



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2016 – 12:09 PM GMT

PDB ID : 4WRO
Title : Complex of 70S ribosome with tRNA-Phe and mRNA with C-A mismatch in the second position in the A-site
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2014-10-24
Resolution : 3.05 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

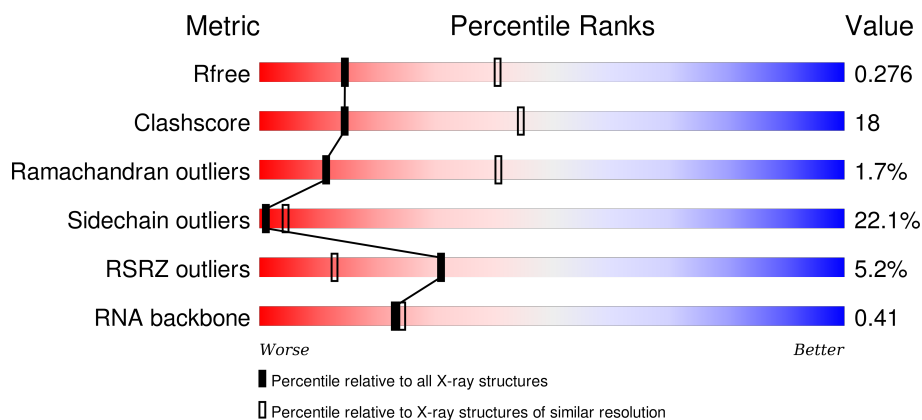
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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.



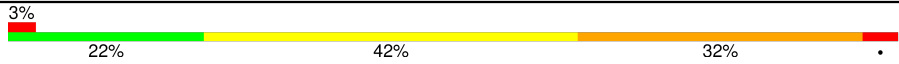

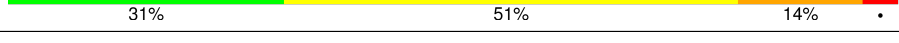
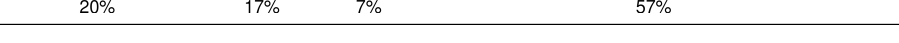
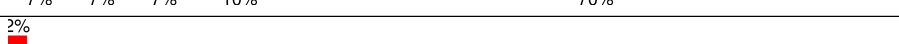
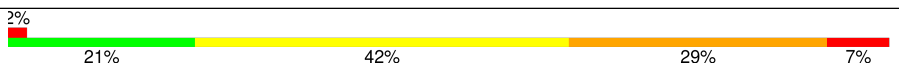
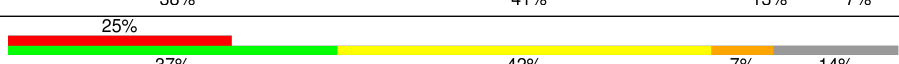


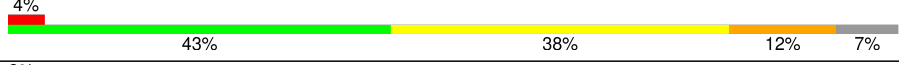

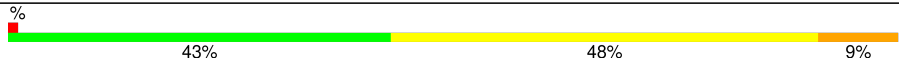
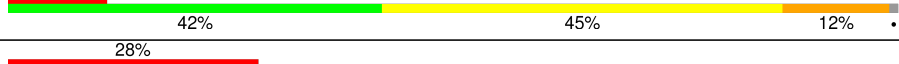
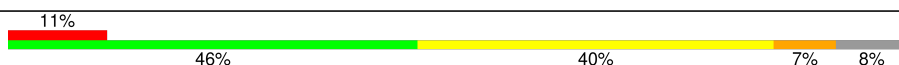

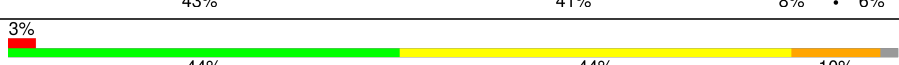


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)
RNA backbone	2183	1035 (3.50-2.62)

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. 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	13	1522	
1	1G	1522	
2	1L	76	
2	3K	76	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	3L	76	
3	2K	77	
3	2L	77	
4	4K	30	
4	4L	30	
5	14	2917	
5	1H	2917	
6	12	256	
6	1E	256	
7	22	239	
7	2E	239	
8	32	209	
8	3E	209	
9	4E	162	
10	5E	101	
11	6E	156	
12	7E	138	
13	8E	128	
14	1I	105	
15	2I	129	
16	3I	132	
17	4I	126	
18	5I	61	
19	6I	89	
20	7I	88	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
21	8I	105	
22	9I	88	
23	AI	93	
24	BI	106	
25	1F	27	
26	1K	76	
27	16	122	
27	1J	122	
28	11	276	
29	21	206	
30	31	210	
31	41	182	
32	51	180	
33	61	148	
34	58	140	
35	68	122	
36	78	150	
37	88	141	
38	98	118	
39	A8	112	
40	B8	146	
41	C8	118	
42	D8	101	
43	E8	113	
44	F8	96	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
45	G8	110	
46	H8	206	
47	I8	85	
48	J8	98	
49	K8	72	
50	L8	60	
51	M8	71	
52	N8	60	
53	O8	54	
54	P8	49	
55	Q8	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	13	1601	-	-	-	X
56	MG	13	1606	-	-	-	X
56	MG	13	1608	-	-	-	X
56	MG	13	1611	-	-	-	X
56	MG	13	1613	-	-	-	X
56	MG	13	1615	-	-	-	X
56	MG	13	1621	-	-	-	X
56	MG	13	1626	-	-	-	X
56	MG	13	1630	-	-	-	X
56	MG	13	1631	-	-	-	X
56	MG	13	1641	-	-	-	X
56	MG	13	1643	-	-	-	X
56	MG	13	1648	-	-	-	X
56	MG	13	1659	-	-	-	X
56	MG	13	1664	-	-	-	X
56	MG	13	1670	-	-	-	X
56	MG	13	1671	-	-	-	X
56	MG	13	1673	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	13	1676	-	-	-	X
56	MG	13	1682	-	-	-	X
56	MG	13	1691	-	-	-	X
56	MG	13	1707	-	-	-	X
56	MG	13	1722	-	-	-	X
56	MG	14	3011	-	-	-	X
56	MG	14	3021	-	-	-	X
56	MG	14	3022	-	-	-	X
56	MG	14	3023	-	-	-	X
56	MG	14	3027	-	-	-	X
56	MG	14	3035	-	-	-	X
56	MG	14	3036	-	-	-	X
56	MG	14	3037	-	-	-	X
56	MG	14	3040	-	-	-	X
56	MG	14	3041	-	-	-	X
56	MG	14	3042	-	-	-	X
56	MG	14	3052	-	-	-	X
56	MG	14	3056	-	-	-	X
56	MG	14	3068	-	-	-	X
56	MG	14	3073	-	-	-	X
56	MG	14	3076	-	-	-	X
56	MG	14	3095	-	-	-	X
56	MG	14	3096	-	-	-	X
56	MG	14	3107	-	-	-	X
56	MG	14	3121	-	-	-	X
56	MG	14	3122	-	-	-	X
56	MG	14	3125	-	-	-	X
56	MG	14	3156	-	-	-	X
56	MG	14	3160	-	-	-	X
56	MG	14	3175	-	-	-	X
56	MG	14	3182	-	-	-	X
56	MG	14	3191	-	-	-	X
56	MG	14	3198	-	-	-	X
56	MG	14	3227	-	-	-	X
56	MG	14	3230	-	-	-	X
56	MG	14	3240	-	-	-	X
56	MG	16	201	-	-	-	X
56	MG	16	206	-	-	-	X
56	MG	1G	1601	-	-	-	X
56	MG	1G	1602	-	-	-	X
56	MG	1G	1609	-	-	-	X
56	MG	1G	1617	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1G	1620	-	-	-	X
56	MG	1G	1640	-	-	-	X
56	MG	1G	1663	-	-	-	X
56	MG	1G	1669	-	-	-	X
56	MG	1G	1675	-	-	-	X
56	MG	1H	3001	-	-	-	X
56	MG	1H	3004	-	-	-	X
56	MG	1H	3010	-	-	-	X
56	MG	1H	3011	-	-	-	X
56	MG	1H	3015	-	-	-	X
56	MG	1H	3020	-	-	-	X
56	MG	1H	3021	-	-	-	X
56	MG	1H	3023	-	-	-	X
56	MG	1H	3025	-	-	-	X
56	MG	1H	3026	-	-	-	X
56	MG	1H	3027	-	-	-	X
56	MG	1H	3032	-	-	-	X
56	MG	1H	3033	-	-	-	X
56	MG	1H	3036	-	-	-	X
56	MG	1H	3037	-	-	-	X
56	MG	1H	3041	-	-	-	X
56	MG	1H	3045	-	-	-	X
56	MG	1H	3047	-	-	-	X
56	MG	1H	3048	-	-	-	X
56	MG	1H	3052	-	-	-	X
56	MG	1H	3054	-	-	-	X
56	MG	1H	3057	-	-	-	X
56	MG	1H	3058	-	-	-	X
56	MG	1H	3065	-	-	-	X
56	MG	1H	3066	-	-	-	X
56	MG	1H	3072	-	-	-	X
56	MG	1H	3078	-	-	-	X
56	MG	1H	3081	-	-	-	X
56	MG	1H	3082	-	-	-	X
56	MG	1H	3085	-	-	-	X
56	MG	1H	3089	-	-	-	X
56	MG	1H	3092	-	-	-	X
56	MG	1H	3095	-	-	-	X
56	MG	1H	3098	-	-	-	X
56	MG	1H	3101	-	-	-	X
56	MG	1H	3103	-	-	-	X
56	MG	1H	3108	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1H	3109	-	-	-	X
56	MG	1H	3111	-	-	-	X
56	MG	1H	3118	-	-	-	X
56	MG	1H	3124	-	-	-	X
56	MG	1H	3128	-	-	-	X
56	MG	1H	3132	-	-	-	X
56	MG	1H	3133	-	-	-	X
56	MG	1H	3136	-	-	-	X
56	MG	1H	3138	-	-	-	X
56	MG	1H	3142	-	-	-	X
56	MG	1H	3145	-	-	-	X
56	MG	1H	3146	-	-	-	X
56	MG	1H	3149	-	-	-	X
56	MG	1H	3151	-	-	-	X
56	MG	1H	3152	-	-	-	X
56	MG	1H	3164	-	-	-	X
56	MG	1H	3167	-	-	-	X
56	MG	1H	3176	-	-	-	X
56	MG	1H	3185	-	-	-	X
56	MG	1H	3186	-	-	-	X
56	MG	1H	3189	-	-	-	X
56	MG	1H	3199	-	-	-	X
56	MG	1H	3203	-	-	-	X
56	MG	1H	3204	-	-	-	X
56	MG	1H	3221	-	-	-	X
56	MG	1H	3230	-	-	-	X
56	MG	1H	3232	-	-	-	X
56	MG	1H	3240	-	-	-	X
56	MG	1H	3258	-	-	-	X
56	MG	1H	3263	-	-	-	X
56	MG	1H	3278	-	-	-	X
56	MG	1H	3305	-	-	-	X
56	MG	1H	3312	-	-	-	X
56	MG	1H	3323	-	-	-	X
56	MG	1H	3358	-	-	-	X
56	MG	1H	3366	-	-	-	X
56	MG	1H	3389	-	-	-	X
56	MG	1H	3392	-	-	-	X
56	MG	1H	3416	-	-	-	X
56	MG	1H	3482	-	-	-	X
56	MG	1H	3532	-	-	-	X
56	MG	1J	204	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2I	302	-	-	-	X
56	MG	2K	101	-	-	-	X
56	MG	2K	103	-	-	-	X
56	MG	3I	201	-	-	-	X
56	MG	J8	101	-	-	-	X
57	ZN	3E	303	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 260090 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			
1	1G	1497	Total	C	N	O	P	0	0	0
			32182	14324	5968	10394	1496			

- Molecule 2 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	1L	76	Total	C	N	O	P	S	0	0	0
			1627	730	290	530	75	2			
2	3L	76	Total	C	N	O	P	S	0	0	0
			1627	730	290	530	75	2			
2	3K	76	Total	C	N	O	P	S	0	0	0
			1627	730	290	530	75	2			

- Molecule 3 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	2L	77	Total	C	N	O	P	S	0	0	0
			1645	734	298	535	77	1			
3	2K	77	Total	C	N	O	P	S	0	0	0
			1645	734	298	535	77	1			

- Molecule 4 is a RNA chain called RNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4L	9	Total	C	N	O	P	0	0	0
			191	86	35	61	9			
4	4K	13	Total	C	N	O	P	0	0	0
			279	126	55	85	13			

- Molecule 5 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	14	2909	Total	C	N	O	P	0	0	0
			62647	27884	11716	20139	2908			
5	1H	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
14	161	U	-	insertion	GB 48268
14	493	G	-	insertion	GB 48268
14	1228	G	-	insertion	GB 48268
1H	161	U	-	insertion	GB 48268
1H	493	G	-	insertion	GB 48268
1H	1228	G	-	insertion	GB 48268

- Molecule 6 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1E	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
6	12	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 7 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
7	22	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 8 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	3E	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			
8	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

- Molecule 9 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	4E	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 10 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	5E	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

- Molecule 11 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	6E	155	Total	C	N	O	S	0	0	0
			1256	781	252	217	6			

- Molecule 12 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	7E	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			

- Molecule 13 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	8E	127	Total	C	N	O	0	0	0
			1009	639	197	173			

- Molecule 14 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1I	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 15 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	2I	119	Total	C	N	O	S	0	0	0
			884	549	168	164	3			

- Molecule 16 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	3I	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 17 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4I	118	Total	C	N	O	S	0	0	0
			938	580	193	163	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4I	119	ALA	GLY	conflict	UNP P80377

- Molecule 18 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	5I	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			

- Molecule 19 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	6I	88	Total	C	N	O	S	0	0	0
			733	459	147	125	2			

- Molecule 20 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	7I	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 21 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	8I	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 22 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	9I	72	Total	C	N	O	0	0	0
			590	376	117	97			

- Molecule 23 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AI	81	Total	C	N	O	S	0	0	0
			647	413	119	113	2			

- Molecule 24 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BI	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

- Molecule 25 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	1F	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 26 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
26	1K	74	Total	C	N	O	P	S	0	0	0
			1587	712	286	514	73	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
27	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	11	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	21	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	41	181	Total	C	N	O	S	0	0	0
			1473	942	268	259	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	51	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	61	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	58	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	78	150	Total	C	N	O	S	0	0	0
			1144	712	232	197	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	88	138	Total	C	N	O	S	0	0	0
			1086	693	208	179	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	A8	111	Total	C	N	O	S	0	0	0
			881	556	176	149				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B8	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	C8	117	Total	C	N	O	S	0	0	0
			963	610	202	150	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	D8	101	Total	C	N	O	S	0	0	0
			778	501	142	134	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	E8	113	Total	C	N	O	S	0	0	0
			899	566	177	154	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	F8	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	G8	104	Total	C	N	O	S	0	0	0
			791	510	149	127	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	H8	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	I8	80	Total	C	N	O	S	0	0	0
			626	388	132	105	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I8	6	ALA	GLY	conflict	UNP P60493
I8	8	ALA	GLY	conflict	UNP P60493

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	J8	97	Total	C	N	O	S	0	0	0
			762	481	150	130	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	K8	67	Total	C	N	O	S	0	0	0
			563	349	114	99	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	L8	57	Total	C	N	O		0	0	0
			452	288	88	76				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M8	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	N8	58	Total	C	N	O	S	0	0	0
			453	285	89	74	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	O8	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	P8	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	Q8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	P8	1	Total Mg 1 1	0	0
56	13	149	Total Mg 149 149	0	0
56	1J	7	Total Mg 7 7	0	0
56	5I	1	Total Mg 1 1	0	0
56	16	13	Total Mg 13 13	0	0
56	21	2	Total Mg 2 2	0	0
56	2K	8	Total Mg 8 8	0	0
56	L8	1	Total Mg 1 1	0	0
56	3I	1	Total Mg 1 1	0	0
56	I8	1	Total Mg 1 1	0	0
56	5E	1	Total Mg 1 1	0	0
56	78	1	Total Mg 1 1	0	0
56	J8	1	Total Mg 1 1	0	0
56	1L	1	Total Mg 1 1	0	0
56	1G	96	Total Mg 96 96	0	0
56	11	2	Total Mg 2 2	0	0
56	1H	537	Total Mg 537 537	0	0
56	88	2	Total Mg 2 2	0	0
56	14	421	Total Mg 421 421	0	0
56	3E	2	Total Mg 2 2	0	0
56	3L	3	Total Mg 3 3	0	0
56	1K	2	Total Mg 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	41	2	Total	Mg	0	0
			2	2		
56	2L	4	Total	Mg	0	0
			4	4		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	14	1	Total	Zn	0	0
			1	1		
57	32	1	Total	Zn	0	0
			1	1		
57	3E	1	Total	Zn	0	0
			1	1		
57	1G	1	Total	Zn	0	0
			1	1		
57	G8	1	Total	Zn	0	0
			1	1		
57	5I	1	Total	Zn	0	0
			1	1		

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	13	230	Total	O	0	0
			230	230		
58	2L	1	Total	O	0	0
			1	1		
58	4L	2	Total	O	0	0
			2	2		
58	14	863	Total	O	0	0
			863	863		
58	3E	1	Total	O	0	0
			1	1		
58	4E	3	Total	O	0	0
			3	3		
58	8E	2	Total	O	0	0
			2	2		
58	1I	1	Total	O	0	0
			1	1		
58	3I	1	Total	O	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	5I	1	Total 1	O 1	0	0
58	6I	1	Total 1	O 1	0	0
58	7I	1	Total 1	O 1	0	0
58	BI	1	Total 1	O 1	0	0
58	1K	6	Total 6	O 6	0	0
58	2K	8	Total 8	O 8	0	0
58	3K	1	Total 1	O 1	0	0
58	4K	4	Total 4	O 4	0	0
58	1H	1212	Total 1212	O 1212	0	0
58	1J	12	Total 12	O 12	0	0
58	16	21	Total 21	O 21	0	0
58	11	9	Total 9	O 9	0	0
58	21	3	Total 3	O 3	0	0
58	31	8	Total 8	O 8	0	0
58	58	3	Total 3	O 3	0	0
58	78	6	Total 6	O 6	0	0
58	98	1	Total 1	O 1	0	0
58	B8	1	Total 1	O 1	0	0
58	C8	3	Total 3	O 3	0	0
58	D8	1	Total 1	O 1	0	0
58	E8	2	Total 2	O 2	0	0

Continued on next page...

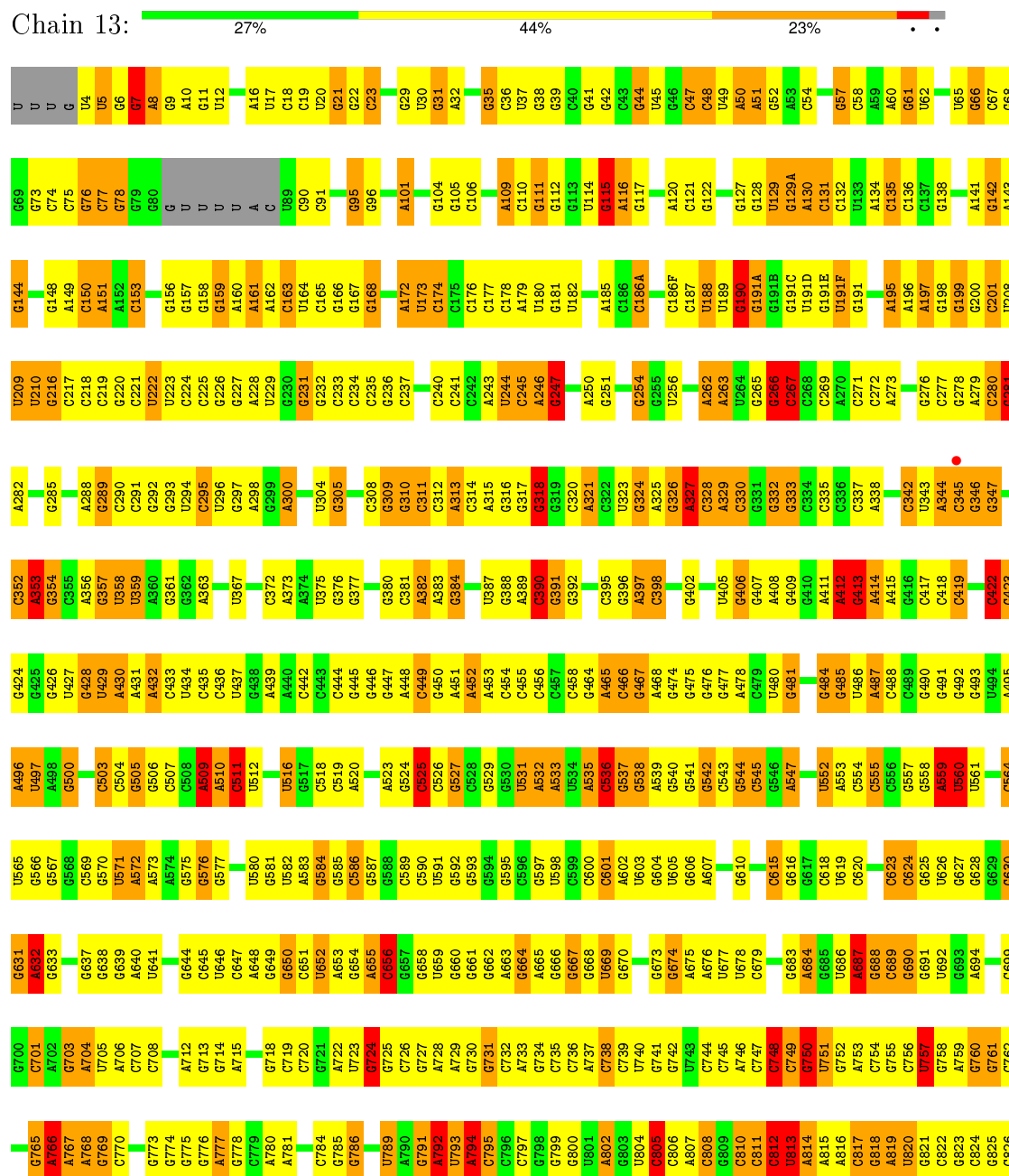
Continued from previous page...

