366	1/1	0.99	0.08	50,50,50,50	0
54	MG	BA	3323	1/1	0.99	0.09	40,40,40,40	0
54	MG	DA	3004	1/1	0.99	0.14	59,59,59,59	0
54	MG	B5	102	1/1	0.99	0.08	42,42,42,42	0
54	MG	BA	3600	1/1	0.99	0.20	31,31,31,31	0
55	ZN	B5	103	1/1	0.99	0.14	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
54	MG	BA	3393	1/1	0.99	0.19	38,38,38,38	0
54	MG	BA	3504	1/1	0.99	0.39	28,28,28,28	0
54	MG	BA	3443	1/1	0.99	0.25	41,41,41,41	0
54	MG	DA	3281	1/1	0.99	0.09	36,36,36,36	0
54	MG	BA	3560	1/1	0.99	0.12	29,29,29,29	0
54	MG	DA	3418	1/1	0.99	0.07	39,39,39,39	0
55	ZN	B6	101	1/1	0.99	0.12	54,54,54,54	0
54	MG	BA	3368	1/1	0.99	0.31	34,34,34,34	0
54	MG	DA	3373	1/1	0.99	0.27	38,38,38,38	0
54	MG	BA	3245	1/1	0.99	0.12	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.