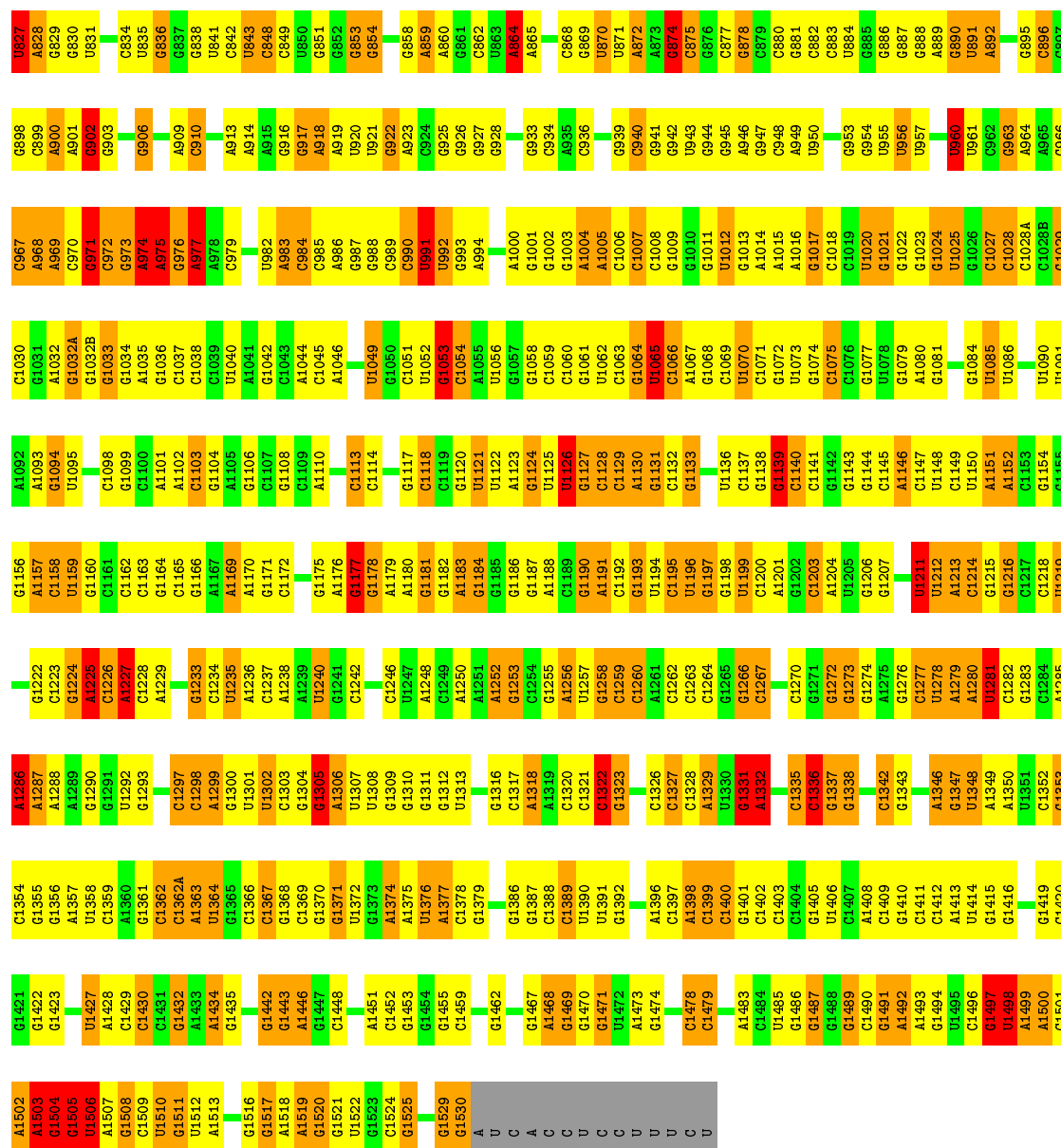
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	F8	2	Total	O	0	0
			2	2		
58	G8	3	Total	O	0	0
			3	3		
58	I8	5	Total	O	0	0
			5	5		
58	J8	1	Total	O	0	0
			1	1		
58	L8	1	Total	O	0	0
			1	1		
58	P8	4	Total	O	0	0
			4	4		
58	Q8	1	Total	O	0	0
			1	1		
58	1G	106	Total	O	0	0
			106	106		

3 Residue-property plots

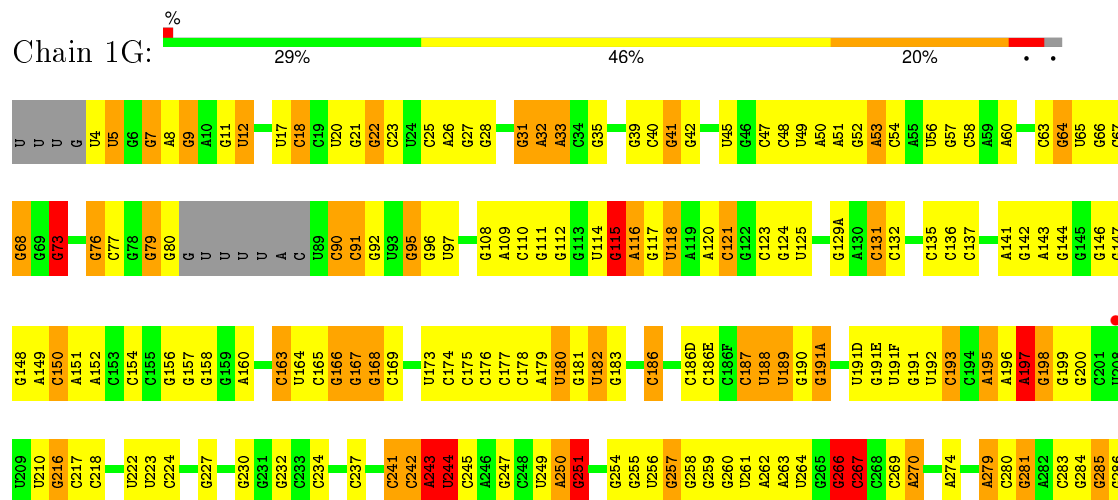
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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

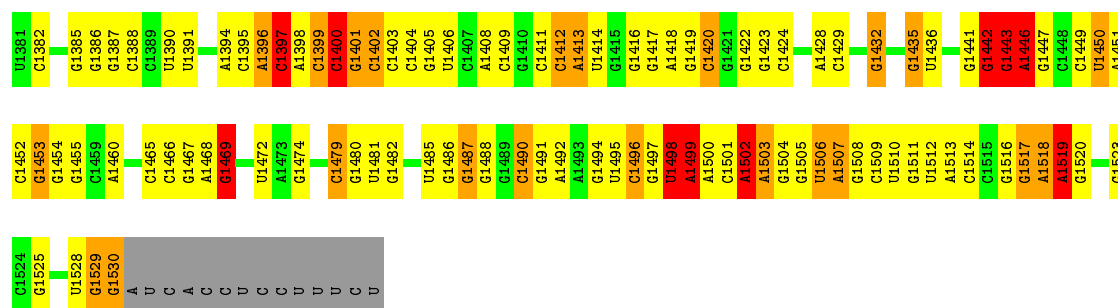




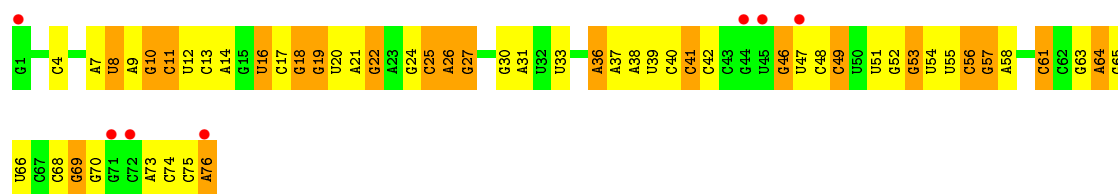
• Molecule 1: 16S ribosomal RNA



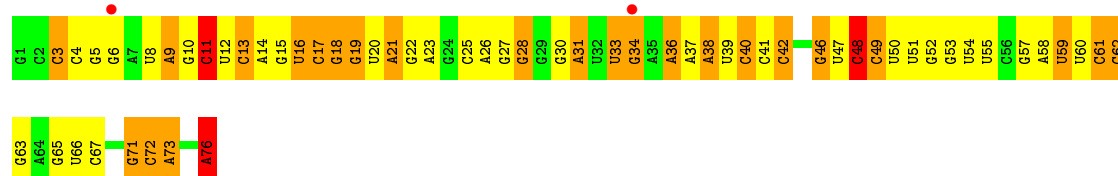
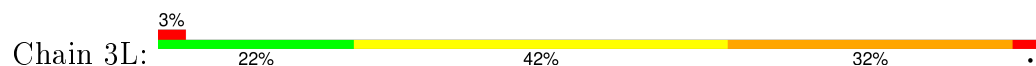
C1320	A1256	C1189	G1124	G1053	G993	C932	U863	U788	G719	G639	A574	C511	C436	G361	G289
C1321	U1257	G1190	U1125	C1054	A994	G933	A864	U789	C719	A640	G575	U512	U437	G362	G289
C1322	C1258	A1191	U1126	U1056	C995	C934	A865	A790	C720	U641	G576	C513	G438	G363	C290
C1323	C1259	G1192	G1127	U1055		A935	C866	A791	G721	A642	G577	C514	A439		C291
A1324	C1260	G1193	C1128	G1058	G998	C936	G867	A792	U723	C645	C578	G517	C442	C366	G297
C1325	A1261	U1194	C1129	G1059	U999	A937	C868	A793	U722	U646	G579	C518	C443	U367	A298
C1326	C1262	G1195	A1130	C1059	U999	A938	C869	A794	U724	C647	U580	C519	C444	U368	A299
C1327	C1263	U1196	G1131	C1060	A1000	G939			G725	U647	G581	A520	C445	C370	A300
C1328		G1197	G1132	G1061	G1001	C940	A872	G800	C726	A648	U582	A521	G446	C371	G301
A1329	C1266	G1198	G1133	U1062	G1002	G941	A873	U801	C727	G649	G583	C522	G447	C372	G302
U1330	C1267	U1199	G1134	C1063	G1003	G942	G874	A802	U728	G650	G584	A523	G448	C373	A303
G1331	A1268	G1200	U1135	G1064	A1004	U943	C875	G803	U729	G651		G524	A448	A373	U304
A1332	A1269	C1201	U1136	U1065	A1005	G944		U804	C730	U652	G587	C525	C449	A374	U304
A1333	C1270	G1202	C1137	C1066	C1006	G945	C879	C805	C731	A653	G588	C526	G450	U375	G305
G1334	G1271	C1203	G1138	A1067	A946	A946	C880	C806	C732	A654	C589	G527	A451	G377	G306
C1335	G1272	A1204	G1139	G1068	G1009	G947	G881	A807	U733	A655	C590	G528	A452	G376	
C1336	G1273	U1205	C1140	C1069	G1010	C948	C882		C734		U591	G529	A453		G309
G1337	G1274	G1206	C1141	C1070	G1013	A949	C883	C810	C735	G660	G592	G530		A382	G310
A1275	G1207	C1208	G1142	C1071	U1013	U950	U884	C811	C736	G661		U531		A383	C311
G1276	C1209	G1208	G1143	G1072	A1014	G951	G885	C812	A737	G662	G595	A532		C384	C312
C1277	C1209	G1208	G1144	U1073	A1015	U952	G886	U813	C738	A663	C596	A533		C385	A313
U1278	C1210	C1211	C1145	G1074	G1016	G953	G887	A814	C739	G664	C597	U534		C386	C314
A1279	U1211	G1212	A1146	C1075	G1017	G954	G888	A815	U740	A665	U598	A535		U387	A315
U1280	C1212	U1212	C1147	U1076		U955	G889	A816	G741	G666	C599	C536		G316	
A1281	A1213	A1213	U1148	G1077	U1020	U956	G890	C817	G742	G667	C600	G537		C390	G317
C1282	C1214	C1214	C1149	G1078		U957	U891	G818	U743	G668	C601	G538		C391	G318
G1283	G1215	U1150	U1150	G1081	G1023	A958	A892	A819	C744		A602	A539		G392	G319
C1284	C1216	A1151	G1024	G1082	G1024	A959	C893	U820		G673	U603	G540		C401	C320
A1285	C1217	A1152	U1025	U1085	U1025	G960	G894	U821	C748	G674	U604	G541		C402	A321
A1286	C1218	C1218	G1026	U1086	G1026	U961	G895	G829	C749	A675	U605	G542		G394	
A1287	U1219	U1219	C1027	U1086	C1027	C962	C896	C822	G750	A676	G606	C543		A397	U323
C1288	G1220	G1220	C1028	G1087	C1028	C963	C897	G825	U751	U677	A607	G544		C398	G324
A1289	G1221	G1221	C1028A	G1087	A964	A964	G898	C826		U678	A608	C545		A325	A325
G1290	G1222	G1222	C1028B	A1092	A965	A965	C899	U827	C754	C679	A609	G546		G401	G326
G1291	C1223	C1223	G1029	G1094	A966	A966	A900	A828	C755	C680	A610	A547		C402	A327
U1292	G1224	G1224	C1030	U1095	C967	C967	A901	G829	C756	G681	C483	G548		C403	
G1293	A1225	A1225	G1031	U1095	A968	A968		G830	U757	G682	C484	C549		U405	
G1294			A1032	C1096	A969	A969	C904	U831	G758	G683		G550		G406	C330
G1295	C1228	C1228	G1032A	C1097	G1032A	C970	U905			A684				G407	G331
C1296	A1229	A1229	G1032B	C1098	G1032B	G971	G906	G836	G760		G617	A553		A408	G332
C1297			G1033	G1099	G1033	C972		G837		A687	C618	C554		G409	C337
A1298	U1232	U1232	G1034	C1100	A1035	G973	A909	G838	G765	C669	U619	C555		G410	
G1300	G1233	G1233	A1169	A1101	A1036	A974	C910	U841	A766	C690	C620	C556		A411	U340
U1301	U1234	U1234	G1170	G1104	G1036	A975	U911	U842	A767	G691	A621	G557		A412	C341
U1302	U1235	U1235	C1038	A1105	C1038	G976	C912	U843	A768	G692	C622	G558		G413	C342
G1304	A1236	A1236	C1039	G1106	C1039	A977	A913	C849	G769	U692	C624	A559		A414	U343
G1305	C1237	C1237	U1040	C1107	G1039	C979	A915	U850	C770	A694	G625	U560			A344
U1306	U1238	U1238	A1041	G1108	A1041	C980	G916	G851	U772		U626	C562		U421	C422
U1307	G1241	G1241	G1042	C1109	G1042	U981	G917	G852	G773	U697	G627	A563		G423	G346
			C1043	A1110	C1043	U982	A918	G853				C564		G424	G347
			A1044	A1111	A1044	A983	A919	G854	A777	A702	C630	U565		G425	G350
	C1246	C1246	C1045	C1112	C1045	C984	U920	G855	G778	C708	C631	G566		G426	G351
A1374	U1247	U1247	A1046	C1113	A1046	C985	U921	C856	C779	G709	A633	G567		C352	C352
U1375	A1248	A1248	G1047	C1114	G1047	A986		G857	A780	G710	C634	G568		U429	A353
U1376	U1315	U1315	G1048	G987	G1048	G987	C924	G858	C783	G711	C635	C569		A430	A353
G1377	G1316	G1316	U1049	G988	U1049	G988	G925	A859	C784	A712	G636	G570		C433	G354
G1378	A1252	A1252	G1050	C1051	G1050		G926	A860	G785	A713	U637	U571		U434	U359
U1380	G1379	G1379	U991	U991	U991	U991	G927	A861		G714	G638	A572		C435	A360
	U1380	U1380	U1052	U992	U1052	U992		C862				A573			



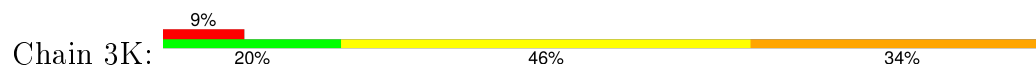
- Molecule 2: tRNA-Phe



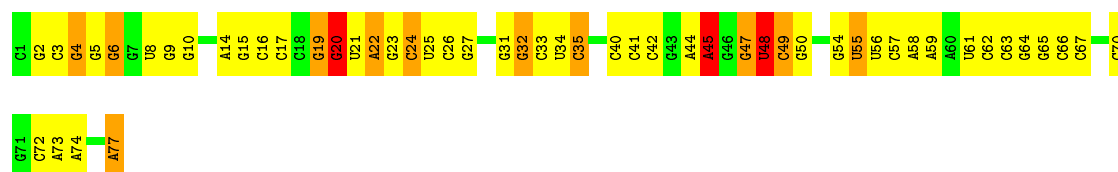
- Molecule 2: tRNA-Phe



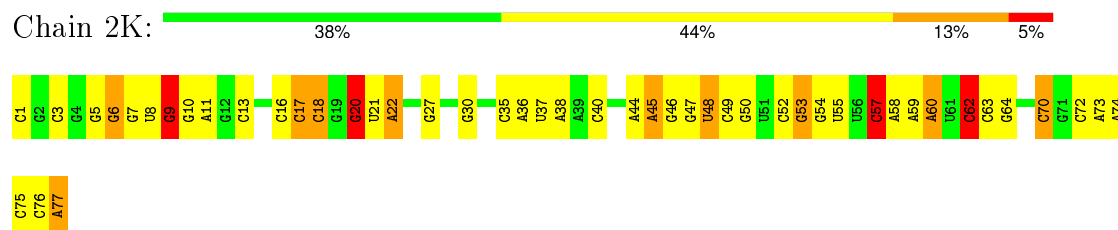
- Molecule 2: tRNA-Phe



- Molecule 3: tRNA-fMet



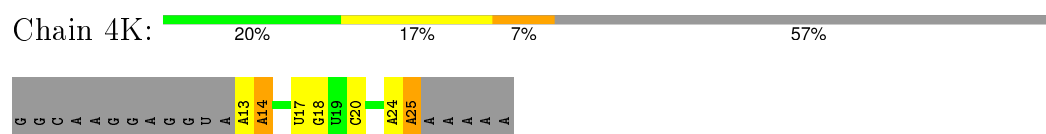
- Molecule 3: tRNA-fMet



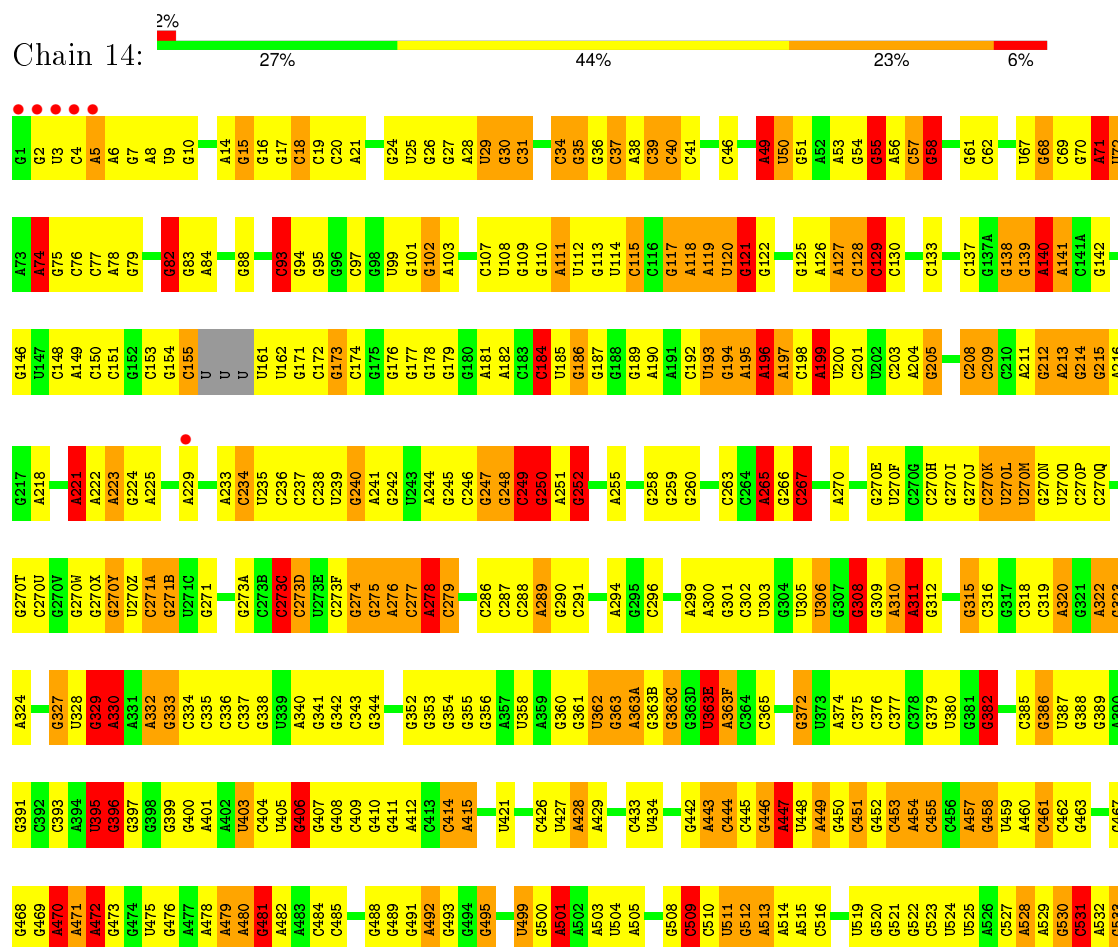
- Molecule 4: RNA (30-MER)



- Molecule 4: RNA (30-MER)

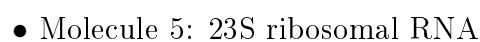


- Molecule 5: 23S ribosomal RNA



G1416	A1354	G1293	C1230	G1161	G1093	A1032	G967	C904	U839	A777	G712	C654K	C605	U534
C1417	G1355	G1296	G1231	G1162	U1094	U1033	G968	U905	C840	G778	G712	G854L	U606	
G1418	G1356	G1297	G1232	G1163	A1095	G1034	U969	G906	A841	U779	G715	G854H	U607	C537
A1419	U1357	G1298	G1233	G1164	A1096	U1035	C970	U907	G842	G780	G715	G854H	A608	C539
U1420	G1358	G1299	U1234	U1165	A1097	G1036	C971	C908	G843	A781	A716	G854D	A609	G540
G1421	A1359	G1299	G1235	C1166	A1098	G1037	G972	A908	C844	A782	G717	G854D	G609A	C541
G1422	A1360	U1300	G1236	U1167	A1099	G1038	A973	A910	G845	A783	A718	C854Q	C610	
G1423	G1361	A1301	A1237	G1168	C1100	G1039	C974A	A911	C846	A784	C719	C854Q	C611	C546
G1424	G1362	A1302	U1240	G1169	U1101	G1040	G977	C912	U847	G785	G720	A654T	A547	
G1425	G1363	G1303	G1170	G1171	A1102	G1041	G978	U913	G848	G786	G721	G856	U613	A548
G1426	A1365	C1304	A1173	G1174	A1103	G1042	G979	C914	A849	U787	A722	G858	U614	A549
A1427	A1366	A1174	A1175	G1175	U1105	G1044	G980	C915	G853	A788	G724	G858	G615	G552
C1428	A1367	U1176	U1177	G1176	G1110	A1045	A980	A937	G854	C790	G725	G859	G617	U553
G1429	G1368	A1177	A1178	G1177	A1111	A1046	A981	A938	G855	C791	G726	G860	G618	U554
C1430	G1369	U1179	C1178	G1178	A1112	G1048	C982	U948	C856	G792	G727	G861	C618A	A556
U1431	U1370	G1180	G1179	G1179	A1113	C1049	A983	G921	C857	A793	G728	C664	G619	U557
G1432	G1371	U1311	G1250	U1113	U1113	A1050	C985	U922	U858	C796	G729	C665	G620	G558
U1433	U1372	U1312	G1251	G1114	G1114	G1051	C986	C923	G859	C797	G730	G666	A621	G559
A1434	A1373	U1313	G1252	G1115	G1115	U1052	C987	C924	U860	C798	G731	G667	G622	C560
G1435	G1374	G1183	A1253	G1116	G1116	G1053	G988	C925	A861	G799	G732	G668	G623	G561
G1436	C1375	G1184	A1254	G1117	G1117	A1054	A988	A926	G862	G799	G733	G669	G624	U562
C1437	C1376	C1185	U1255	G1117	G1117	A1054	G989	G928	A863	A800	A734	A670	G625	G563
U1438	G1377	G1186	G1256	G1120	G1120	G1056	C990	G929	G864	G801	A735	C671	G626	C564
A1439	A1378	G1187	C1257	C1121	C1121	G1057	C991	U930	C865	A802	G736	C672	A627	C565
G1440	A1379	U1188	C1258	G1122	G1122	A1057	C992	C931	A866	U803	C737	C673	G628	U566
G1441	G1380	A1189	G1259	G1125	G1125	U1058	G993	G932	C867	A804	G738	G674	G629	
G1442	G1381	G1192	G1260	G1126	G1126	U1059	C994	A933	U868	G805	G739	A675	G630	U569
G1443	C1382	G1193	A1261	A1128	A1128	U1060	C995	G934	G869	C806	G740	A676	A631	G570
G1444	C1383	U1262	A1262	U1129	U1129	U1061	A996	C935	A870	U807	G741	A677	A632	
A1444A	A1384	A1194	G1263	U1130	U1130	G1062	G997	C936	U871	G808	G746	C678	A633	G573
C1445	G1385	G1264	G1195	U1131	U1131	G1063	C998	U937	A872	G809	A746	C679	C634	C574
G1446	C1386	A1265	U1266	G1131	G1131	C1064	U999	G938	G873	U810	U747	G680	C635	A575
G1447	G1387	G1197	G1267	A1132	A1132	U1065	A1000	G939	G874	U811	G748	G681	G636	U576
A1448	C1388	U1198	U1267	U1133	U1133	U1066	A1001	G940	A878	C812	G749	G682	A637	G577
G1449	U1329	U1199	U1268	C1135	C1135	A1067	G1002	A941	G879	U813	A750	G683	G638	A578
G1449A	C1330	C1200	A1269	G1136	G1136	G1068	G1003	G942	C879	C814	A751	G684	U639	G579
C1450	U1391	C1201	C1270	G1137	G1137	A1069	C1004	U943	G880	C815	A752	A885	C640	C580
C1451	A1392	G1202	G1271	G1138	G1138	U1070	G1005	G944	G881	C816	G753	G686	C641	C581
A1453	G1393	G1203	A1272	C1139	C1139	G1071	G1011	A945	G882	C817	G754	C687	G642	G582
U1454	U1394	A1204	U1273	C1140	C1140	A1072	U1012	G946	C884	A819	C755	U688	C584	G583
G1455	A1395	U1205	A1274	U1141	U1141	A1073	U1013	G948	C885	A820	U757	G690	G585	
	U1396	G1209	A1275	A1142	A1142	G1076	U1014	C949	C886	A821	C758	G691	A646	G585
G1459	U1397	A1210	G1276	A1143	A1143	A1077	U1015	G950	A897	U822	G759	C692	G647	A586
A1460	C1398	A1211	G1277	G1144	G1144	U1078	G1016	C951	C888	G823	G760	C693	G648	C587
G1461	G1399	A1213	A1278	C1145	C1145	U1079	G1017	G952	C889	A824	G760	U694	G649	U588
C1462	G1400	G1213	G1279	G1146	G1146	G1080	C1018	A953	A890			G695	C651	A590
C1463	G1401	U1341	G1280	C1147	C1147	U1081	U1019	G954	G892	U827	G765	G696	G654	C591
G1464	C1402	A1342	G1281	A1148	A1148	U1082	A1020	C955	C893	U828	G766	C697	A654	G592
C1465	C1403	G1343	U1282	G1149	G1149	U1083	A1021	G956	C894	A829	U767	C698	A654A	G593
G1466	G1404	U1283	G1283	A1220	A1220	G1084	G1022	G957	U895	G830	G768	C699	C654B	
C1467	U1405	A1284	A1284	G1150	G1150	A1085	U1023	U958	A896	G831	G769	G700	G654C	U597
G1470	U1406	G1285	G1285	G1151	G1151	A1086	G1024	A959	C897	G832	G770	G701	G654D	G598
A1471	C1407	A1286	A1286	C1152	C1152	G1087	G1025	A960	C898	U833	G771	G702	G654E	G599
	C1408	U1287	G1224	G1153	G1153	A1088	U1026	C961	A899	C834	G772	U703	C654F	G600
C1474	C1409	U1288	G1225	G1154	G1154	A1088	A1027	G962	A900	A835	G773	G704	C654G	C601
G1475	G1410	C1289	G1226	A1155	A1155	G1089	A1028	U963	A901	G836	A774	A705	G654H	G602
C1476	C1411	C1290	A1227	U1159	U1159	U1090	A1029	G966	C902	C837	G775	A706	G654I	A603
A1477	G1413	G1353	G1229A	G1160	G1160	C1092			C903	C838	G776	G707	A654J	G604

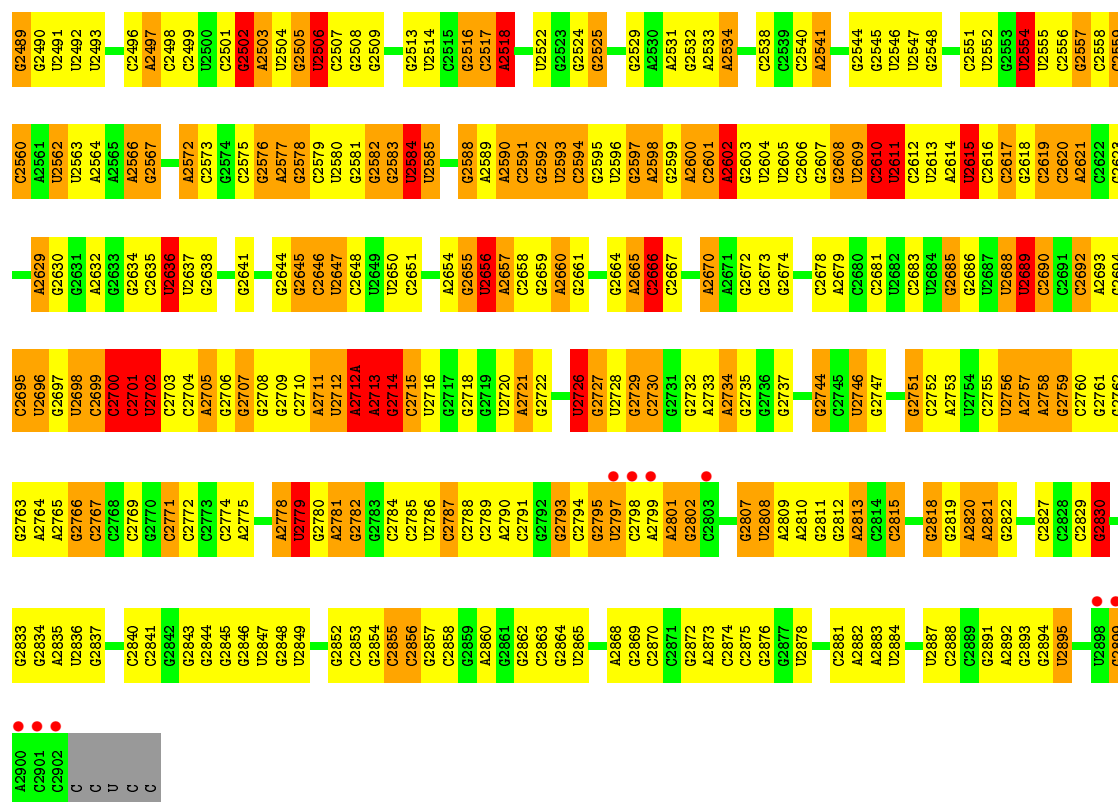




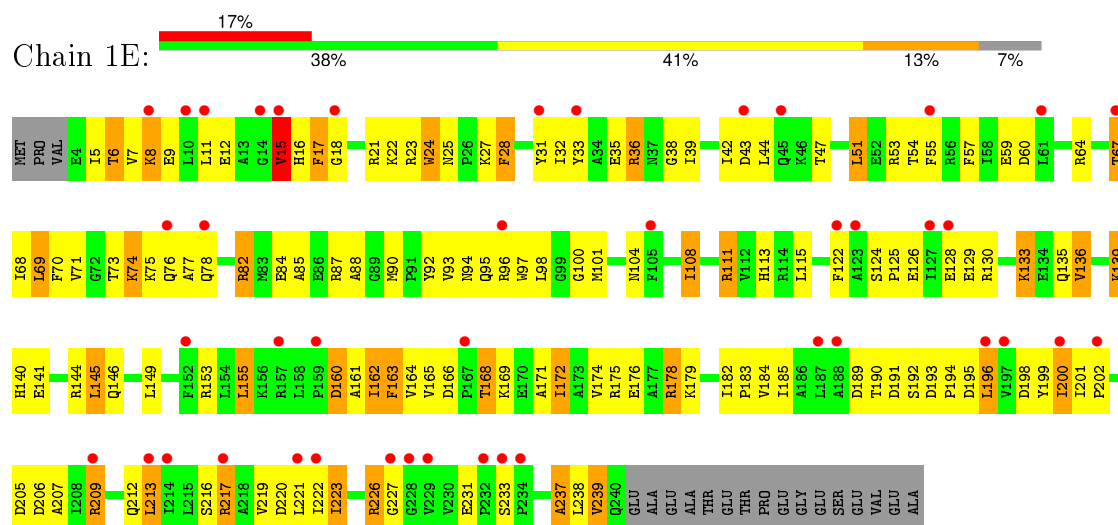
U427	U363E	G301	G261	C198	C130	C66	G1
A428	A363F	C302	A262	A199	G131	U67	G2
A429	C364	U303	C263	U200	G132	G68	U3
G430		G304	C264	C201	G133	C69	C4
U431	G370	U305	A265	U202	C134	G70	A5
A432	A371	U306	G266	C203	G135	A71	A6
	G372	G307	C267	G204	G136	U72	G7
C436	U373	G308	C268	G205	C137	A73	A8
G438	A374	G309	U269	A206	G137A	A74	U9
A439	G375	A310	A270	U207	G138	G75	G10
G440	C376	A311	A270A	C208	G139	C76	G11
U441	C377			C209	A140	C77	U12
G442	C378	G315	G270E	C210	A141		
A443	G379	C316	U270F	G211	C141A	G81	G15
A444	U380	G317	C270G	G212	G142	G82	
C445	G381	C318	G270H	A213	C143	G83	G18
G446	G382	C319	G270I	G214	C144	A84	C19
A447	U383	A320	G270J	G215	G145	G85	C20
U448	U384	G321	C270K	A216	G146	C86	
A449	C385	A322	U270L	G217	U147	C87	G23
G451	U386	G323	U270M	A218	C148	G88	
A452	G387	A324	G270N	G219	A149	G89	G26
G453	G388	G325	U270O	G220	C150	U90	G27
A454	C390	G326	C270P	A221	C151		A28
C455	G391	G327	C270Q	A222	G152	C93	U29
G456	C392	C329	G270R	A223	C153	G94	G30
A457	U393	A330	G270S	G224	G154	G95	C31
G458	C394	A331	G270T	A225	C155	G96	C32
U459	U395	A332	C270U	G226	U161	C97	U83
A460	G396	G333	U270Y	A227	U162	G98	C34
C461	G397	C334	G270Z	A228	U163	U99	G35
G462	G398	C335	C271A	G229	G164	G101	G36
C463	G399	C336	G271B	U230	U165	G102	C37
U464	G400	C337	U271C	C231	G171	A103	A38
G465	A401	G338	G271	G232	C172	U104	C39
A466	A402	U339		A233	G173	G105	C40
G467	U403	A340	G273A	C234	C174	C106	C41
C468	A404			U235	G175	G107	G43
G469	U405	C343	G273F	C236	G176	U108	A44
A470	G406	G344	G274	C237	G177	G109	G45
U471	G407	A345	G275	U239	G179	G110	C46
G472	G408	A476	A276	G240	G179	A111	C47
C473	U409	A347	C277	A241	G180	G48	G48
G474	G410	A348	A278	G242	A181	G113	A49
U475	G411	G352	C279	U243	A182	U114	U50
G476	A412	G353	C280	G245	C183	C115	G51
		G354		G246	C184	G116	A52
C481	A415	G355	C286	C247	U185	C117	A53
A482	C416	G356	C287	G248	G186	G118	G54
G483	U417	A357	C288	G249	C187	U119	G55
C484	G418	U358	A289	G250	G189	U120	A56
G485	G419		G290	A251	C249	G121	C57
C486	G420	G361	G295	G282	A190	G122	G58
	U421	U362	C296		U191	G123	U59
G491	A422	G363	C297	A256	C192	G124	G60
A492	A423	G363A	G298		U193	G125	G61
G493	G424	G363B	C299		G194	A126	C62
C494	G425	G363C	A299		A195	U127	U63
	U426	C363D	A300		A196	C128	A64
					A197	G129	C65



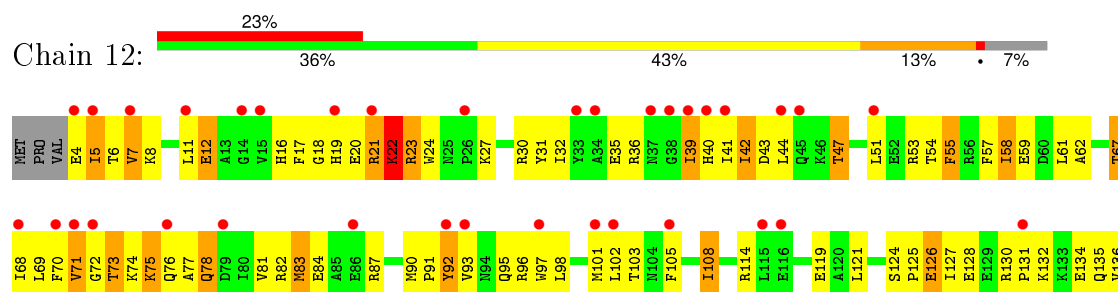
G2421	A2361	C2301	C2240	C2161	G2094	C2026	U1963	A1900	G1824	A1762	G1674	C1548	G2422	G2362	G2302	A2241	C2240	C2161	G2094	C2026	U1963	A1900	G1824	A1762	G1674	C1548
A2422	G2362	G2302	A2241	G2162	C2095	G2027	G1964	A1901	A1825	A1763	C1675	C1549	G2423	G2363	G2303	A2242	C2242	G2163	G2096	G2028	C1965	A1902	A1826	A1764	C1676	C1550
G2424	C2364	G2304	U2243	C2164	G2100	G2029	C1966	G1903	C1827	G1765	A1677	C1551	G2425	G2365	A2305	U2244	G2245	G2165	G2101	G2030	C1967	G1904	G1828	G1766	A1678	G1548
A2426	A2366	G2306	U2245	G2166	G2102	A2031	G1968	G1905	A1829	G1767	U1679	A1554	G2427	G2367	G2307	G2246	G2247	U2167	G2103	G2032	A1869	G1906	C1830	G1768	U1680	A1555
G2428	C2368	G2308	A2247	U2167	G2104	G2033	A1970	G1908	G1831	G1769	G1681	C1556	G2429	C2369	G2309	G2248	A2248	C2168	G2105	U2034	A1971	G1907	C1832	G1770	C1557	A1493
G2430	G2370	A2310	U2249	A2169	C2105	G2035	A1972	C1908	U1832	C1684	U1682	C1558	G2431	G2371	A2311	U2250	G2250	A2170	G2106	G2036	G1973	C1684	G1622	A1494	A1496	A1496
U2431	G2371	G2311	G2250	A2171	C2107	G2036	G1974	G1915	G1835	A1773	C1685	A1497	A2432	G2372	U2312	G2252	G2252	U2172	G2108	C2039	G1975	A1774	G1623	G1560	C1498	A1498
A2433	G2373	G2313	G2253	U2173	U2109	G2040	U1976	U1917	G1838	U1775	C1686	A1499	A2434	C2374	G2314	G2254	G2254	C2174	G2111	U2041	A1978	G1776	G1624	C1561	C1499	G1500
G2435	G2375	G2315	G2255	C2175	G2112	G2042	A1978	U1918	G1839	G1777	U1683	C1562	G2436	A2376	G2316	G2256	G2256	A2176	U2113	A2042	A1979	G1778	G1625	C1563	G1501	C1502
U2437	A2377	G2317	G2257	C2177	U2114	G2043	C1979	A1919	G1840	U1779	U1684	A1566	A2438	A2378	G2318	G2258	G2258	C2178	G2115	G2044	G1980	U1779	G1626	C1564	G1502	G1502
A2439	G2379	G2319	G2258	C2179	G2116	G2045	A1981	G1921	G1842	U1780	U1685	A1567	A2440	G2380	A2320	G2259	G2259	U2180	G2117	G2048	G1982	U1781	G1627	C1565	G1503	G1503
G2441	C2381	G2321	G2260	U2181	G2118	G2049	C1983	U1923	G1843	C1762	C1689	A1568	G2442	G2382	G2322	G2261	G2261	C2182	U2118	G2050	C1984	U1924	A1632	A1507	A1508	A1508
C2443	G2383	A2323	U2262	G2183	U2119	A2051	C1984	U1925	A1847	G1763	G1695	A1509	C2444	G2384	G2324	U2263	U2263	C2184	G2052	G1926	C1925	A1633	A1570	A1510	A1511	A1511
G2445	G2385	G2325	C2264	C2185	G2120	G2053	U1991	A1928	G1849	A1765	G1696	A1512	G2446	C2386	G2326	U2265	U2265	C2186	G1927	G1850	A1766	G1697	A1571	G1512	G1513	G1513
G2447	U2376	A2327	A2266	G2186	G2121	G2054	C1990	A1929	G1851	A1767	U1700	C1574	G2448	G2388	G2328	A2267	A2267	G2190	G2056	G1930	A1853	G1702	C1575	C1575	C1575	C1575
U2449	G2378	G2329	A2268	G2193	G2122	G2056	U1992	A1930	G1852	A1768	U1701	C1576	G2450	G2389	G2330	A2269	A2269	G2193	G2057	G1931	A1854	G1703	C1577	G1517	G1518	G1518
A2451	G2391	U2331	G2270	G2194	U2130	A2059	U1993	A1932	G1855	A1770	U1702	C1577	G2452	G2392	U2332	G2271	G2271	C2205	U2132	A2062	C1996	G1933	A1641	C1578	G1519	G1519
C2452	A2393	A2333	U2272	A2198	U2131	G2060	G1997	C1934	G1857	G1793	U1706	A1580	G2454	A2394	A2334	U2273	A2273	C2206	G1998	C1999	A1859	C1712	G1644	G1520	G1521	G1521
G2454	G2395	G2335	A2274	C2206	U2133	A2063	C1999	A1936	G1860	C1795	U1794	G1581	G2456	G2396	A2336	G2275	G2275	G2210	G2065	A2001	G1938	C1712	G1645	G1522	G1522	G1522
G2455	G2397	G2337	G2276	G2211	A2134	C2064	A2001	A1938	G1861	C1797	U1796	A1582	G2457	G2397	G2337	G2277	G2277	G2211	G2066	G2002	U1939	C1712	G1646	G1523	G1523	G1523
G2458	U2398	G2338	A2278	G2212	C2136	C2066	G2003	U1940	G1862	U1798	U1727	C1526	G2460	G2400	G2339	A2279	A2279	G2213	G2067	G2005	C1941	G1728	G1649	G1527	G1527	G1527
C2461	U2401	G2340	G2280	U2214	C2138	U2068	G2004	C1942	C1870	G1801	U1728	C1527	G2462	G2402	G2342	G2281	G2281	G2215	G2069	U1943	A1872	U1729	G1650	G1528	G1528	G1528
G2463	C2402	G2342	G2282	G2216	C2140	G2070	C2006	U1944	G1878	A1803	G1731	A1529	G2465	G2403	G2343	G2282	G2282	G2216	C2141	C2007	U1944	G1731	G1652	A1530	A1530	A1530
G2466	G2404	U2344	G2283	G2217	U2144	A2071	G2009	U1946	C1879	U1804	A1732	C1531	G2467	G2405	U2345	G2284	G2284	G2217	G2149	A2014	U1951	G1661	G1531	G1531	G1531	G1531
G2468	U2406	G2346	A2285	G2218	C2145	C2072	G2010	C1947	G1883	C1806	G1746	C1533	G2469	G2407	G2347	A2286	A2286	G2218	G2146	G2074	G1948	G1747	G1534	G1534	G1534	G1534
G2470	U2408	G2348	A2287	G2219	G2147	U2075	G1950	C1886	A1884	U1808	G1748	C1535	G2472	G2409	G2349	A2288	A2288	G2220	G2148	U2076	G1951	G1662	G1536	G1536	G1536	G1536
G2475	G2410	G2350	G2289	G2220	G2149	U2079	A2015	U1952	G1888	U1812	C1751	C1538	G2477	G2411	G2351	G2290	G2290	G2221	U2150	U2079	U1953	C1752	G1539	G1539	G1539	G1539
A2476	A2411	G2352	U2291	G2230	G2151	G2080	U2016	A1953	A1889	G1813	C1752	C1539	G2481	G2412	G2353	G2291	G2291	G2231	G2152	G2081	G1954	G1753	G1601	G1540	G1540	G1540
C2477	G2413	G2354	C2282	U2232	G2153	A2082	U1955	C1890	G1891	A1815	C1754	C1541	G2482	G2414	G2355	G2292	G2292	U2233	G2154	G2083	G1956	G1755	G1602	G1541	G1541	G1541
G2481	G2415	G2356	G2295	G2234	G2155	C2084	A2020	C1957	G1892	G1817	C1756	C1542	G2483	G2416	G2357	G2296	G2296	G2235	G2156	G2085	G1958	G1757	G1603	G1543	G1543	G1543
G2485	C2417	U2357	C2297	G2236	G2157	U2086	U2022	G1959	C1895	A1819	G1768	C1544	G2486	G2418	G2359	A2298	A2298	G2237	G2158	G2086	U2023	G1769	G1604	G1544	G1544	G1544
G2487	U2419	G2359	G2299	G2238	A2158	U2092	G2024	A1960	U1898	A1821	C1769	C1545	G2488	G2420	A2360	G2300	G2300	G2239	G2159	G2024	A1961	A1760	G1605	G1545	G1545	G1545
A2488	G2420	A2360	G2300	G2239	G2160	G2093	C2025	C1962	G1899	U1899	C1761	C1547											A1608	G1606	G1546	G1546



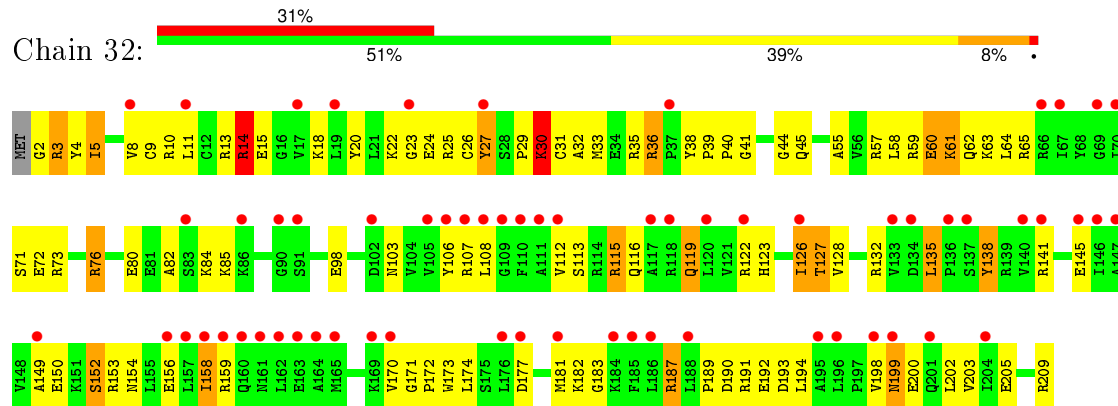
• Molecule 6: 30S ribosomal protein S2



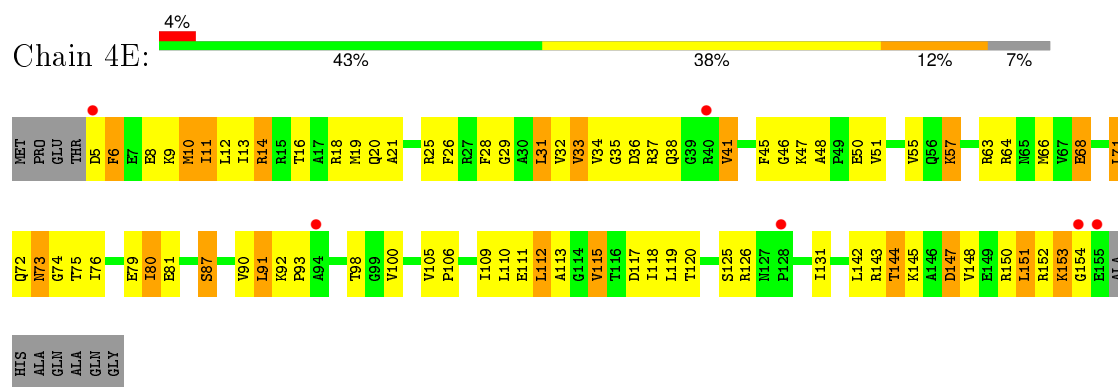
• Molecule 6: 30S ribosomal protein S2



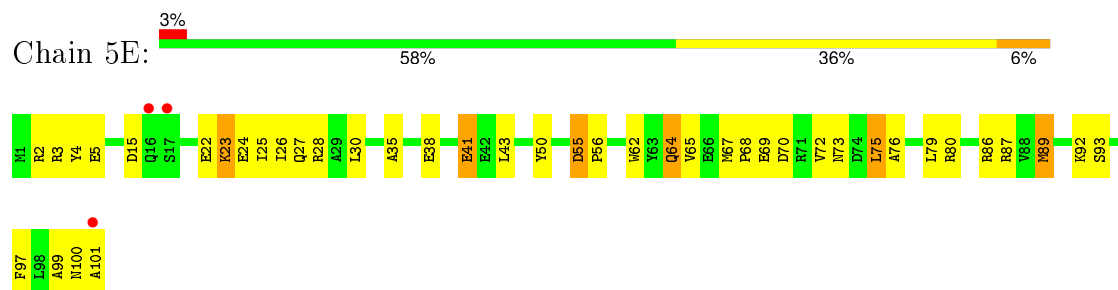
- Molecule 8: 30S ribosomal protein S4



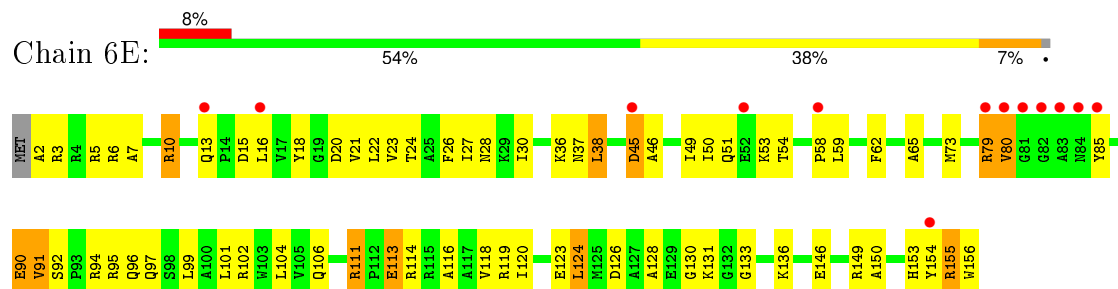
- Molecule 9: 30S ribosomal protein S5



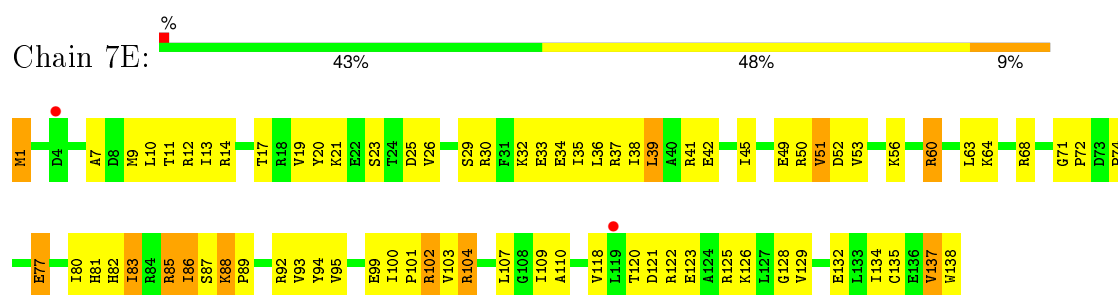
- Molecule 10: 30S ribosomal protein S6



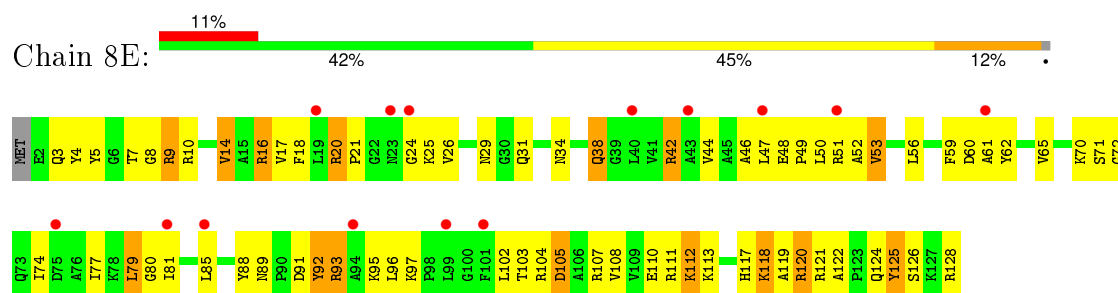
- Molecule 11: 30S ribosomal protein S7



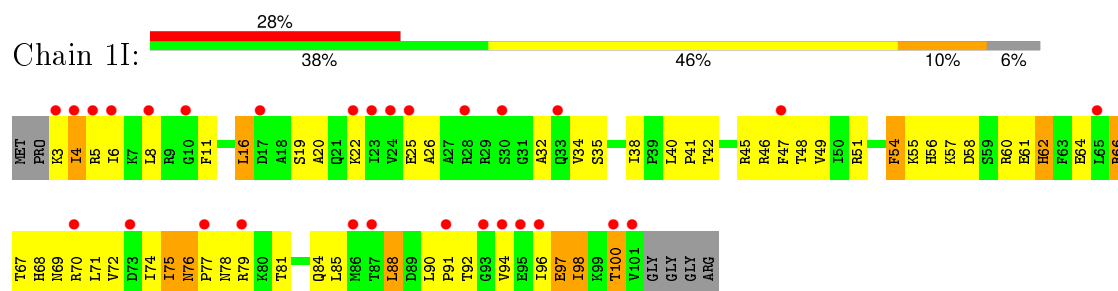
- Molecule 12: 30S ribosomal protein S8



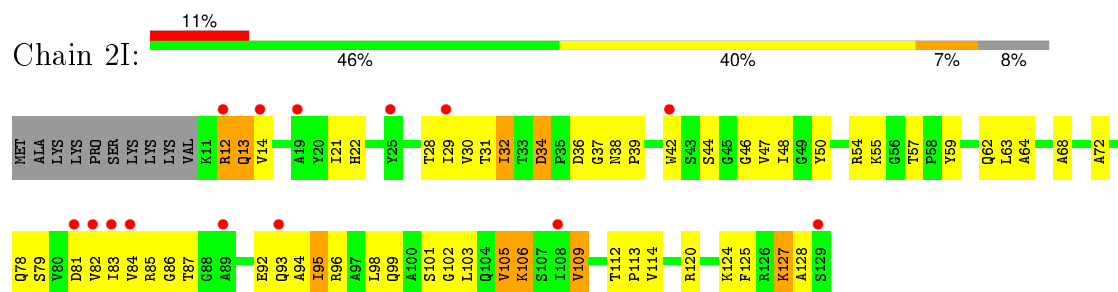
• Molecule 13: 30S ribosomal protein S9



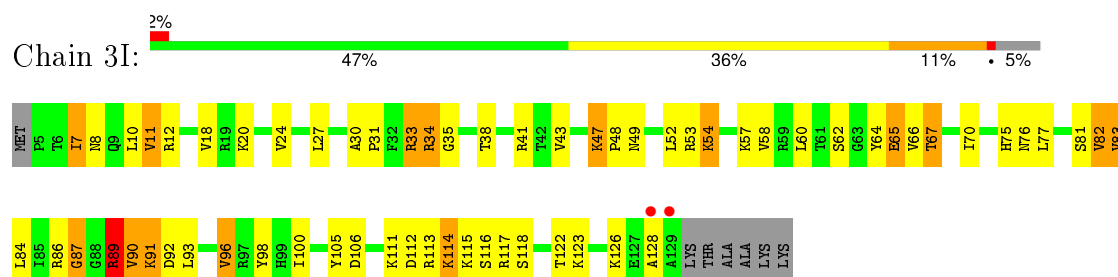
• Molecule 14: 30S ribosomal protein S10



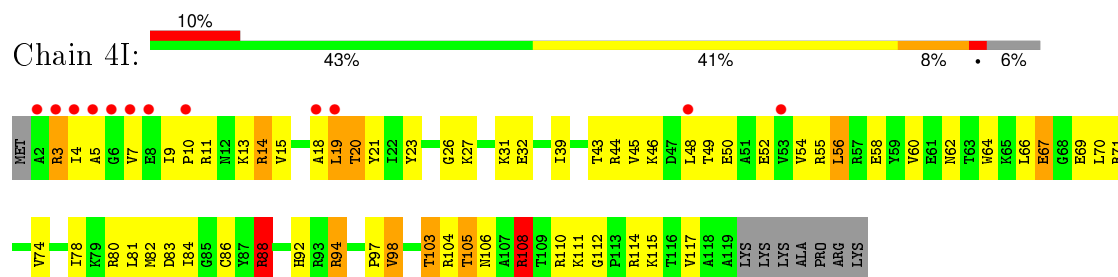
• Molecule 15: 30S ribosomal protein S11



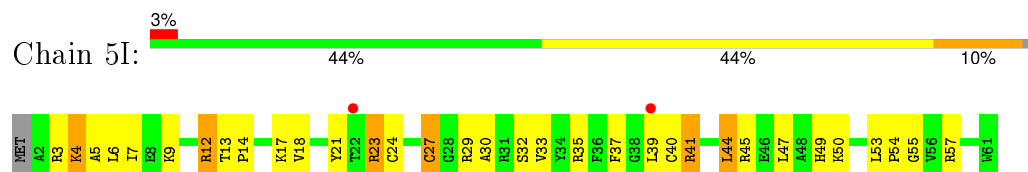
• Molecule 16: 30S ribosomal protein S12



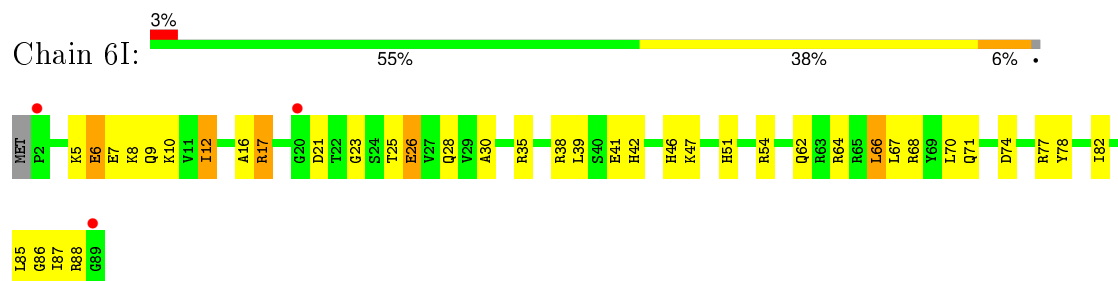
- Molecule 17: 30S ribosomal protein S13



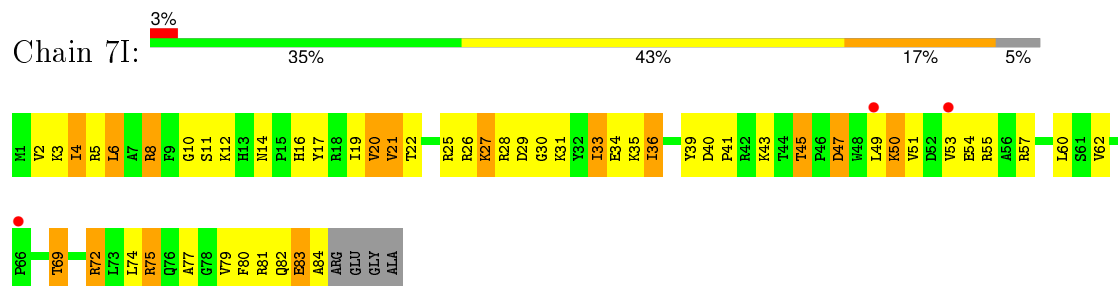
- Molecule 18: 30S ribosomal protein S14 type Z



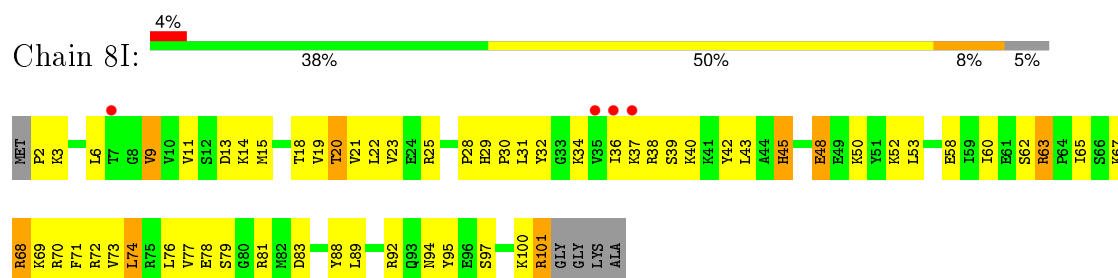
- Molecule 19: 30S ribosomal protein S15



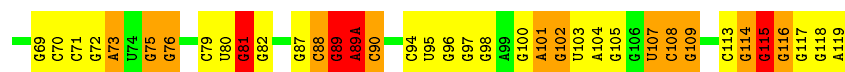
- Molecule 20: 30S ribosomal protein S16



- Molecule 21: 30S ribosomal protein S17



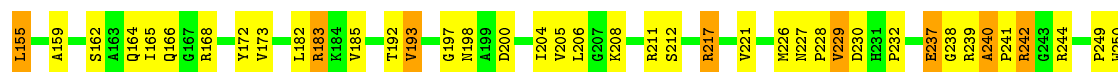
- Molecule 22: 30S ribosomal protein S18



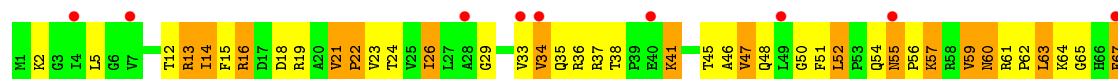
• Molecule 27: 5S ribosomal RNA



• Molecule 28: 50S ribosomal protein L2

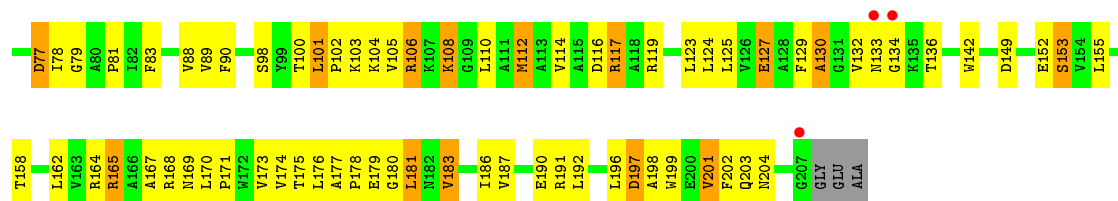


• Molecule 29: 50S ribosomal protein L3

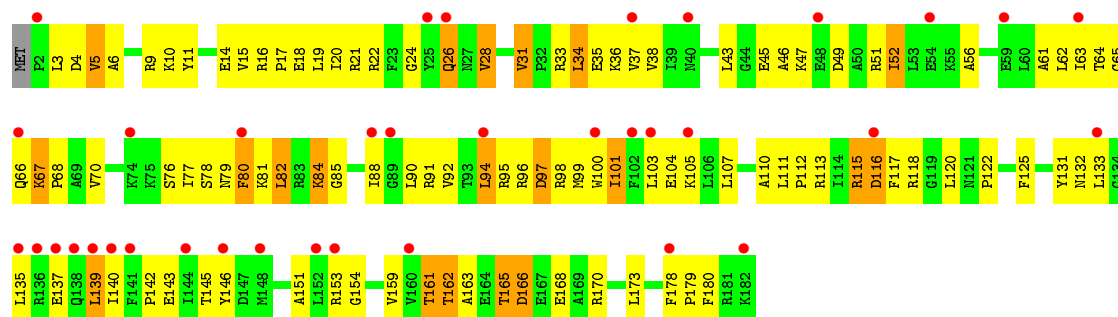


• Molecule 30: 50S ribosomal protein L4

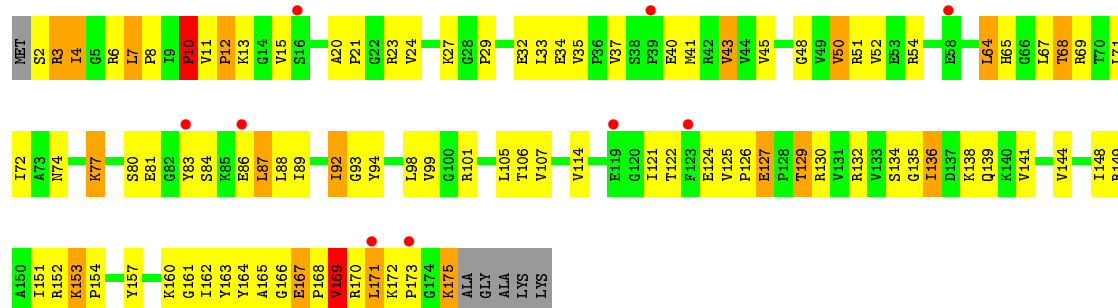
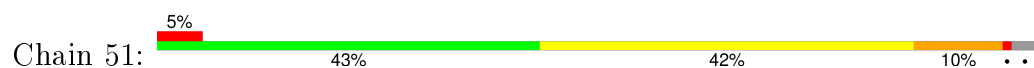




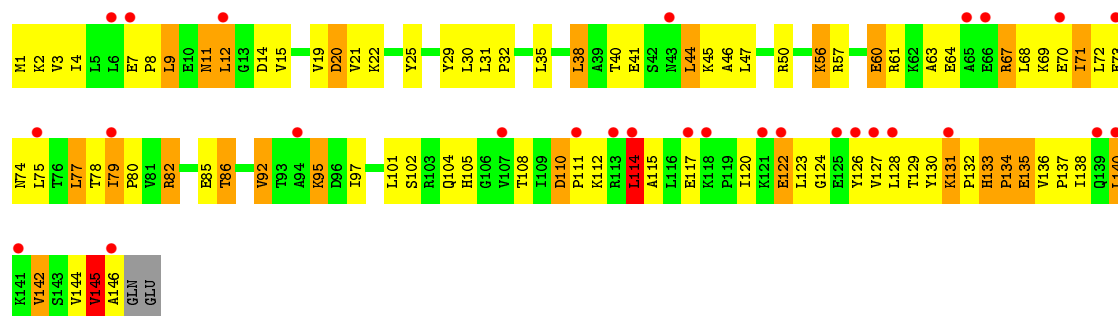
• Molecule 31: 50S ribosomal protein L5



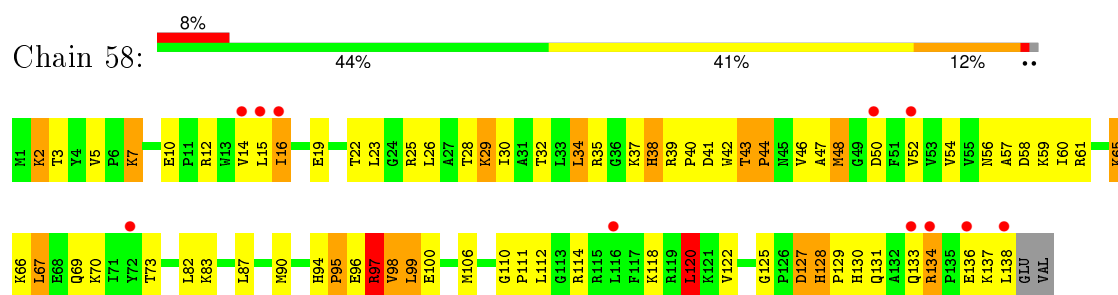
• Molecule 32: 50S ribosomal protein L6



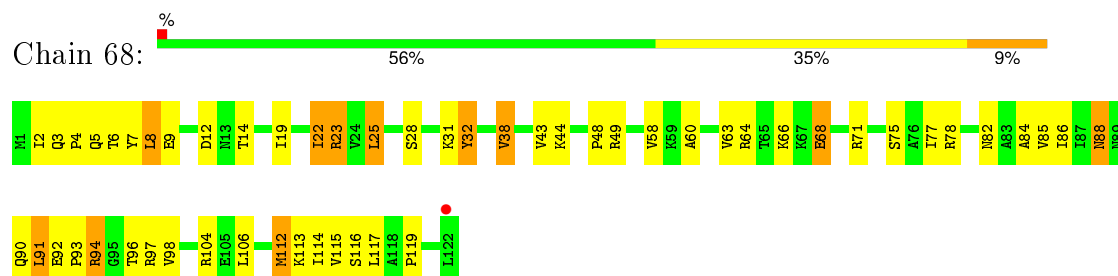
• Molecule 33: 50S ribosomal protein L9



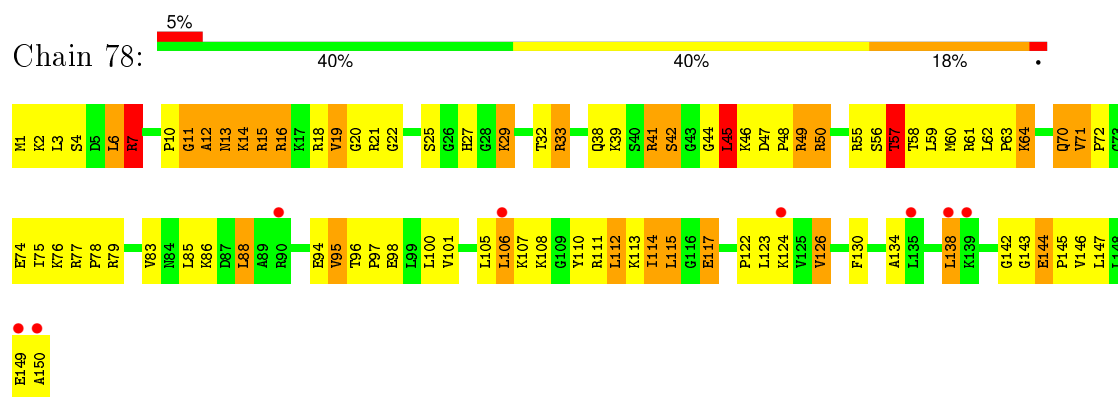
• Molecule 34: 50S ribosomal protein L13



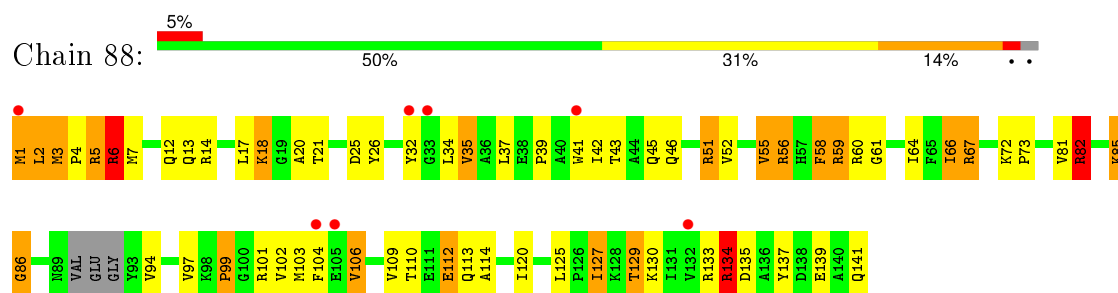
- Molecule 35: 50S ribosomal protein L14



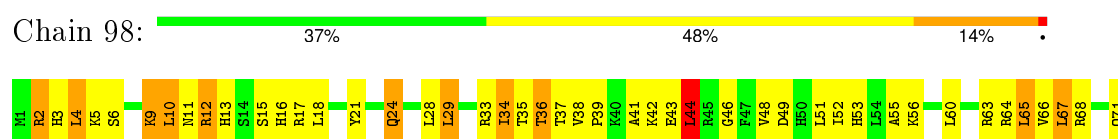
- Molecule 36: 50S ribosomal protein L15



- Molecule 37: 50S ribosomal protein L16

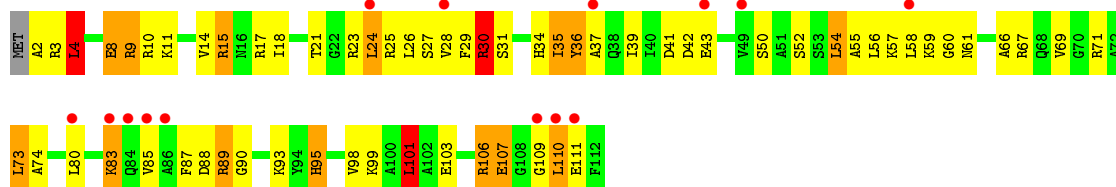


- Molecule 38: 50S ribosomal protein L17

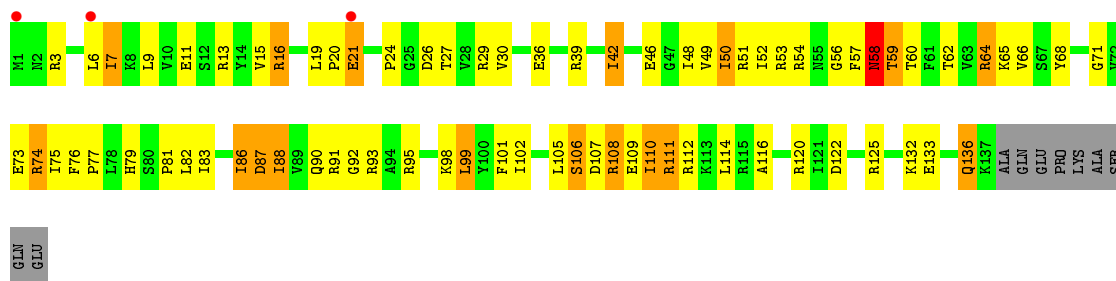




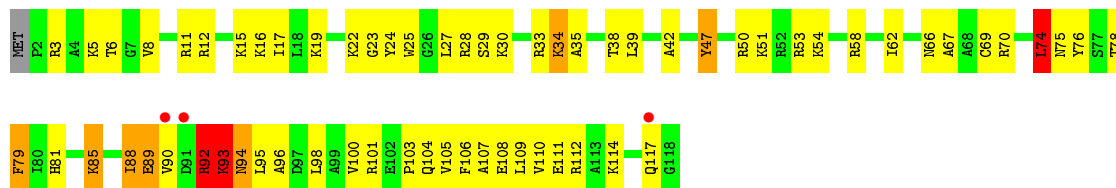
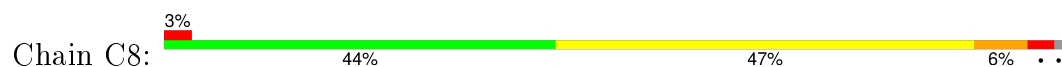
• Molecule 39: 50S ribosomal protein L18



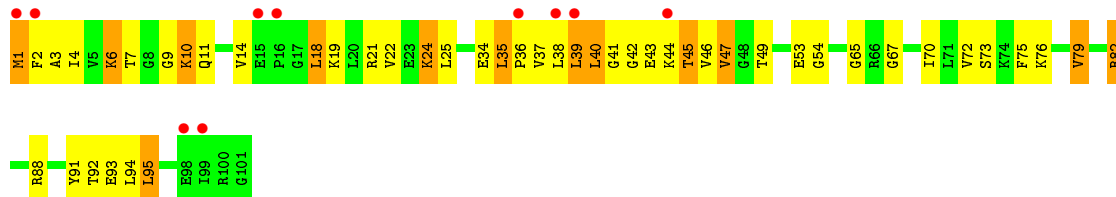
• Molecule 40: 50S ribosomal protein L19



• Molecule 41: 50S ribosomal protein L20

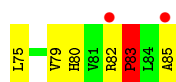


• Molecule 42: 50S ribosomal protein L21

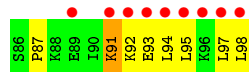
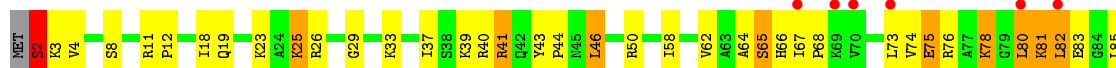


• Molecule 43: 50S ribosomal protein L22

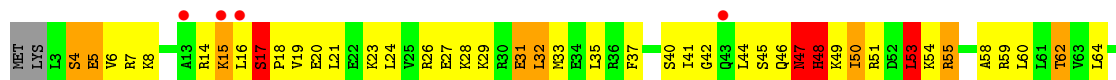




- Molecule 48: 50S ribosomal protein L28



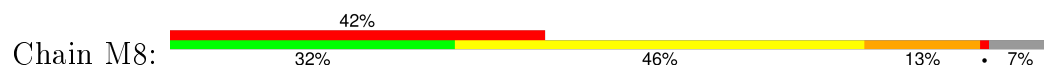
- Molecule 49: 50S ribosomal protein L29



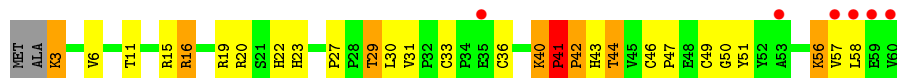
- Molecule 50: 50S ribosomal protein L30



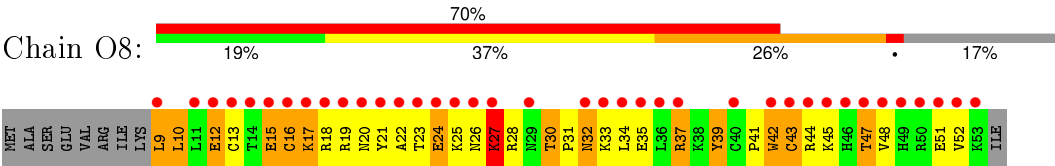
- Molecule 51: 50S ribosomal protein L31



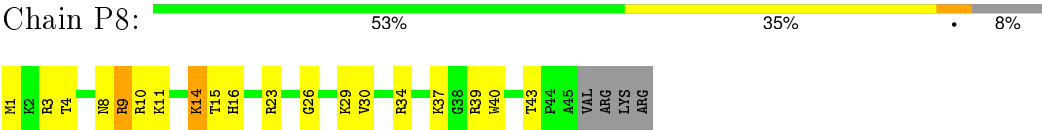
- Molecule 52: 50S ribosomal protein L32



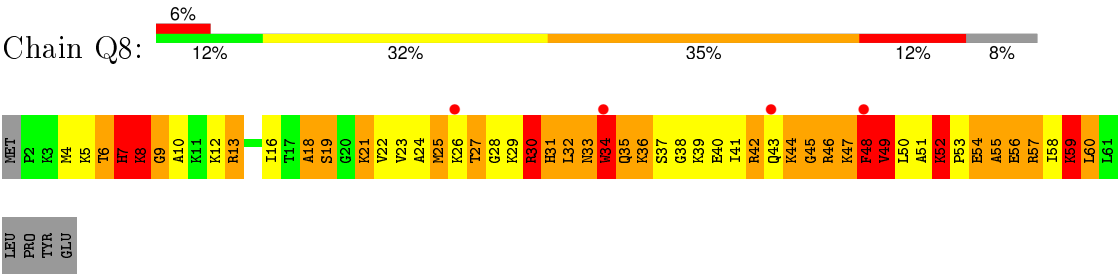
- Molecule 53: 50S ribosomal protein L33



• Molecule 54: 50S ribosomal protein L34



• Molecule 55: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.40 Å 447.70 Å 619.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.96 – 3.05 254.70 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (151.96-3.05) 92.8 (254.70-3.05)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.07 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.193 , 0.231 0.250 , 0.276	Depositor DCC
R_{free} test set	2000 reflections (0.20%)	DCC
Wilson B-factor (Å ²)	88.3	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 77.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 1092032 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	260090	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: OMC, ZN, MIA, MG, H2U, 4SU, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	13	0.87	14/36028 (0.0%)	1.59	679/56231 (1.2%)
1	1G	0.75	2/36025 (0.0%)	1.44	481/56227 (0.9%)
2	1L	0.51	1/1625 (0.1%)	1.02	1/2531 (0.0%)
2	3K	0.57	0/1625	1.17	11/2531 (0.4%)
2	3L	0.63	0/1625	1.20	16/2531 (0.6%)
3	2K	1.02	2/1721 (0.1%)	1.69	42/2682 (1.6%)
3	2L	0.78	1/1721 (0.1%)	1.49	23/2682 (0.9%)
4	4K	1.03	0/313	1.37	4/485 (0.8%)
4	4L	1.26	0/213	1.79	4/329 (1.2%)
5	14	0.99	84/70167 (0.1%)	1.74	2119/109541 (1.9%)
5	1H	1.24	280/70233 (0.4%)	2.01	3566/109643 (3.3%)
6	12	0.40	0/1959	0.68	2/2642 (0.1%)
6	1E	0.48	0/1959	0.74	0/2642
7	22	0.45	0/1636	0.67	1/2205 (0.0%)
7	2E	0.58	0/1629	0.74	0/2195
8	32	0.53	0/1732	0.76	1/2318 (0.0%)
8	3E	0.65	2/1732 (0.1%)	0.80	3/2318 (0.1%)
9	4E	0.62	0/1171	0.81	0/1576
10	5E	0.61	0/855	0.78	0/1154
11	6E	0.56	0/1275	0.70	0/1709
12	7E	0.59	0/1135	0.79	0/1527
13	8E	0.52	0/1028	0.75	1/1379 (0.1%)
14	1I	0.54	0/814	0.75	0/1095
15	2I	0.64	0/899	0.85	1/1213 (0.1%)
16	3I	0.79	0/991	1.03	4/1327 (0.3%)
17	4I	0.59	0/948	0.84	2/1272 (0.2%)
18	5I	0.83	1/500 (0.2%)	0.85	1/664 (0.2%)
19	6I	0.62	0/744	0.84	0/992
20	7I	0.56	0/721	0.77	0/970
21	8I	0.60	0/847	0.77	0/1131
22	9I	0.58	0/595	0.79	0/790
23	AI	0.60	0/661	0.84	0/890

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
24	BI	0.47	0/764	0.73	1/1007 (0.1%)
25	1F	0.52	0/221	0.81	0/288
26	1K	0.56	0/1602	1.16	9/2493 (0.4%)
27	16	0.97	2/2928 (0.1%)	1.87	95/4568 (2.1%)
27	1J	0.80	1/2928 (0.0%)	1.48	31/4568 (0.7%)
28	11	0.96	3/2165 (0.1%)	1.09	6/2919 (0.2%)
29	21	0.78	0/1601	0.99	3/2160 (0.1%)
30	31	0.88	1/1620 (0.1%)	1.02	6/2194 (0.3%)
31	41	0.65	0/1498	0.86	1/2016 (0.0%)
32	51	0.68	0/1362	0.92	3/1841 (0.2%)
33	61	0.59	0/1151	0.83	0/1558
34	58	0.69	0/1131	0.88	1/1525 (0.1%)
35	68	0.75	0/942	0.85	1/1269 (0.1%)
36	78	0.82	0/1161	1.14	3/1544 (0.2%)
37	88	0.94	0/1106	1.13	4/1478 (0.3%)
38	98	0.66	0/981	1.00	1/1312 (0.1%)
39	A8	0.74	0/891	1.05	6/1187 (0.5%)
40	B8	0.77	0/1155	0.92	0/1542
41	C8	0.82	0/981	0.93	1/1306 (0.1%)
42	D8	0.69	0/789	0.93	2/1057 (0.2%)
43	E8	0.77	0/910	0.98	2/1220 (0.2%)
44	F8	1.00	2/756 (0.3%)	1.04	4/1014 (0.4%)
45	G8	0.83	0/804	1.11	6/1073 (0.6%)
46	H8	0.54	0/1427	0.84	1/1935 (0.1%)
47	I8	0.86	0/634	1.01	0/847
48	J8	0.84	0/769	1.03	4/1022 (0.4%)
49	K8	0.99	2/565 (0.4%)	1.16	4/748 (0.5%)
50	L8	0.70	0/457	0.99	1/613 (0.2%)
51	M8	0.58	0/545	0.84	0/733
52	N8	0.69	0/467	0.98	1/632 (0.2%)
53	O8	0.81	1/396 (0.3%)	0.97	0/529
54	P8	0.98	0/399	1.12	1/526 (0.2%)
55	Q8	1.30	3/486 (0.6%)	1.71	9/638 (1.4%)
All	All	0.96	402/280719 (0.1%)	1.64	7169/426784 (1.7%)

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
6	12	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
6	1E	0	3
8	32	0	2
8	3E	0	1
13	8E	0	1
16	3I	0	1
17	4I	0	1
20	7I	0	1
23	AI	0	2
28	11	0	1
29	21	0	3
30	31	0	2
31	41	0	2
33	61	0	4
36	78	0	3
37	88	0	1
38	98	0	1
39	A8	0	1
40	B8	0	1
41	C8	0	1
45	G8	0	4
46	H8	0	2
47	I8	0	2
48	J8	0	1
49	K8	0	2
51	M8	0	1
52	N8	0	2
53	O8	0	3
55	Q8	0	8
All	All	0	58

The worst 5 of 402 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1H	2430	A	N9-C4	-15.74	1.28	1.37
5	1H	774	A	N9-C4	-13.11	1.29	1.37
5	1H	1786	A	N9-C4	-13.10	1.29	1.37
18	5I	27	CYS	CB-SG	-12.07	1.61	1.82
5	14	783	A	N9-C4	-11.82	1.30	1.37

The worst 5 of 7169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1H	1899	G	N3-C4-N9	-27.85	109.29	126.00
5	1H	1786	A	C2-N3-C4	-22.12	99.54	110.60
5	1H	917	A	N1-C2-N3	21.20	139.90	129.30
5	1H	1332	G	N3-C4-N9	-21.08	113.35	126.00
5	1H	1899	G	N3-C4-C5	21.00	139.10	128.60

There are no chirality outliers.

5 of 58 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1E	15	VAL	Peptide
6	1E	169	LYS	Peptide
6	1E	237	ALA	Peptide
8	3E	31	CYS	Peptide
13	8E	110	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	13	32185	0	16244	835	0
1	1G	32182	0	16243	773	1
2	1L	1627	0	842	40	0
2	3K	1627	0	842	51	0
2	3L	1627	0	842	53	0
3	2K	1645	0	845	23	0
3	2L	1645	0	845	38	0
4	4K	279	0	142	6	0
4	4L	191	0	98	8	0
5	14	62647	0	31582	1217	0
5	1H	62707	0	31606	1584	1
6	12	1924	0	1975	116	0
6	1E	1924	0	1975	112	0
7	22	1612	0	1677	87	0
7	2E	1605	0	1668	48	0
8	32	1702	0	1763	87	0
8	3E	1702	0	1763	82	0
9	4E	1155	0	1213	67	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	5E	842	0	857	29	0
11	6E	1256	0	1296	51	0
12	7E	1115	0	1177	61	0
13	8E	1009	0	1037	60	0
14	1I	801	0	849	56	0
15	2I	884	0	904	39	0
16	3I	975	0	1062	47	0
17	4I	938	0	997	54	0
18	5I	491	0	529	28	0
19	6I	733	0	771	32	0
20	7I	705	0	725	50	0
21	8I	834	0	904	58	0
22	9I	590	0	662	25	0
23	AI	647	0	665	50	0
24	BI	762	0	861	35	0
25	1F	217	0	234	19	0
26	1K	1587	0	822	25	0
27	16	2617	0	1328	74	0
27	1J	2617	0	1328	81	0
28	11	2115	0	2195	102	0
29	21	1568	0	1634	92	0
30	31	1585	0	1632	93	0
31	41	1473	0	1535	99	0
32	51	1336	0	1418	73	0
33	61	1136	0	1223	66	0
34	58	1104	0	1180	60	0
35	68	932	0	996	42	0
36	78	1144	0	1228	96	0
37	88	1086	0	1129	57	0
38	98	967	0	1033	61	0
39	A8	881	0	943	61	0
40	B8	1141	0	1202	70	0
41	C8	963	0	1022	68	0
42	D8	778	0	852	39	0
43	E8	899	0	964	30	0
44	F8	742	0	803	46	0
45	G8	791	0	881	61	0
46	H8	1397	0	1430	78	0
47	I8	626	0	642	38	0
48	J8	762	0	848	37	0
49	K8	563	0	612	30	0
50	L8	452	0	503	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	M8	533	0	526	38	0
52	N8	453	0	475	29	0
53	O8	389	0	404	35	0
54	P8	391	0	432	17	0
55	Q8	480	0	549	106	0
56	11	2	0	0	0	0
56	13	149	0	0	0	0
56	14	421	0	0	0	0
56	16	13	0	0	0	0
56	1G	96	0	0	0	0
56	1H	537	0	0	0	0
56	1J	7	0	0	0	0
56	1K	2	0	0	0	0
56	1L	1	0	0	0	0
56	21	2	0	0	0	0
56	2K	8	0	0	0	0
56	2L	4	0	0	0	0
56	3E	2	0	0	0	0
56	3I	1	0	0	0	0
56	3L	3	0	0	0	0
56	41	2	0	0	0	0
56	5E	1	0	0	0	0
56	5I	1	0	0	0	0
56	78	1	0	0	0	0
56	88	2	0	0	0	0
56	I8	1	0	0	0	0
56	J8	1	0	0	0	0
56	L8	1	0	0	0	0
56	P8	1	0	0	0	0
57	14	1	0	0	0	0
57	1G	1	0	0	0	0
57	32	1	0	0	0	0
57	3E	1	0	0	0	0
57	5I	1	0	0	0	0
57	G8	1	0	0	0	0
58	11	9	0	0	3	0
58	13	230	0	0	36	0
58	14	863	0	0	119	0
58	16	21	0	0	3	0
58	1G	106	0	0	22	0
58	1H	1212	0	0	257	0
58	1I	1	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1J	12	0	0	4	0
58	1K	6	0	0	0	0
58	2I	3	0	0	2	0
58	2K	8	0	0	1	0
58	2L	1	0	0	0	0
58	3I	8	0	0	0	0
58	3E	1	0	0	0	0
58	3I	1	0	0	0	0
58	3K	1	0	0	0	0
58	4E	3	0	0	0	0
58	4K	4	0	0	0	0
58	4L	2	0	0	0	0
58	58	3	0	0	0	0
58	5I	1	0	0	0	0
58	6I	1	0	0	0	0
58	78	6	0	0	0	0
58	7I	1	0	0	0	0
58	8E	2	0	0	0	0
58	98	1	0	0	1	0
58	B8	1	0	0	0	0
58	BI	1	0	0	0	0
58	C8	3	0	0	2	0
58	D8	1	0	0	0	0
58	E8	2	0	0	0	0
58	F8	2	0	0	0	0
58	G8	3	0	0	0	0
58	I8	5	0	0	1	0
58	J8	1	0	0	0	0
58	L8	1	0	0	1	0
58	P8	4	0	0	0	0
58	Q8	1	0	0	0	0
All	All	260090	0	157464	7103	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 18.

The worst 5 of 7103 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)
5:1H:567:A:OP1	58:1H:3610:HOH:O	1.72	1.07
5:1H:2714:G:OP2	58:1H:3679:HOH:O	1.74	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1H:987:G:OP2	58:1H:4091:HOH:O	1.74	1.03
36:78:19:VAL:HG12	36:78:21:ARG:H	1.24	1.02
5:1H:945:A:OP1	58:1H:4240:HOH:O	1.80	1.00

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)
5:1H:2137:C:OP1	1:1G:999:U:O2'[4_555]	2.11	0.09

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	
6	12	235/256 (92%)	196 (83%)	35 (15%)	4 (2%)	11	41
6	1E	235/256 (92%)	199 (85%)	33 (14%)	3 (1%)	15	48
7	22	204/239 (85%)	185 (91%)	19 (9%)	0	100	100
7	2E	203/239 (85%)	182 (90%)	21 (10%)	0	100	100
8	32	206/209 (99%)	181 (88%)	23 (11%)	2 (1%)	19	56
8	3E	206/209 (99%)	186 (90%)	18 (9%)	2 (1%)	19	56
9	4E	149/162 (92%)	138 (93%)	10 (7%)	1 (1%)	26	64
10	5E	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
11	6E	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
12	7E	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	26	64
13	8E	125/128 (98%)	105 (84%)	20 (16%)	0	100	100
14	1I	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
15	2I	117/129 (91%)	102 (87%)	14 (12%)	1 (1%)	21	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	3I	123/132 (93%)	103 (84%)	20 (16%)	0	100	100
17	4I	116/126 (92%)	97 (84%)	18 (16%)	1 (1%)	21	58
18	5I	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	5	23
19	6I	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
20	7I	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
21	8I	98/105 (93%)	94 (96%)	4 (4%)	0	100	100
22	9I	70/88 (80%)	60 (86%)	8 (11%)	2 (3%)	6	27
23	AI	79/93 (85%)	66 (84%)	9 (11%)	4 (5%)	2	14
24	BI	97/106 (92%)	80 (82%)	17 (18%)	0	100	100
25	1F	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
28	11	270/276 (98%)	252 (93%)	15 (6%)	3 (1%)	17	53
29	21	203/206 (98%)	164 (81%)	29 (14%)	10 (5%)	3	15
30	31	200/210 (95%)	182 (91%)	16 (8%)	2 (1%)	19	56
31	41	179/182 (98%)	156 (87%)	20 (11%)	3 (2%)	11	41
32	51	172/180 (96%)	143 (83%)	22 (13%)	7 (4%)	3	19
33	61	144/148 (97%)	117 (81%)	24 (17%)	3 (2%)	9	35
34	58	136/140 (97%)	117 (86%)	15 (11%)	4 (3%)	6	27
35	68	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
36	78	148/150 (99%)	116 (78%)	27 (18%)	5 (3%)	5	23
37	88	134/141 (95%)	110 (82%)	20 (15%)	4 (3%)	5	26
38	98	116/118 (98%)	100 (86%)	15 (13%)	1 (1%)	21	58
39	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	21	58
40	B8	135/146 (92%)	120 (89%)	14 (10%)	1 (1%)	26	64
41	C8	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	7	29
42	D8	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	19	56
43	E8	111/113 (98%)	101 (91%)	10 (9%)	0	100	100
44	F8	92/96 (96%)	83 (90%)	7 (8%)	2 (2%)	8	34
45	G8	102/110 (93%)	80 (78%)	16 (16%)	6 (6%)	2	11
46	H8	173/206 (84%)	141 (82%)	24 (14%)	8 (5%)	3	16
47	I8	78/85 (92%)	66 (85%)	11 (14%)	1 (1%)	15	48
48	J8	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	9	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	K8	65/72 (90%)	57 (88%)	6 (9%)	2 (3%)	5	25
50	L8	55/60 (92%)	50 (91%)	4 (7%)	1 (2%)	11	39
51	M8	64/71 (90%)	40 (62%)	22 (34%)	2 (3%)	5	25
52	N8	56/60 (93%)	46 (82%)	8 (14%)	2 (4%)	4	22
53	O8	43/54 (80%)	28 (65%)	13 (30%)	2 (5%)	3	16
54	P8	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
55	Q8	58/65 (89%)	33 (57%)	19 (33%)	6 (10%)	1	3
All	All	6312/6731 (94%)	5477 (87%)	730 (12%)	105 (2%)	11	41

5 of 105 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	21	83	ASP
32	51	169	VAL
36	78	57	THR
45	G8	54	LYS
49	K8	48	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	12	205/220 (93%)	155 (76%)	50 (24%)	1	2
6	1E	205/220 (93%)	157 (77%)	48 (23%)	1	3
7	22	160/188 (85%)	130 (81%)	30 (19%)	2	7
7	2E	159/188 (85%)	131 (82%)	28 (18%)	2	9
8	32	180/181 (99%)	149 (83%)	31 (17%)	2	10
8	3E	180/181 (99%)	143 (79%)	37 (21%)	1	6
9	4E	116/123 (94%)	87 (75%)	29 (25%)	1	2
10	5E	90/90 (100%)	79 (88%)	11 (12%)	6	22
11	6E	126/127 (99%)	101 (80%)	25 (20%)	1	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	7E	119/119 (100%)	98 (82%)	21 (18%)	2	9
13	8E	98/99 (99%)	74 (76%)	24 (24%)	1	2
14	1I	89/92 (97%)	71 (80%)	18 (20%)	1	6
15	2I	90/99 (91%)	76 (84%)	14 (16%)	3	13
16	3I	104/109 (95%)	83 (80%)	21 (20%)	1	6
17	4I	94/101 (93%)	70 (74%)	24 (26%)	1	2
18	5I	49/50 (98%)	41 (84%)	8 (16%)	3	11
19	6I	79/80 (99%)	67 (85%)	12 (15%)	3	14
20	7I	72/74 (97%)	54 (75%)	18 (25%)	1	2
21	8I	95/97 (98%)	79 (83%)	16 (17%)	2	10
22	9I	63/77 (82%)	58 (92%)	5 (8%)	15	46
23	AI	70/80 (88%)	50 (71%)	20 (29%)	0	1
24	BI	76/82 (93%)	60 (79%)	16 (21%)	1	5
25	1F	20/22 (91%)	19 (95%)	1 (5%)	30	66
28	11	214/218 (98%)	169 (79%)	45 (21%)	1	5
29	21	165/166 (99%)	125 (76%)	40 (24%)	1	3
30	31	161/166 (97%)	127 (79%)	34 (21%)	1	5
31	41	155/156 (99%)	125 (81%)	30 (19%)	2	7
32	51	145/148 (98%)	110 (76%)	35 (24%)	1	3
33	61	122/124 (98%)	87 (71%)	35 (29%)	0	1
34	58	117/119 (98%)	92 (79%)	25 (21%)	1	5
35	68	100/100 (100%)	85 (85%)	15 (15%)	3	14
36	78	116/116 (100%)	82 (71%)	34 (29%)	0	1
37	88	104/111 (94%)	75 (72%)	29 (28%)	0	1
38	98	101/101 (100%)	72 (71%)	29 (29%)	0	1
39	A8	87/88 (99%)	68 (78%)	19 (22%)	1	5
40	B8	120/127 (94%)	93 (78%)	27 (22%)	1	4
41	C8	93/94 (99%)	76 (82%)	17 (18%)	2	8
42	D8	82/82 (100%)	63 (77%)	19 (23%)	1	3
43	E8	92/92 (100%)	71 (77%)	21 (23%)	1	4
44	F8	76/78 (97%)	61 (80%)	15 (20%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	G8	85/91 (93%)	56 (66%)	29 (34%)	0	0
46	H8	154/179 (86%)	114 (74%)	40 (26%)	0	2
47	I8	61/67 (91%)	47 (77%)	14 (23%)	1	4
48	J8	82/83 (99%)	65 (79%)	17 (21%)	1	6
49	K8	62/67 (92%)	39 (63%)	23 (37%)	0	0
50	L8	49/52 (94%)	40 (82%)	9 (18%)	2	8
51	M8	59/63 (94%)	42 (71%)	17 (29%)	0	1
52	N8	51/52 (98%)	37 (72%)	14 (28%)	0	1
53	O8	44/52 (85%)	31 (70%)	13 (30%)	0	1
54	P8	38/42 (90%)	32 (84%)	6 (16%)	3	12
55	Q8	50/55 (91%)	31 (62%)	19 (38%)	0	0
All	All	5324/5588 (95%)	4147 (78%)	1177 (22%)	1	4

5 of 1177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	41	84	LYS
36	78	13	ASN
6	12	76	GLN
32	51	10	PRO
33	61	82	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
23	AI	56	GLN
29	21	135	HIS
47	I8	29	GLN
15	2I	93	GLN
44	F8	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1495/1522 (98%)	353 (23%)	38 (2%)
1	1G	1495/1522 (98%)	374 (25%)	37 (2%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1L	74/76 (97%)	32 (43%)	3 (4%)
2	3K	74/76 (97%)	36 (48%)	5 (6%)
2	3L	74/76 (97%)	32 (43%)	1 (1%)
26	1K	70/76 (92%)	32 (45%)	2 (2%)
27	16	121/122 (99%)	26 (21%)	3 (2%)
27	1J	121/122 (99%)	31 (25%)	3 (2%)
3	2K	76/77 (98%)	15 (19%)	2 (2%)
3	2L	76/77 (98%)	17 (22%)	3 (3%)
4	4K	12/30 (40%)	2 (16%)	0
4	4L	9/30 (30%)	4 (44%)	2 (22%)
5	14	2908/2917 (99%)	754 (25%)	46 (1%)
5	1H	2911/2917 (99%)	685 (23%)	62 (2%)
All	All	9516/9640 (98%)	2393 (25%)	207 (2%)

5 of 2393 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	5	U
1	13	6	G
1	13	7	G
1	13	8	A
1	13	9	G

5 of 207 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1K	10	G
5	1H	685	A
1	1G	812	C
3	2K	48	U
5	1H	196	A

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

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

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

the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	H2U	1K	16	26	17,21,22	2.55	5 (29%)	23,30,33	2.95	6 (26%)
26	PSU	1K	32	26,56	15,21,22	1.08	2 (13%)	16,30,33	2.02	3 (18%)
26	MIA	1K	37	26	22,31,32	0.97	1 (4%)	26,44,47	1.58	5 (19%)
26	PSU	1K	39	26	15,21,22	0.90	1 (6%)	16,30,33	2.15	4 (25%)
26	7MG	1K	46	26	20,26,27	3.35	6 (30%)	23,39,42	2.28	7 (30%)
26	PSU	1K	55	26	15,21,22	1.10	1 (6%)	16,30,33	2.20	3 (18%)
26	4SU	1K	8	26	12,21,22	3.13	2 (16%)	15,30,33	1.10	1 (6%)
2	H2U	1L	16	2	17,21,22	2.33	5 (29%)	23,30,33	3.03	6 (26%)
2	H2U	1L	20	2	17,21,22	2.23	4 (23%)	23,30,33	2.71	5 (21%)
2	PSU	1L	32	2	15,21,22	1.27	2 (13%)	16,30,33	2.40	4 (25%)
2	MIA	1L	37	2	22,31,32	1.30	2 (9%)	26,44,47	1.66	5 (19%)
2	PSU	1L	39	2	15,21,22	1.12	1 (6%)	16,30,33	2.07	3 (18%)
2	7MG	1L	46	2	20,26,27	3.34	5 (25%)	23,39,42	2.13	7 (30%)
2	PSU	1L	55	2	15,21,22	1.29	1 (6%)	16,30,33	2.24	2 (12%)
2	4SU	1L	8	2	12,21,22	3.15	2 (16%)	15,30,33	1.41	1 (6%)
3	H2U	2K	21	3	17,21,22	2.80	3 (17%)	23,30,33	2.76	5 (21%)
3	OMC	2K	33	3	15,22,23	2.29	4 (26%)	20,31,34	2.18	3 (15%)
3	7MG	2K	47	3	20,26,27	3.28	6 (30%)	23,39,42	2.03	5 (21%)
3	PSU	2K	56	3	15,21,22	1.24	2 (13%)	16,30,33	1.91	2 (12%)
3	4SU	2K	8	3	12,21,22	3.35	2 (16%)	15,30,33	1.07	1 (6%)
3	H2U	2L	21	3	17,21,22	2.21	4 (23%)	23,30,33	2.59	4 (17%)
3	OMC	2L	33	3	15,22,23	2.15	4 (26%)	20,31,34	2.00	3 (15%)
3	7MG	2L	47	3	20,26,27	3.19	5 (25%)	23,39,42	2.10	5 (21%)
3	PSU	2L	56	3	15,21,22	1.30	1 (6%)	16,30,33	1.95	3 (18%)
3	4SU	2L	8	3	12,21,22	3.57	2 (16%)	15,30,33	0.81	1 (6%)
2	H2U	3K	16	2	17,21,22	2.27	4 (23%)	23,30,33	2.86	5 (21%)
2	H2U	3K	20	2	17,21,22	2.29	4 (23%)	23,30,33	2.88	5 (21%)
2	PSU	3K	32	2	15,21,22	1.14	1 (6%)	16,30,33	1.95	5 (31%)
2	MIA	3K	37	2	22,31,32	1.49	2 (9%)	26,44,47	3.35	4 (15%)
2	PSU	3K	39	2	15,21,22	1.17	1 (6%)	16,30,33	2.17	3 (18%)
2	7MG	3K	46	2	20,26,27	3.32	5 (25%)	23,39,42	2.23	7 (30%)
2	PSU	3K	55	2	15,21,22	1.13	3 (20%)	16,30,33	2.03	4 (25%)
2	4SU	3K	8	2	12,21,22	3.34	2 (16%)	15,30,33	0.99	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	H2U	3L	16	2	17,21,22	2.24	4 (23%)	23,30,33	2.72	4 (17%)
2	H2U	3L	20	2	17,21,22	2.31	4 (23%)	23,30,33	3.10	6 (26%)
2	PSU	3L	32	2	15,21,22	1.26	1 (6%)	16,30,33	1.91	4 (25%)
2	MIA	3L	37	2	22,31,32	1.80	2 (9%)	26,44,47	3.27	5 (19%)
2	PSU	3L	39	2	15,21,22	1.17	1 (6%)	16,30,33	2.01	2 (12%)
2	7MG	3L	46	2	20,26,27	3.41	5 (25%)	23,39,42	2.16	6 (26%)
2	PSU	3L	55	2	15,21,22	0.97	1 (6%)	16,30,33	1.85	3 (18%)
2	4SU	3L	8	2	12,21,22	3.32	2 (16%)	15,30,33	1.32	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	H2U	1K	16	26	-	0/7/38/39	0/2/2/2
26	PSU	1K	32	26,56	-	0/7/25/26	0/2/2/2
26	MIA	1K	37	26	-	0/11/33/34	0/3/3/3
26	PSU	1K	39	26	-	0/7/25/26	0/2/2/2
26	7MG	1K	46	26	-	0/7/37/38	0/3/3/3
26	PSU	1K	55	26	-	0/7/25/26	0/2/2/2
26	4SU	1K	8	26	-	0/3/25/26	0/2/2/2
2	H2U	1L	16	2	-	0/7/38/39	0/2/2/2
2	H2U	1L	20	2	-	0/7/38/39	0/2/2/2
2	PSU	1L	32	2	-	1/7/25/26	0/2/2/2
2	MIA	1L	37	2	-	2/11/33/34	0/3/3/3
2	PSU	1L	39	2	-	0/7/25/26	0/2/2/2
2	7MG	1L	46	2	-	0/7/37/38	0/3/3/3
2	PSU	1L	55	2	-	0/7/25/26	0/2/2/2
2	4SU	1L	8	2	-	0/3/25/26	0/2/2/2
3	H2U	2K	21	3	-	0/7/38/39	0/2/2/2
3	OMC	2K	33	3	-	0/5/27/28	0/2/2/2
3	7MG	2K	47	3	-	0/7/37/38	0/3/3/3
3	PSU	2K	56	3	-	0/7/25/26	0/2/2/2
3	4SU	2K	8	3	-	0/3/25/26	0/2/2/2
3	H2U	2L	21	3	-	0/7/38/39	0/2/2/2
3	OMC	2L	33	3	-	0/5/27/28	0/2/2/2
3	7MG	2L	47	3	-	0/7/37/38	0/3/3/3
3	PSU	2L	56	3	-	0/7/25/26	0/2/2/2
3	4SU	2L	8	3	-	0/3/25/26	0/2/2/2
2	H2U	3K	16	2	-	0/7/38/39	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	H2U	3K	20	2	-	0/7/38/39	0/2/2/2
2	PSU	3K	32	2	-	0/7/25/26	0/2/2/2
2	MIA	3K	37	2	-	0/11/33/34	0/3/3/3
2	PSU	3K	39	2	-	0/7/25/26	0/2/2/2
2	7MG	3K	46	2	-	0/7/37/38	0/3/3/3
2	PSU	3K	55	2	-	0/7/25/26	0/2/2/2
2	4SU	3K	8	2	-	0/3/25/26	0/2/2/2
2	H2U	3L	16	2	-	0/7/38/39	0/2/2/2
2	H2U	3L	20	2	-	0/7/38/39	0/2/2/2
2	PSU	3L	32	2	-	0/7/25/26	0/2/2/2
2	MIA	3L	37	2	-	0/11/33/34	0/3/3/3
2	PSU	3L	39	2	-	0/7/25/26	0/2/2/2
2	7MG	3L	46	2	-	0/7/37/38	0/3/3/3
2	PSU	3L	55	2	-	0/7/25/26	0/2/2/2
2	4SU	3L	8	2	-	0/3/25/26	0/2/2/2

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1K	46	7MG	C5-C4	-5.65	1.24	1.39
2	3L	46	7MG	C5-C4	-5.60	1.24	1.39
2	1L	46	7MG	C5-C4	-5.58	1.24	1.39
3	2K	47	7MG	C5-C4	-5.46	1.24	1.39
2	3K	46	7MG	C5-C4	-5.39	1.24	1.39

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1K	46	7MG	C5-C4-N3	-6.94	119.67	126.74
2	3K	46	7MG	C5-C4-N3	-6.89	119.72	126.74
2	1L	20	H2U	C4-N3-C2	-6.42	119.95	125.77
2	3L	46	7MG	C5-C4-N3	-6.28	120.34	126.74
3	2K	47	7MG	C5-C4-N3	-6.21	120.41	126.74

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1L	37	MIA	N1-C2-S10-C11
2	1L	37	MIA	N3-C2-S10-C11
2	1L	32	PSU	O4'-C1'-C5-C4

There are no ring outliers.

26 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	1K	16	H2U	1	0
26	1K	37	MIA	1	0
26	1K	46	7MG	1	0
26	1K	8	4SU	1	0
2	1L	16	H2U	1	0
2	1L	37	MIA	1	0
2	1L	39	PSU	3	0
2	1L	46	7MG	2	0
2	1L	55	PSU	1	0
2	1L	8	4SU	4	0
3	2K	47	7MG	5	0
3	2K	8	4SU	1	0
3	2L	33	OMC	3	0
3	2L	47	7MG	2	0
3	2L	56	PSU	2	0
3	2L	8	4SU	2	0
2	3K	20	H2U	1	0
2	3K	37	MIA	4	0
2	3K	39	PSU	1	0
2	3K	55	PSU	3	0
2	3L	16	H2U	1	0
2	3L	20	H2U	4	0
2	3L	37	MIA	2	0
2	3L	46	7MG	2	0
2	3L	55	PSU	1	0
2	3L	8	4SU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1265 ligands modelled in this entry, 1265 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	13	1497/1522 (98%)	-0.47	1 (0%) 95 91	62, 106, 190, 319	0
1	1G	1497/1522 (98%)	-0.38	20 (1%) 79 59	78, 126, 199, 313	0
2	1L	68/76 (89%)	0.30	7 (10%) 9 3	144, 237, 271, 321	0
2	3K	68/76 (89%)	0.35	7 (10%) 9 3	76, 227, 273, 285	0
2	3L	68/76 (89%)	-0.22	2 (2%) 55 29	95, 217, 254, 268	0
3	2K	72/77 (93%)	-0.42	0 100 100	74, 96, 125, 136	0
3	2L	72/77 (93%)	-0.76	0 100 100	87, 122, 154, 170	0
4	4K	13/30 (43%)	-0.40	0 100 100	74, 92, 138, 142	0
4	4L	9/30 (30%)	-0.28	0 100 100	104, 111, 123, 125	0
5	14	2909/2917 (99%)	-0.34	57 (1%) 68 44	59, 96, 254, 399	0
5	1H	2912/2917 (99%)	-0.09	53 (1%) 71 47	45, 78, 243, 371	0
6	12	237/256 (92%)	1.33	59 (24%) 1 0	143, 177, 205, 218	0
6	1E	237/256 (92%)	0.75	43 (18%) 2 1	114, 148, 178, 191	0
7	22	206/239 (86%)	1.52	59 (28%) 1 0	139, 159, 187, 204	0
7	2E	205/239 (85%)	0.42	16 (7%) 16 5	92, 114, 150, 155	0
8	32	208/209 (99%)	1.44	64 (30%) 1 0	103, 127, 150, 155	0
8	3E	208/209 (99%)	0.03	10 (4%) 34 15	87, 115, 142, 155	0
9	4E	151/162 (93%)	0.22	6 (3%) 42 19	82, 104, 128, 177	0
10	5E	101/101 (100%)	0.53	3 (2%) 54 27	85, 108, 131, 146	0
11	6E	155/156 (99%)	0.53	13 (8%) 14 5	104, 120, 156, 189	0
12	7E	138/138 (100%)	0.23	2 (1%) 78 57	98, 116, 128, 138	0
13	8E	127/128 (99%)	0.68	14 (11%) 7 2	91, 137, 163, 179	0
14	1I	99/105 (94%)	1.16	29 (29%) 1 0	86, 134, 171, 177	0
15	2I	119/129 (92%)	0.77	14 (11%) 6 2	79, 110, 145, 183	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
16	3I	125/132 (94%)	-0.18	2 (1%) 74 52	73, 84, 121, 204	0
17	4I	118/126 (93%)	0.50	12 (10%) 9 3	85, 123, 147, 162	0
18	5I	60/61 (98%)	0.31	2 (3%) 50 24	91, 103, 123, 133	0
19	6I	88/89 (98%)	0.22	3 (3%) 49 23	85, 109, 123, 143	0
20	7I	84/88 (95%)	0.01	3 (3%) 46 21	108, 119, 153, 170	0
21	8I	100/105 (95%)	-0.12	4 (4%) 42 19	96, 114, 125, 129	0
22	9I	72/88 (81%)	1.21	13 (18%) 2 1	93, 111, 145, 177	0
23	AI	81/93 (87%)	0.33	3 (3%) 45 21	99, 123, 149, 161	0
24	BI	99/106 (93%)	-0.03	0 100 100	113, 127, 166, 172	0
25	1F	25/27 (92%)	-0.05	0 100 100	99, 111, 125, 154	0
26	1K	67/76 (88%)	-0.01	2 (2%) 54 27	92, 192, 262, 271	0
27	16	122/122 (100%)	-0.27	2 (1%) 74 52	73, 96, 118, 204	0
27	1J	122/122 (100%)	-0.43	0 100 100	94, 140, 168, 212	0
28	11	272/276 (98%)	0.11	1 (0%) 93 84	46, 70, 87, 96	0
29	21	205/206 (99%)	0.53	22 (10%) 8 2	56, 97, 145, 164	0
30	31	202/210 (96%)	0.31	11 (5%) 29 12	52, 80, 120, 139	0
31	41	181/182 (99%)	1.02	36 (19%) 1 0	84, 107, 142, 155	0
32	51	174/180 (96%)	0.39	9 (5%) 31 13	86, 110, 126, 154	0
33	61	146/148 (98%)	1.04	28 (19%) 2 0	81, 136, 154, 161	0
34	58	138/140 (98%)	0.52	11 (7%) 15 5	71, 96, 137, 154	0
35	68	122/122 (100%)	0.17	1 (0%) 87 72	64, 83, 101, 116	0
36	78	150/150 (100%)	0.32	8 (5%) 30 12	51, 84, 109, 169	0
37	88	138/141 (97%)	0.29	7 (5%) 32 13	58, 84, 104, 139	0
38	98	118/118 (100%)	0.06	0 100 100	70, 90, 114, 121	0
39	A8	111/112 (99%)	0.77	14 (12%) 5 2	78, 94, 125, 141	0
40	B8	137/146 (93%)	0.04	3 (2%) 65 40	79, 99, 157, 179	0
41	C8	117/118 (99%)	0.16	3 (2%) 59 33	60, 83, 118, 150	0
42	D8	101/101 (100%)	0.70	10 (9%) 9 3	63, 106, 143, 159	0
43	E8	113/113 (100%)	0.40	4 (3%) 48 22	64, 80, 116, 169	0
44	F8	94/96 (97%)	0.34	3 (3%) 51 25	59, 75, 98, 115	0
45	G8	104/110 (94%)	0.36	1 (0%) 84 66	76, 98, 138, 169	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
46	H8	175/206 (84%)	0.83	24 (13%) 4 1	88, 128, 212, 220	0
47	I8	80/85 (94%)	0.36	4 (5%) 32 13	61, 76, 110, 122	0
48	J8	97/98 (98%)	0.77	15 (15%) 3 1	57, 77, 129, 175	0
49	K8	67/72 (93%)	0.29	4 (5%) 25 10	66, 84, 101, 143	0
50	L8	57/60 (95%)	0.34	2 (3%) 48 22	66, 85, 111, 117	0
51	M8	66/71 (92%)	2.18	30 (45%) 0 0	119, 163, 218, 238	0
52	N8	58/60 (96%)	0.87	6 (10%) 9 3	57, 104, 195, 203	0
53	O8	45/54 (83%)	5.46	38 (84%) 0 0	115, 146, 171, 183	0
54	P8	45/49 (91%)	-0.25	0 100 100	46, 55, 70, 82	0
55	Q8	60/65 (92%)	0.52	4 (6%) 21 7	62, 77, 102, 118	0
All	All	15912/16371 (97%)	0.06	824 (5%) 31 13	45, 103, 202, 399	0

The worst 5 of 824 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
52	N8	59	GLU	15.7
5	14	654(J)	A	15.0
5	1H	2901	C	14.1
5	14	654(I)	C	13.7
5	1H	2902	C	13.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PSU	3L	55	20/21	0.74	0.12	-	180,202,212,213	0
26	PSU	1K	32	20/21	0.91	0.13	-	107,112,124,131	0
2	7MG	3K	46	24/25	0.58	0.20	-	193,206,217,221	0
3	H2U	2K	21	20/21	0.81	0.23	-	114,124,134,134	0
2	H2U	3L	16	20/21	0.62	0.19	-	181,194,205,211	0
26	H2U	1K	16	20/21	0.77	0.26	-	122,160,190,196	0
2	7MG	3L	46	24/25	0.70	0.14	-	190,197,206,218	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	H2U	3K	16	20/21	0.75	0.27	-	165,195,210,211	0
2	H2U	3L	20	20/21	0.59	0.20	-	180,188,201,202	0
2	7MG	1L	46	24/25	0.78	0.16	-	172,200,218,231	0
26	MIA	1K	37	29/30	0.95	0.18	-	84,92,107,113	0
2	MIA	3L	37	29/30	0.74	0.25	-	148,168,178,187	0
3	4SU	2L	8	20/21	0.90	0.11	-	115,120,123,126	0
2	MIA	1L	37	29/30	0.88	0.22	-	131,147,155,157	0
3	PSU	2L	56	20/21	0.90	0.10	-	123,130,136,139	0
3	7MG	2K	47	24/25	0.93	0.13	-	97,106,114,116	0
2	4SU	1L	8	20/21	0.74	0.12	-	185,201,207,213	0
3	OMC	2K	33	21/22	0.96	0.17	-	75,80,86,87	0
2	MIA	3K	37	29/30	0.91	0.21	-	123,142,147,157	0
2	H2U	1L	16	20/21	0.58	0.32	-	157,192,217,227	0
2	PSU	3K	55	20/21	0.62	0.15	-	190,210,228,233	0
3	4SU	2K	8	20/21	0.94	0.17	-	89,95,103,105	0
3	H2U	2L	21	20/21	0.79	0.18	-	135,143,147,157	0
2	4SU	3K	8	20/21	0.50	0.18	-	200,207,220,233	0
2	PSU	3K	39	20/21	0.90	0.15	-	117,127,130,138	0
2	PSU	3L	39	20/21	0.73	0.21	-	134,144,154,160	0
26	4SU	1K	8	20/21	0.73	0.12	-	164,174,189,190	0
3	7MG	2L	47	24/25	0.92	0.12	-	126,134,139,140	0
2	H2U	1L	20	20/21	0.54	0.36	-	141,165,187,195	0
3	OMC	2L	33	21/22	0.96	0.14	-	104,109,112,118	0
2	4SU	3L	8	20/21	0.69	0.12	-	191,196,208,218	0
3	PSU	2K	56	20/21	0.92	0.17	-	101,106,113,119	0
2	PSU	1L	39	20/21	0.89	0.10	-	140,150,158,160	0
26	7MG	1K	46	24/25	0.84	0.12	-	149,160,172,176	0
2	PSU	1L	55	20/21	0.56	0.21	-	165,197,211,225	0
2	PSU	3L	32	20/21	0.71	0.16	-	133,144,152,153	0
2	PSU	3K	32	20/21	0.83	0.17	-	127,135,142,151	0
26	PSU	1K	55	20/21	0.81	0.21	-	133,151,166,168	0
2	PSU	1L	32	20/21	0.71	0.19	-	149,152,163,169	0
26	PSU	1K	39	20/21	0.96	0.13	-	86,100,107,110	0
2	H2U	3K	20	20/21	0.66	0.44	-	140,167,205,206	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	MG	1H	3204	1/1	0.92	0.46	38.60	70,70,70,70	0
56	MG	1H	3078	1/1	0.90	0.45	36.94	80,80,80,80	0
56	MG	1H	3176	1/1	0.96	0.47	34.92	76,76,76,76	0
56	MG	1H	3258	1/1	0.72	0.45	32.89	63,63,63,63	0
56	MG	1H	3263	1/1	0.56	0.51	30.77	87,87,87,87	0
56	MG	2K	103	1/1	0.42	0.32	26.55	88,88,88,88	0
56	MG	13	1707	1/1	0.89	0.38	26.48	98,98,98,98	0
56	MG	1H	3138	1/1	0.51	0.36	25.73	72,72,72,72	0
56	MG	13	1664	1/1	0.96	0.36	25.17	88,88,88,88	0
56	MG	1H	3149	1/1	0.90	0.40	21.49	60,60,60,60	0
56	MG	1H	3054	1/1	0.76	0.40	20.33	67,67,67,67	0
56	MG	1H	3203	1/1	0.87	0.48	20.14	101,101,101,101	0
56	MG	1H	3085	1/1	0.83	0.29	19.59	64,64,64,64	0
56	MG	1H	3045	1/1	0.79	0.39	19.51	66,66,66,66	0
56	MG	13	1641	1/1	0.97	0.31	18.44	80,80,80,80	0
56	MG	1H	3047	1/1	0.98	0.33	17.72	62,62,62,62	0
56	MG	1H	3136	1/1	0.89	0.32	16.44	69,69,69,69	0
56	MG	13	1626	1/1	0.86	0.32	16.26	56,56,56,56	0
56	MG	1H	3133	1/1	0.90	0.38	16.14	69,69,69,69	0
56	MG	13	1648	1/1	0.86	0.36	15.90	91,91,91,91	0
56	MG	1H	3108	1/1	0.93	0.38	15.56	44,44,44,44	0
56	MG	1H	3145	1/1	0.94	0.27	15.38	70,70,70,70	0
56	MG	14	3056	1/1	0.89	0.28	15.15	69,69,69,69	0
56	MG	1H	3072	1/1	0.95	0.39	15.11	52,52,52,52	0
56	MG	16	201	1/1	0.93	0.33	14.91	91,91,91,91	0
56	MG	14	3036	1/1	0.94	0.32	14.82	80,80,80,80	0
56	MG	13	1643	1/1	0.64	0.32	14.69	96,96,96,96	0
56	MG	13	1621	1/1	0.96	0.47	14.54	64,64,64,64	0
56	MG	14	3073	1/1	0.90	0.27	14.13	64,64,64,64	0
56	MG	1H	3011	1/1	0.98	0.33	13.50	51,51,51,51	0
56	MG	1H	3312	1/1	0.57	0.29	13.41	83,83,83,83	0
56	MG	1G	1617	1/1	0.91	0.27	13.31	90,90,90,90	0
56	MG	14	3076	1/1	0.99	0.28	13.21	60,60,60,60	0
56	MG	1H	3048	1/1	0.95	0.35	12.86	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	13	1613	1/1	0.94	0.31	12.60	79,79,79,79	0
56	MG	1H	3015	1/1	0.98	0.36	12.02	54,54,54,54	0
56	MG	1H	3001	1/1	0.98	0.37	11.96	49,49,49,49	0
56	MG	1H	3103	1/1	0.92	0.31	11.84	60,60,60,60	0
56	MG	1H	3023	1/1	0.84	0.28	11.70	85,85,85,85	0
56	MG	1G	1640	1/1	0.89	0.23	11.37	107,107,107,107	0
56	MG	2K	101	1/1	0.98	0.28	11.19	74,74,74,74	0
56	MG	1G	1669	1/1	0.81	0.34	10.93	105,105,105,105	0
56	MG	1H	3041	1/1	0.95	0.43	10.86	75,75,75,75	0
56	MG	1H	3109	1/1	0.78	0.35	10.71	79,79,79,79	0
56	MG	13	1691	1/1	0.73	0.30	10.64	87,87,87,87	0
56	MG	1H	3323	1/1	0.87	0.30	10.58	100,100,100,100	0
56	MG	1G	1675	1/1	0.88	0.23	10.23	93,93,93,93	0
56	MG	16	206	1/1	0.86	0.20	10.22	88,88,88,88	0
56	MG	14	3040	1/1	0.94	0.32	9.91	86,86,86,86	0
56	MG	14	3156	1/1	0.69	0.34	9.87	92,92,92,92	0
56	MG	13	1608	1/1	0.95	0.34	9.82	79,79,79,79	0
56	MG	14	3095	1/1	0.94	0.21	9.77	87,87,87,87	0
56	MG	1H	3058	1/1	0.83	0.33	9.73	80,80,80,80	0
56	MG	1H	3189	1/1	0.78	0.32	9.59	67,67,67,67	0
56	MG	1H	3124	1/1	0.79	0.26	9.22	72,72,72,72	0
56	MG	13	1631	1/1	0.96	0.30	9.17	62,62,62,62	0
56	MG	1H	3004	1/1	0.96	0.32	9.15	63,63,63,63	0
56	MG	14	3042	1/1	0.91	0.21	9.09	69,69,69,69	0
56	MG	1H	3033	1/1	0.96	0.33	9.07	72,72,72,72	0
56	MG	1H	3146	1/1	0.93	0.34	8.61	81,81,81,81	0
56	MG	1H	3199	1/1	0.91	0.47	8.56	101,101,101,101	0
56	MG	1H	3164	1/1	0.86	0.27	8.52	56,56,56,56	0
56	MG	13	1671	1/1	0.94	0.20	8.35	92,92,92,92	0
56	MG	1H	3186	1/1	0.43	0.26	8.28	74,74,74,74	0
56	MG	1H	3032	1/1	0.81	0.33	8.20	79,79,79,79	0
56	MG	1H	3240	1/1	0.89	0.32	8.17	82,82,82,82	0
56	MG	1H	3089	1/1	0.79	0.25	8.09	56,56,56,56	0
56	MG	1H	3128	1/1	0.81	0.27	7.76	69,69,69,69	0
56	MG	13	1659	1/1	0.97	0.30	7.35	94,94,94,94	0
56	MG	1H	3027	1/1	0.96	0.24	7.16	58,58,58,58	0
56	MG	1H	3230	1/1	0.94	0.28	7.01	73,73,73,73	0
56	MG	1H	3052	1/1	0.98	0.31	6.95	77,77,77,77	0
56	MG	1J	204	1/1	0.72	0.26	6.72	108,108,108,108	0
56	MG	14	3052	1/1	0.95	0.31	6.70	75,75,75,75	0
56	MG	21	302	1/1	0.91	0.35	6.69	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3041	1/1	0.88	0.28	6.32	59,59,59,59	0
56	MG	14	3021	1/1	0.85	0.26	6.30	81,81,81,81	0
56	MG	1H	3036	1/1	0.95	0.24	6.29	59,59,59,59	0
56	MG	1H	3151	1/1	0.70	0.23	6.07	60,60,60,60	0
56	MG	1H	3167	1/1	0.78	0.27	5.93	59,59,59,59	0
56	MG	1H	3232	1/1	0.96	0.30	5.92	46,46,46,46	0
56	MG	1H	3118	1/1	0.88	0.25	5.91	87,87,87,87	0
56	MG	14	3027	1/1	0.93	0.25	5.90	89,89,89,89	0
56	MG	1H	3081	1/1	0.99	0.26	5.82	54,54,54,54	0
56	MG	1G	1620	1/1	0.98	0.27	5.58	93,93,93,93	0
56	MG	1H	3305	1/1	0.92	0.26	5.49	76,76,76,76	0
56	MG	14	3096	1/1	0.89	0.22	5.40	64,64,64,64	0
56	MG	1H	3221	1/1	0.86	0.44	5.24	88,88,88,88	0
56	MG	1H	3152	1/1	0.61	0.24	5.15	75,75,75,75	0
56	MG	14	3107	1/1	0.79	0.19	5.07	74,74,74,74	0
56	MG	1G	1663	1/1	0.81	0.33	5.02	120,120,120,120	0
56	MG	14	3011	1/1	0.97	0.23	5.01	65,65,65,65	0
56	MG	14	3122	1/1	0.91	0.21	4.94	77,77,77,77	0
56	MG	13	1611	1/1	0.76	0.20	4.89	79,79,79,79	0
56	MG	14	3037	1/1	0.66	0.23	4.82	62,62,62,62	0
56	MG	1G	1602	1/1	0.91	0.26	4.76	76,76,76,76	0
56	MG	14	3068	1/1	0.98	0.23	4.73	64,64,64,64	0
56	MG	13	1676	1/1	0.68	0.20	4.65	89,89,89,89	0
56	MG	13	1630	1/1	0.90	0.20	4.65	80,80,80,80	0
56	MG	1H	3278	1/1	0.68	0.38	4.65	74,74,74,74	0
56	MG	1H	3185	1/1	0.71	0.20	4.53	70,70,70,70	0
56	MG	1H	3066	1/1	0.94	0.23	4.50	48,48,48,48	0
56	MG	13	1606	1/1	0.86	0.27	4.43	83,83,83,83	0
56	MG	1H	3532	1/1	0.85	0.37	4.38	116,116,116,116	0
56	MG	1H	3021	1/1	0.99	0.26	4.15	84,84,84,84	0
56	MG	13	1601	1/1	0.95	0.27	4.14	71,71,71,71	0
56	MG	1H	3358	1/1	0.94	0.25	4.04	65,65,65,65	0
56	MG	13	1682	1/1	0.95	0.19	4.03	135,135,135,135	0
56	MG	14	3035	1/1	0.99	0.23	3.84	68,68,68,68	0
56	MG	14	3198	1/1	0.86	0.19	3.82	90,90,90,90	0
56	MG	1H	3020	1/1	0.96	0.22	3.68	67,67,67,67	0
56	MG	13	1670	1/1	0.95	0.20	3.68	95,95,95,95	0
56	MG	1H	3095	1/1	0.90	0.26	3.66	87,87,87,87	0
56	MG	1G	1601	1/1	0.98	0.21	3.64	90,90,90,90	0
56	MG	13	1722	1/1	0.96	0.19	3.62	87,87,87,87	0
56	MG	14	3022	1/1	0.96	0.19	3.57	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3111	1/1	0.89	0.23	3.53	67,67,67,67	0
56	MG	3I	201	1/1	0.69	0.26	3.51	68,68,68,68	0
56	MG	1H	3082	1/1	0.91	0.23	3.37	40,40,40,40	0
56	MG	1H	3010	1/1	0.94	0.32	3.33	46,46,46,46	0
56	MG	14	3227	1/1	0.87	0.16	3.28	106,106,106,106	0
56	MG	1H	3037	1/1	0.93	0.29	3.26	51,51,51,51	0
56	MG	1H	3026	1/1	0.84	0.22	3.23	61,61,61,61	0
56	MG	14	3125	1/1	0.55	0.16	3.06	77,77,77,77	0
56	MG	1H	3132	1/1	0.85	0.22	3.03	71,71,71,71	0
56	MG	14	3160	1/1	0.86	0.20	3.00	81,81,81,81	0
56	MG	13	1673	1/1	0.97	0.21	2.95	84,84,84,84	0
56	MG	1H	3057	1/1	0.97	0.21	2.92	64,64,64,64	0
56	MG	14	3182	1/1	0.94	0.19	2.83	66,66,66,66	0
57	ZN	3E	303	1/1	0.96	0.41	2.82	127,127,127,127	0
56	MG	1H	3416	1/1	0.97	0.21	2.81	48,48,48,48	0
56	MG	1H	3065	1/1	0.97	0.25	2.80	51,51,51,51	0
56	MG	14	3023	1/1	0.92	0.22	2.73	67,67,67,67	0
56	MG	1H	3389	1/1	0.88	0.21	2.71	98,98,98,98	0
56	MG	14	3230	1/1	0.69	0.16	2.69	86,86,86,86	0
56	MG	14	3191	1/1	0.96	0.20	2.69	90,90,90,90	0
56	MG	1H	3392	1/1	0.96	0.23	2.65	67,67,67,67	0
56	MG	1H	3142	1/1	0.95	0.23	2.61	82,82,82,82	0
56	MG	14	3175	1/1	0.74	0.17	2.57	83,83,83,83	0
56	MG	1H	3366	1/1	0.65	0.21	2.48	74,74,74,74	0
56	MG	1H	3092	1/1	0.69	0.19	2.46	66,66,66,66	0
56	MG	13	1615	1/1	0.93	0.27	2.42	100,100,100,100	0
56	MG	J8	101	1/1	0.95	0.37	2.34	67,67,67,67	0
56	MG	1H	3098	1/1	0.99	0.27	2.34	63,63,63,63	0
56	MG	14	3240	1/1	0.62	0.23	2.31	90,90,90,90	0
56	MG	14	3121	1/1	0.81	0.15	2.23	91,91,91,91	0
56	MG	1G	1609	1/1	0.98	0.17	2.18	96,96,96,96	0
56	MG	1H	3025	1/1	0.88	0.18	2.12	67,67,67,67	0
56	MG	1H	3482	1/1	0.97	0.19	2.04	81,81,81,81	0
56	MG	1H	3101	1/1	0.92	0.20	2.02	57,57,57,57	0
56	MG	14	3031	1/1	0.92	0.16	1.96	83,83,83,83	0
56	MG	14	3029	1/1	0.85	0.15	1.95	86,86,86,86	0
56	MG	1H	3399	1/1	0.98	0.20	1.91	50,50,50,50	0
56	MG	1H	3188	1/1	0.76	0.18	1.89	67,67,67,67	0
56	MG	1G	1665	1/1	0.74	0.17	1.84	99,99,99,99	0
56	MG	1H	3028	1/1	0.94	0.23	1.78	59,59,59,59	0
56	MG	14	3412	1/1	0.84	0.20	1.75	93,93,93,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3038	1/1	0.97	0.25	1.70	78,78,78,78	0
56	MG	1H	3042	1/1	0.77	0.22	1.65	62,62,62,62	0
56	MG	88	201	1/1	0.96	0.34	1.64	73,73,73,73	0
56	MG	14	3162	1/1	0.83	0.21	1.60	107,107,107,107	0
56	MG	1H	3107	1/1	0.81	0.18	1.42	84,84,84,84	0
56	MG	14	3187	1/1	0.95	0.16	1.40	63,63,63,63	0
56	MG	14	3189	1/1	0.93	0.16	1.30	72,72,72,72	0
56	MG	1H	3174	1/1	0.84	0.16	1.26	63,63,63,63	0
56	MG	1J	205	1/1	0.66	0.26	1.24	113,113,113,113	0
56	MG	14	3169	1/1	0.95	0.16	1.22	65,65,65,65	0
56	MG	14	3034	1/1	0.94	0.19	1.16	78,78,78,78	0
56	MG	14	3090	1/1	0.98	0.16	1.13	87,87,87,87	0
56	MG	1H	3202	1/1	0.94	0.29	1.09	87,87,87,87	0
56	MG	14	3114	1/1	0.62	0.15	1.04	69,69,69,69	0
56	MG	13	1706	1/1	0.52	0.23	1.03	93,93,93,93	0
56	MG	13	1680	1/1	0.74	0.18	0.97	107,107,107,107	0
56	MG	1H	3008	1/1	0.96	0.26	0.89	41,41,41,41	0
56	MG	1H	3219	1/1	0.96	0.18	0.89	73,73,73,73	0
56	MG	14	3183	1/1	0.61	0.19	0.83	74,74,74,74	0
56	MG	13	1715	1/1	0.96	0.17	0.82	85,85,85,85	0
56	MG	1G	1621	1/1	0.76	0.16	0.78	122,122,122,122	0
56	MG	1H	3365	1/1	0.93	0.19	0.76	71,71,71,71	0
56	MG	2L	101	1/1	0.96	0.17	0.72	86,86,86,86	0
56	MG	78	201	1/1	0.88	0.17	0.70	79,79,79,79	0
56	MG	13	1632	1/1	0.98	0.17	0.67	74,74,74,74	0
56	MG	1H	3061	1/1	0.95	0.20	0.65	52,52,52,52	0
56	MG	1G	1644	1/1	0.87	0.21	0.64	102,102,102,102	0
56	MG	14	3320	1/1	0.98	0.16	0.64	84,84,84,84	0
56	MG	14	3014	1/1	0.93	0.17	0.62	73,73,73,73	0
56	MG	1H	3398	1/1	0.93	0.19	0.62	58,58,58,58	0
56	MG	1H	3147	1/1	0.86	0.20	0.59	69,69,69,69	0
56	MG	14	3246	1/1	0.63	0.14	0.56	97,97,97,97	0
56	MG	1H	3239	1/1	0.72	0.16	0.51	88,88,88,88	0
56	MG	14	3004	1/1	0.98	0.15	0.48	61,61,61,61	0
56	MG	14	3127	1/1	0.86	0.15	0.48	88,88,88,88	0
56	MG	14	3013	1/1	0.81	0.17	0.47	65,65,65,65	0
56	MG	14	3084	1/1	0.92	0.16	0.39	70,70,70,70	0
56	MG	14	3351	1/1	0.94	0.15	0.33	70,70,70,70	0
56	MG	1G	1670	1/1	0.89	0.14	0.33	96,96,96,96	0
56	MG	13	1654	1/1	0.88	0.22	0.31	125,125,125,125	0
56	MG	13	1605	1/1	0.97	0.17	0.28	82,82,82,82	0
56	MG	1H	3252	1/1	0.93	0.16	0.21	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	ZN	32	301	1/1	0.98	0.32	0.16	119,119,119,119	0
56	MG	13	1724	1/1	0.91	0.16	0.13	116,116,116,116	0
56	MG	1H	3076	1/1	0.90	0.17	0.11	64,64,64,64	0
56	MG	13	1663	1/1	0.81	0.13	0.10	107,107,107,107	0
56	MG	16	205	1/1	0.89	0.15	0.10	87,87,87,87	0
56	MG	14	3190	1/1	0.70	0.15	-0.00	90,90,90,90	0
56	MG	13	1616	1/1	0.88	0.17	-0.01	95,95,95,95	0
57	ZN	G8	201	1/1	0.63	0.24	-0.04	176,176,176,176	0
56	MG	13	1609	1/1	0.93	0.15	-0.04	83,83,83,83	0
56	MG	41	202	1/1	0.87	0.20	-0.11	85,85,85,85	0
56	MG	14	3097	1/1	0.83	0.15	-0.17	71,71,71,71	0
56	MG	13	1667	1/1	0.87	0.15	-0.19	91,91,91,91	0
56	MG	1G	1603	1/1	0.97	0.17	-0.24	77,77,77,77	0
57	ZN	5I	102	1/1	0.99	0.20	-0.25	96,96,96,96	0
56	MG	13	1627	1/1	0.97	0.16	-0.36	64,64,64,64	0
56	MG	16	210	1/1	0.88	0.15	-0.40	105,105,105,105	0
56	MG	11	302	1/1	0.96	0.20	-0.40	42,42,42,42	0
56	MG	1G	1618	1/1	0.83	0.15	-0.42	102,102,102,102	0
56	MG	13	1604	1/1	0.92	0.14	-0.45	80,80,80,80	0
56	MG	14	3055	1/1	0.98	0.14	-0.45	59,59,59,59	0
56	MG	14	3252	1/1	0.87	0.12	-0.47	74,74,74,74	0
56	MG	1H	3235	1/1	0.94	0.17	-0.47	61,61,61,61	0
56	MG	14	3032	1/1	0.95	0.13	-0.53	87,87,87,87	0
56	MG	1H	3063	1/1	0.89	0.17	-0.63	54,54,54,54	0
56	MG	1H	3383	1/1	0.96	0.15	-0.73	59,59,59,59	0
56	MG	14	3171	1/1	0.96	0.12	-0.79	84,84,84,84	0
56	MG	5I	101	1/1	0.78	0.15	-0.80	82,82,82,82	0
56	MG	1H	3345	1/1	0.86	0.15	-0.85	66,66,66,66	0
56	MG	14	3110	1/1	0.90	0.16	-0.91	61,61,61,61	0
56	MG	13	1637	1/1	0.79	0.14	-0.92	71,71,71,71	0
56	MG	14	3217	1/1	0.81	0.15	-0.94	159,159,159,159	0
56	MG	1G	1615	1/1	0.80	0.13	-0.97	86,86,86,86	0
56	MG	1H	3162	1/1	0.89	0.17	-1.02	69,69,69,69	0
56	MG	13	1709	1/1	0.94	0.14	-1.04	72,72,72,72	0
56	MG	1H	3330	1/1	0.97	0.17	-1.10	53,53,53,53	0
56	MG	14	3193	1/1	0.81	0.14	-1.11	78,78,78,78	0
56	MG	3E	301	1/1	0.96	0.14	-1.12	116,116,116,116	0
56	MG	1H	3327	1/1	0.97	0.17	-1.13	61,61,61,61	0
56	MG	1G	1642	1/1	0.95	0.15	-1.14	130,130,130,130	0
56	MG	1H	3528	1/1	0.97	0.13	-1.19	61,61,61,61	0
56	MG	1H	3064	1/1	0.98	0.16	-1.20	52,52,52,52	0
56	MG	14	3019	1/1	0.96	0.14	-1.20	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3447	1/1	0.97	0.12	-1.20	74,74,74,74	0
56	MG	1H	3412	1/1	0.93	0.13	-1.21	70,70,70,70	0
56	MG	1H	3452	1/1	0.95	0.15	-1.26	50,50,50,50	0
56	MG	14	3277	1/1	0.96	0.13	-1.27	54,54,54,54	0
56	MG	1H	3208	1/1	0.81	0.17	-1.28	53,53,53,53	0
56	MG	1H	3166	1/1	0.95	0.17	-1.31	53,53,53,53	0
56	MG	14	3116	1/1	0.88	0.12	-1.38	75,75,75,75	0
56	MG	14	3173	1/1	0.92	0.12	-1.41	66,66,66,66	0
56	MG	1H	3071	1/1	0.84	0.16	-1.42	38,38,38,38	0
56	MG	1H	3537	1/1	0.89	0.14	-1.50	55,55,55,55	0
56	MG	13	1686	1/1	0.94	0.15	-1.53	84,84,84,84	0
56	MG	14	3167	1/1	0.93	0.12	-1.57	67,67,67,67	0
56	MG	1H	3116	1/1	0.99	0.15	-1.57	66,66,66,66	0
56	MG	1H	3343	1/1	0.98	0.17	-1.61	52,52,52,52	0
56	MG	1H	3337	1/1	0.93	0.16	-1.62	65,65,65,65	0
56	MG	1H	3404	1/1	0.96	0.15	-1.62	74,74,74,74	0
56	MG	1H	3117	1/1	0.71	0.15	-1.64	57,57,57,57	0
56	MG	1H	3395	1/1	0.91	0.16	-1.65	59,59,59,59	0
56	MG	1H	3341	1/1	0.99	0.16	-1.65	43,43,43,43	0
56	MG	14	3159	1/1	0.94	0.13	-1.66	64,64,64,64	0
56	MG	1G	1652	1/1	0.96	0.12	-1.67	81,81,81,81	0
56	MG	1H	3414	1/1	0.96	0.17	-1.68	67,67,67,67	0
56	MG	41	201	1/1	0.85	0.19	-1.69	85,85,85,85	0
56	MG	1H	3129	1/1	0.80	0.15	-1.70	57,57,57,57	0
56	MG	13	1739	1/1	0.94	0.12	-1.70	103,103,103,103	0
56	MG	14	3153	1/1	0.69	0.12	-1.72	82,82,82,82	0
56	MG	1H	3408	1/1	0.90	0.16	-1.81	60,60,60,60	0
56	MG	5E	201	1/1	0.93	0.17	-1.81	93,93,93,93	0
56	MG	14	3202	1/1	0.94	0.11	-1.85	106,106,106,106	0
56	MG	14	3007	1/1	0.95	0.15	-1.85	69,69,69,69	0
56	MG	13	1735	1/1	0.91	0.09	-1.85	78,78,78,78	0
56	MG	1H	3153	1/1	0.98	0.15	-1.86	77,77,77,77	0
56	MG	1H	3468	1/1	0.70	0.12	-1.86	115,115,115,115	0
56	MG	13	1647	1/1	0.86	0.06	-1.86	83,83,83,83	0
56	MG	13	1675	1/1	0.73	0.10	-1.87	131,131,131,131	0
56	MG	13	1701	1/1	0.50	0.14	-1.88	71,71,71,71	0
56	MG	13	1713	1/1	0.96	0.09	-1.89	99,99,99,99	0
56	MG	14	3150	1/1	0.89	0.12	-1.89	57,57,57,57	0
56	MG	13	1746	1/1	0.93	0.07	-1.90	102,102,102,102	0
56	MG	14	3300	1/1	0.96	0.12	-1.91	69,69,69,69	0
56	MG	1H	3396	1/1	0.96	0.14	-1.95	61,61,61,61	0
56	MG	1H	3448	1/1	0.96	0.14	-1.95	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3083	1/1	0.97	0.15	-1.96	51,51,51,51	0
56	MG	1H	3355	1/1	0.95	0.14	-1.97	72,72,72,72	0
56	MG	14	3264	1/1	0.93	0.09	-1.99	78,78,78,78	0
56	MG	1H	3264	1/1	0.86	0.13	-2.03	68,68,68,68	0
56	MG	1H	3536	1/1	0.93	0.07	-2.04	43,43,43,43	0
56	MG	14	3286	1/1	0.95	0.12	-2.05	62,62,62,62	0
56	MG	1G	1688	1/1	0.71	0.10	-2.08	122,122,122,122	0
56	MG	14	3328	1/1	0.93	0.11	-2.10	73,73,73,73	0
56	MG	1H	3405	1/1	0.89	0.12	-2.10	78,78,78,78	0
56	MG	16	204	1/1	0.84	0.11	-2.14	68,68,68,68	0
56	MG	1H	3456	1/1	0.92	0.14	-2.17	69,69,69,69	0
56	MG	1G	1637	1/1	0.96	0.11	-2.18	89,89,89,89	0
56	MG	13	1721	1/1	0.96	0.14	-2.24	99,99,99,99	0
56	MG	1H	3093	1/1	0.96	0.12	-2.26	56,56,56,56	0
56	MG	14	3360	1/1	0.88	0.08	-2.31	104,104,104,104	0
56	MG	1H	3331	1/1	0.97	0.16	-2.33	49,49,49,49	0
56	MG	1H	3432	1/1	0.95	0.15	-2.35	69,69,69,69	0
56	MG	1H	3339	1/1	1.00	0.11	-2.38	60,60,60,60	0
56	MG	1J	201	1/1	0.96	0.10	-2.42	123,123,123,123	0
56	MG	13	1710	1/1	0.90	0.13	-2.43	61,61,61,61	0
56	MG	1H	3437	1/1	0.96	0.14	-2.48	70,70,70,70	0
56	MG	14	3047	1/1	0.96	0.09	-2.54	68,68,68,68	0
56	MG	14	3357	1/1	0.94	0.10	-2.61	82,82,82,82	0
56	MG	14	3275	1/1	0.98	0.12	-2.67	58,58,58,58	0
56	MG	1H	3351	1/1	0.96	0.12	-2.74	65,65,65,65	0
56	MG	14	3323	1/1	0.96	0.14	-2.77	59,59,59,59	0
56	MG	1H	3391	1/1	0.95	0.10	-2.79	58,58,58,58	0
56	MG	1H	3342	1/1	0.96	0.12	-2.79	60,60,60,60	0
56	MG	1H	3397	1/1	0.93	0.12	-2.83	52,52,52,52	0
56	MG	1H	3442	1/1	0.91	0.11	-2.92	74,74,74,74	0
56	MG	13	1633	1/1	0.96	0.12	-2.93	84,84,84,84	0
56	MG	14	3283	1/1	0.91	0.07	-2.98	78,78,78,78	0
56	MG	1H	3380	1/1	0.91	0.11	-3.00	44,44,44,44	0
56	MG	14	3308	1/1	0.95	0.10	-3.00	69,69,69,69	0
56	MG	14	3314	1/1	0.86	0.10	-3.04	59,59,59,59	0
56	MG	14	3420	1/1	0.59	0.12	-3.14	91,91,91,91	0
56	MG	1G	1605	1/1	0.94	0.10	-3.22	95,95,95,95	0
56	MG	14	3074	1/1	0.85	0.10	-3.24	89,89,89,89	0
56	MG	1H	3378	1/1	0.88	0.14	-3.29	77,77,77,77	0
56	MG	14	3371	1/1	0.92	0.10	-3.30	102,102,102,102	0
56	MG	1G	1683	1/1	0.89	0.11	-3.34	97,97,97,97	0
56	MG	13	1620	1/1	0.85	0.10	-3.40	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3430	1/1	0.95	0.09	-3.41	50,50,50,50	0
56	MG	1H	3155	1/1	0.93	0.11	-3.43	65,65,65,65	0
56	MG	14	3092	1/1	0.85	0.09	-3.44	61,61,61,61	0
56	MG	14	3378	1/1	0.42	0.07	-3.49	126,126,126,126	0
56	MG	1H	3102	1/1	0.94	0.15	-3.50	45,45,45,45	0
56	MG	14	3318	1/1	0.97	0.09	-3.54	69,69,69,69	0
56	MG	14	3177	1/1	0.75	0.11	-3.55	81,81,81,81	0
56	MG	1G	1685	1/1	0.90	0.10	-3.58	91,91,91,91	0
56	MG	1H	3286	1/1	0.71	0.13	-3.60	88,88,88,88	0
56	MG	14	3025	1/1	0.95	0.09	-3.80	87,87,87,87	0
56	MG	1H	3350	1/1	0.96	0.12	-3.84	52,52,52,52	0
56	MG	14	3394	1/1	0.80	0.10	-3.85	102,102,102,102	0
56	MG	14	3322	1/1	0.89	0.08	-3.86	80,80,80,80	0
56	MG	14	3285	1/1	0.92	0.09	-3.97	68,68,68,68	0
56	MG	14	3393	1/1	0.81	0.08	-3.98	111,111,111,111	0
56	MG	14	3324	1/1	0.93	0.08	-4.07	63,63,63,63	0
56	MG	1H	3521	1/1	0.45	0.12	-4.13	89,89,89,89	0
56	MG	1H	3367	1/1	0.92	0.13	-4.19	50,50,50,50	0
56	MG	13	1726	1/1	0.74	0.08	-4.20	96,96,96,96	0
56	MG	14	3392	1/1	0.93	0.10	-4.32	77,77,77,77	0
56	MG	1H	3326	1/1	0.95	0.13	-4.35	54,54,54,54	0
56	MG	1H	3087	1/1	0.98	0.12	-4.43	69,69,69,69	0
56	MG	14	3294	1/1	0.94	0.07	-4.45	59,59,59,59	0
56	MG	16	213	1/1	0.77	0.09	-4.57	102,102,102,102	0
56	MG	1H	3332	1/1	0.95	0.15	-4.58	64,64,64,64	0
56	MG	14	3321	1/1	0.96	0.07	-4.62	62,62,62,62	0
56	MG	13	1678	1/1	0.93	0.10	-4.63	85,85,85,85	0
56	MG	1H	3435	1/1	0.95	0.13	-4.64	52,52,52,52	0
56	MG	1H	3348	1/1	0.98	0.12	-4.75	60,60,60,60	0
56	MG	1H	3074	1/1	0.97	0.15	-4.77	46,46,46,46	0
56	MG	14	3184	1/1	0.89	0.08	-4.79	79,79,79,79	0
56	MG	14	3289	1/1	0.87	0.10	-4.80	77,77,77,77	0
56	MG	14	3411	1/1	0.93	0.07	-4.83	106,106,106,106	0
56	MG	1H	3334	1/1	0.97	0.07	-4.86	56,56,56,56	0
56	MG	1H	3390	1/1	0.95	0.11	-4.93	61,61,61,61	0
56	MG	14	3319	1/1	0.90	0.08	-5.03	86,86,86,86	0
56	MG	14	3388	1/1	0.87	0.06	-5.08	90,90,90,90	0
56	MG	14	3210	1/1	0.92	0.09	-5.20	100,100,100,100	0
56	MG	1G	1657	1/1	0.80	0.08	-5.20	112,112,112,112	0
56	MG	14	3306	1/1	0.96	0.08	-5.24	66,66,66,66	0
56	MG	14	3333	1/1	0.97	0.06	-5.30	74,74,74,74	0
56	MG	14	3354	1/1	0.92	0.05	-5.31	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3024	1/1	0.95	0.08	-5.38	61,61,61,61	0
56	MG	1H	3329	1/1	0.95	0.11	-5.46	52,52,52,52	0
56	MG	14	3379	1/1	0.75	0.06	-5.58	126,126,126,126	0
56	MG	1H	3493	1/1	0.97	0.11	-5.59	68,68,68,68	0
56	MG	14	3089	1/1	0.93	0.06	-5.64	54,54,54,54	0
56	MG	1H	3169	1/1	0.94	0.10	-5.72	49,49,49,49	0
56	MG	14	3389	1/1	0.87	0.09	-5.84	72,72,72,72	0
56	MG	14	3276	1/1	0.95	0.09	-5.90	85,85,85,85	0
56	MG	1H	3359	1/1	0.90	0.10	-6.45	93,93,93,93	0
56	MG	1H	3484	1/1	0.83	0.08	-6.54	105,105,105,105	0
56	MG	1H	3385	1/1	0.96	0.11	-6.64	62,62,62,62	0
56	MG	1H	3451	1/1	0.93	0.07	-6.66	88,88,88,88	0
56	MG	1H	3450	1/1	0.90	0.12	-6.77	88,88,88,88	0
56	MG	1H	3357	1/1	0.90	0.08	-7.19	72,72,72,72	0
56	MG	14	3292	1/1	0.98	0.09	-7.25	73,73,73,73	0
56	MG	1H	3518	1/1	0.86	0.06	-7.36	89,89,89,89	0
56	MG	2K	108	1/1	0.88	0.07	-7.45	92,92,92,92	0
56	MG	13	1717	1/1	0.97	0.06	-7.60	64,64,64,64	0
56	MG	1H	3533	1/1	0.92	0.05	-7.67	106,106,106,106	0
56	MG	13	1728	1/1	0.95	0.07	-7.78	80,80,80,80	0
56	MG	14	3149	1/1	0.97	0.09	-8.31	58,58,58,58	0
56	MG	1H	3511	1/1	0.94	0.11	-8.35	84,84,84,84	0
56	MG	1H	3407	1/1	0.92	0.06	-8.56	59,59,59,59	0
56	MG	1H	3349	1/1	0.99	0.06	-10.34	68,68,68,68	0
56	MG	1H	3441	1/1	0.89	0.05	-10.73	73,73,73,73	0
56	MG	1H	3384	1/1	0.97	0.10	-11.27	50,50,50,50	0
56	MG	1H	3379	1/1	0.88	0.07	-12.05	90,90,90,90	0
56	MG	1H	3363	1/1	0.62	0.06	-13.08	83,83,83,83	0
56	MG	14	3365	1/1	0.82	0.07	-13.13	89,89,89,89	0
56	MG	1H	3513	1/1	0.91	0.06	-14.76	104,104,104,104	0
56	MG	1H	3182	1/1	0.73	0.40	-	69,69,69,69	0
56	MG	14	3259	1/1	0.65	0.39	-	104,104,104,104	0
56	MG	13	1700	1/1	0.85	0.36	-	103,103,103,103	0
56	MG	1H	3340	1/1	0.95	0.12	-	76,76,76,76	0
56	MG	1H	3259	1/1	0.82	0.29	-	79,79,79,79	0
56	MG	1H	3055	1/1	0.89	0.27	-	77,77,77,77	0
56	MG	14	3251	1/1	0.80	0.32	-	83,83,83,83	0
56	MG	1H	3419	1/1	0.83	0.09	-	86,86,86,86	0
56	MG	1H	3449	1/1	0.97	0.08	-	91,91,91,91	0
56	MG	14	3020	1/1	0.95	0.20	-	62,62,62,62	0
56	MG	1H	3243	1/1	0.86	0.57	-	85,85,85,85	0
56	MG	13	1692	1/1	0.65	0.29	-	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3292	1/1	0.91	0.10	-	80,80,80,80	0
56	MG	14	3267	1/1	0.84	0.27	-	79,79,79,79	0
56	MG	1H	3049	1/1	0.98	0.28	-	59,59,59,59	0
56	MG	1H	3455	1/1	0.82	0.05	-	101,101,101,101	0
56	MG	14	3146	1/1	0.89	0.35	-	91,91,91,91	0
56	MG	14	3287	1/1	0.94	0.07	-	70,70,70,70	0
56	MG	1H	3295	1/1	0.85	0.32	-	72,72,72,72	0
56	MG	14	3272	1/1	0.35	0.25	-	100,100,100,100	0
56	MG	1H	3516	1/1	0.86	0.13	-	114,114,114,114	0
56	MG	14	3248	1/1	0.86	0.29	-	91,91,91,91	0
56	MG	1G	1616	1/1	0.81	0.21	-	97,97,97,97	0
56	MG	13	1662	1/1	0.89	0.35	-	94,94,94,94	0
56	MG	14	3406	1/1	0.88	0.21	-	84,84,84,84	0
56	MG	1H	3135	1/1	0.95	0.40	-	74,74,74,74	0
56	MG	14	3060	1/1	0.95	0.24	-	84,84,84,84	0
56	MG	1H	3200	1/1	0.96	0.25	-	77,77,77,77	0
56	MG	1H	3311	1/1	0.62	0.39	-	93,93,93,93	0
56	MG	1H	3313	1/1	0.96	0.16	-	86,86,86,86	0
56	MG	1H	3062	1/1	0.86	0.27	-	61,61,61,61	0
56	MG	1H	3526	1/1	0.93	0.06	-	78,78,78,78	0
56	MG	13	1628	1/1	0.92	0.20	-	51,51,51,51	0
56	MG	1H	3178	1/1	0.83	0.26	-	61,61,61,61	0
56	MG	1H	3144	1/1	0.96	0.17	-	63,63,63,63	0
56	MG	1G	1672	1/1	0.71	0.20	-	98,98,98,98	0
56	MG	1H	3502	1/1	0.87	0.08	-	109,109,109,109	0
56	MG	1H	3271	1/1	0.46	0.43	-	100,100,100,100	0
56	MG	1H	3175	1/1	0.82	0.41	-	69,69,69,69	0
56	MG	1K	102	1/1	0.90	0.10	-	107,107,107,107	0
56	MG	14	3224	1/1	0.95	0.12	-	66,66,66,66	0
56	MG	1H	3280	1/1	0.58	0.40	-	101,101,101,101	0
56	MG	1H	3470	1/1	0.90	0.08	-	81,81,81,81	0
56	MG	13	1640	1/1	0.87	0.26	-	81,81,81,81	0
56	MG	1H	3104	1/1	0.96	0.31	-	57,57,57,57	0
56	MG	1G	1658	1/1	0.88	0.32	-	91,91,91,91	0
56	MG	14	3049	1/1	0.97	0.16	-	60,60,60,60	0
56	MG	14	3303	1/1	0.90	0.04	-	92,92,92,92	0
56	MG	1H	3333	1/1	0.91	0.14	-	64,64,64,64	0
56	MG	14	3071	1/1	0.75	0.20	-	63,63,63,63	0
56	MG	3L	103	1/1	0.89	0.26	-	99,99,99,99	0
56	MG	14	3219	1/1	0.61	0.31	-	100,100,100,100	0
56	MG	14	3088	1/1	0.94	0.24	-	88,88,88,88	0
56	MG	1H	3262	1/1	0.89	0.23	-	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3388	1/1	0.90	0.09	-	90,90,90,90	0
56	MG	1H	3483	1/1	0.81	0.17	-	116,116,116,116	0
56	MG	14	3305	1/1	0.91	0.07	-	89,89,89,89	0
56	MG	1H	3209	1/1	0.96	0.15	-	68,68,68,68	0
56	MG	13	1694	1/1	0.89	0.12	-	94,94,94,94	0
56	MG	14	3353	1/1	0.87	0.19	-	94,94,94,94	0
56	MG	1H	3039	1/1	0.97	0.23	-	87,87,87,87	0
56	MG	14	3083	1/1	0.69	0.22	-	86,86,86,86	0
56	MG	1G	1667	1/1	0.80	0.32	-	124,124,124,124	0
56	MG	1H	3019	1/1	0.96	0.17	-	48,48,48,48	0
56	MG	1H	3479	1/1	0.96	0.10	-	72,72,72,72	0
56	MG	1H	3043	1/1	0.78	0.41	-	62,62,62,62	0
56	MG	14	3002	1/1	0.98	0.18	-	62,62,62,62	0
56	MG	1H	3425	1/1	0.96	0.08	-	77,77,77,77	0
56	MG	14	3263	1/1	0.82	0.16	-	97,97,97,97	0
56	MG	14	3235	1/1	0.80	0.26	-	92,92,92,92	0
56	MG	14	3315	1/1	0.71	0.11	-	76,76,76,76	0
56	MG	14	3336	1/1	0.86	0.46	-	114,114,114,114	0
56	MG	1H	3328	1/1	0.94	0.12	-	75,75,75,75	0
56	MG	13	1603	1/1	0.96	0.27	-	67,67,67,67	0
56	MG	14	3062	1/1	0.97	0.09	-	70,70,70,70	0
56	MG	14	3048	1/1	0.93	0.11	-	63,63,63,63	0
56	MG	1H	3266	1/1	0.75	0.33	-	94,94,94,94	0
56	MG	1H	3233	1/1	0.94	0.16	-	65,65,65,65	0
56	MG	14	3128	1/1	0.52	0.31	-	91,91,91,91	0
56	MG	1H	3106	1/1	0.86	0.34	-	70,70,70,70	0
56	MG	14	3194	1/1	0.86	0.13	-	73,73,73,73	0
56	MG	1H	3179	1/1	0.86	0.23	-	75,75,75,75	0
56	MG	14	3383	1/1	0.86	0.14	-	114,114,114,114	0
56	MG	14	3069	1/1	0.97	0.34	-	73,73,73,73	0
56	MG	14	3257	1/1	0.39	0.17	-	93,93,93,93	0
56	MG	13	1651	1/1	0.86	0.28	-	76,76,76,76	0
56	MG	14	3390	1/1	0.91	0.07	-	111,111,111,111	0
56	MG	14	3221	1/1	0.82	0.35	-	99,99,99,99	0
56	MG	1H	3009	1/1	0.97	0.41	-	58,58,58,58	0
56	MG	14	3174	1/1	0.69	0.23	-	82,82,82,82	0
56	MG	16	209	1/1	0.90	0.22	-	74,74,74,74	0
56	MG	14	3102	1/1	0.82	0.47	-	73,73,73,73	0
56	MG	1G	1682	1/1	0.94	0.08	-	86,86,86,86	0
56	MG	1H	3307	1/1	0.75	0.31	-	86,86,86,86	0
56	MG	14	3377	1/1	0.96	0.04	-	88,88,88,88	0
56	MG	13	1704	1/1	0.70	0.26	-	113,113,113,113	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	13	1736	1/1	0.96	0.14	-	95,95,95,95	0
56	MG	1H	3035	1/1	0.96	0.24	-	76,76,76,76	0
56	MG	3L	102	1/1	0.86	0.09	-	146,146,146,146	0
56	MG	14	3199	1/1	0.56	0.23	-	83,83,83,83	0
56	MG	14	3250	1/1	0.72	0.28	-	98,98,98,98	0
56	MG	1G	1607	1/1	0.15	0.26	-	96,96,96,96	0
56	MG	13	1696	1/1	0.81	0.22	-	91,91,91,91	0
56	MG	1H	3509	1/1	0.88	0.06	-	91,91,91,91	0
56	MG	14	3307	1/1	0.90	0.07	-	81,81,81,81	0
56	MG	14	3242	1/1	0.51	0.29	-	89,89,89,89	0
56	MG	14	3278	1/1	0.97	0.07	-	62,62,62,62	0
56	MG	1G	1686	1/1	0.97	0.09	-	117,117,117,117	0
56	MG	14	3268	1/1	0.55	0.20	-	96,96,96,96	0
56	MG	14	3381	1/1	0.91	0.05	-	110,110,110,110	0
56	MG	14	3204	1/1	0.91	0.19	-	87,87,87,87	0
56	MG	14	3295	1/1	0.88	0.03	-	90,90,90,90	0
56	MG	13	1684	1/1	0.54	0.23	-	108,108,108,108	0
56	MG	1H	3091	1/1	0.94	0.35	-	65,65,65,65	0
56	MG	1H	3249	1/1	0.97	0.13	-	75,75,75,75	0
56	MG	1H	3315	1/1	0.90	0.39	-	93,93,93,93	0
56	MG	1H	3068	1/1	0.62	0.44	-	68,68,68,68	0
56	MG	2L	103	1/1	0.87	0.14	-	85,85,85,85	0
56	MG	13	1712	1/1	0.93	0.08	-	84,84,84,84	0
56	MG	14	3385	1/1	0.95	0.07	-	83,83,83,83	0
56	MG	1H	3368	1/1	0.93	0.14	-	58,58,58,58	0
56	MG	1G	1664	1/1	0.83	0.29	-	90,90,90,90	0
56	MG	14	3407	1/1	0.78	0.10	-	110,110,110,110	0
56	MG	1H	3122	1/1	0.53	0.27	-	77,77,77,77	0
56	MG	1H	3504	1/1	0.74	0.12	-	117,117,117,117	0
56	MG	13	1666	1/1	0.98	0.06	-	86,86,86,86	0
56	MG	1H	3050	1/1	0.96	0.30	-	62,62,62,62	0
56	MG	1H	3226	1/1	0.96	0.29	-	87,87,87,87	0
56	MG	1H	3302	1/1	0.53	0.37	-	88,88,88,88	0
56	MG	1H	3299	1/1	0.86	0.40	-	83,83,83,83	0
56	MG	14	3245	1/1	0.70	0.17	-	83,83,83,83	0
56	MG	1H	3268	1/1	0.81	0.32	-	84,84,84,84	0
56	MG	1H	3498	1/1	0.93	0.09	-	74,74,74,74	0
56	MG	1H	3284	1/1	0.91	0.38	-	81,81,81,81	0
56	MG	13	1725	1/1	0.75	0.10	-	114,114,114,114	0
56	MG	14	3126	1/1	0.96	0.32	-	80,80,80,80	0
56	MG	14	3343	1/1	0.94	0.05	-	81,81,81,81	0
56	MG	13	1638	1/1	0.88	0.33	-	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3147	1/1	0.75	0.29	-	93,93,93,93	0
56	MG	13	1639	1/1	0.96	0.19	-	87,87,87,87	0
56	MG	1H	3228	1/1	0.96	0.21	-	67,67,67,67	0
56	MG	13	1644	1/1	0.96	0.39	-	87,87,87,87	0
56	MG	14	3262	1/1	0.55	0.13	-	101,101,101,101	0
56	MG	1H	3207	1/1	0.76	0.34	-	76,76,76,76	0
56	MG	1H	3422	1/1	0.62	0.14	-	99,99,99,99	0
56	MG	1G	1634	1/1	0.84	0.44	-	114,114,114,114	0
56	MG	14	3395	1/1	0.80	0.09	-	105,105,105,105	0
56	MG	1H	3127	1/1	0.92	0.36	-	64,64,64,64	0
56	MG	1H	3191	1/1	0.90	0.23	-	83,83,83,83	0
56	MG	14	3386	1/1	0.83	0.06	-	96,96,96,96	0
56	MG	1G	1692	1/1	0.79	0.06	-	106,106,106,106	0
56	MG	14	3139	1/1	0.93	0.30	-	97,97,97,97	0
56	MG	13	1618	1/1	0.94	0.35	-	67,67,67,67	0
56	MG	14	3358	1/1	0.72	0.16	-	98,98,98,98	0
56	MG	14	3387	1/1	0.97	0.06	-	90,90,90,90	0
56	MG	14	3170	1/1	0.91	0.11	-	77,77,77,77	0
56	MG	14	3130	1/1	0.73	0.26	-	98,98,98,98	0
56	MG	1H	3294	1/1	0.46	0.54	-	88,88,88,88	0
56	MG	14	3065	1/1	0.96	0.15	-	71,71,71,71	0
56	MG	1H	3059	1/1	0.96	0.28	-	70,70,70,70	0
56	MG	1H	3317	1/1	0.93	0.19	-	75,75,75,75	0
56	MG	1H	3376	1/1	0.90	0.09	-	88,88,88,88	0
56	MG	1J	202	1/1	0.82	0.18	-	93,93,93,93	0
56	MG	1G	1648	1/1	0.84	0.32	-	85,85,85,85	0
56	MG	13	1677	1/1	0.55	0.36	-	96,96,96,96	0
56	MG	14	3195	1/1	0.91	0.13	-	51,51,51,51	0
56	MG	1G	1626	1/1	0.96	0.24	-	99,99,99,99	0
56	MG	13	1740	1/1	0.97	0.07	-	83,83,83,83	0
56	MG	14	3409	1/1	0.85	0.09	-	109,109,109,109	0
56	MG	1H	3040	1/1	0.84	0.36	-	72,72,72,72	0
56	MG	1H	3413	1/1	0.95	0.15	-	82,82,82,82	0
56	MG	1H	3387	1/1	0.98	0.10	-	63,63,63,63	0
56	MG	14	3067	1/1	0.94	0.17	-	76,76,76,76	0
56	MG	1H	3494	1/1	0.84	0.07	-	107,107,107,107	0
56	MG	1G	1651	1/1	0.81	0.19	-	95,95,95,95	0
56	MG	1H	3377	1/1	0.95	0.10	-	90,90,90,90	0
56	MG	13	1741	1/1	0.60	0.08	-	99,99,99,99	0
56	MG	1H	3369	1/1	0.86	0.15	-	58,58,58,58	0
56	MG	14	3327	1/1	0.95	0.08	-	70,70,70,70	0
56	MG	14	3342	1/1	0.86	0.08	-	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	MG	1H	3251	1/1	0.94	0.15	-	115,115,115,115	0
56	MG	1H	3110	1/1	0.77	0.36	-	75,75,75,75	0
56	MG	1H	3140	1/1	0.64	0.43	-	87,87,87,87	0
56	MG	14	3082	1/1	0.98	0.23	-	75,75,75,75	0
56	MG	14	3239	1/1	0.79	0.24	-	92,92,92,92	0
56	MG	1H	3097	1/1	0.79	0.18	-	76,76,76,76	0
56	MG	14	3172	1/1	0.91	0.18	-	87,87,87,87	0
56	MG	14	3157	1/1	0.61	0.19	-	68,68,68,68	0
56	MG	14	3290	1/1	0.86	0.13	-	68,68,68,68	0
56	MG	13	1625	1/1	0.92	0.32	-	74,74,74,74	0
56	MG	14	3112	1/1	0.86	0.23	-	85,85,85,85	0
56	MG	1H	3067	1/1	0.92	0.28	-	75,75,75,75	0
56	MG	13	1749	1/1	0.92	0.10	-	107,107,107,107	0
56	MG	1H	3236	1/1	0.89	0.12	-	72,72,72,72	0
56	MG	1H	3044	1/1	0.86	0.26	-	76,76,76,76	0
56	MG	13	1720	1/1	0.94	0.10	-	105,105,105,105	0
56	MG	13	1653	1/1	0.85	0.28	-	91,91,91,91	0
56	MG	1H	3474	1/1	0.88	0.09	-	103,103,103,103	0
56	MG	1H	3206	1/1	0.82	0.38	-	76,76,76,76	0
56	MG	14	3249	1/1	0.96	0.13	-	89,89,89,89	0
56	MG	1H	3297	1/1	0.69	0.29	-	79,79,79,79	0
56	MG	14	3030	1/1	0.86	0.18	-	84,84,84,84	0
56	MG	14	3326	1/1	0.91	0.08	-	58,58,58,58	0
56	MG	1H	3170	1/1	0.78	0.15	-	71,71,71,71	0
56	MG	14	3359	1/1	0.92	0.07	-	117,117,117,117	0
56	MG	1G	1646	1/1	0.93	0.43	-	108,108,108,108	0
56	MG	1H	3510	1/1	0.85	0.07	-	99,99,99,99	0
56	MG	13	1727	1/1	0.97	0.11	-	111,111,111,111	0
56	MG	1G	1610	1/1	0.94	0.09	-	103,103,103,103	0
56	MG	13	1711	1/1	0.70	0.08	-	106,106,106,106	0
56	MG	1H	3177	1/1	0.91	0.43	-	72,72,72,72	0
56	MG	1H	3272	1/1	0.85	0.34	-	92,92,92,92	0
56	MG	14	3368	1/1	0.81	0.07	-	105,105,105,105	0
56	MG	14	3115	1/1	0.79	0.28	-	82,82,82,82	0
56	MG	1H	3356	1/1	0.90	0.14	-	81,81,81,81	0
56	MG	1H	3112	1/1	0.84	0.23	-	72,72,72,72	0
56	MG	14	3093	1/1	0.97	0.23	-	58,58,58,58	0
56	MG	1H	3190	1/1	0.84	0.43	-	85,85,85,85	0
56	MG	14	3135	1/1	0.66	0.17	-	84,84,84,84	0
56	MG	1H	3245	1/1	0.93	0.15	-	73,73,73,73	0
56	MG	1H	3181	1/1	0.96	0.34	-	84,84,84,84	0
56	MG	14	3253	1/1	0.73	0.13	-	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3243	1/1	0.60	0.18	-	93,93,93,93	0
56	MG	1H	3381	1/1	0.87	0.10	-	78,78,78,78	0
56	MG	1H	3496	1/1	0.92	0.08	-	103,103,103,103	0
56	MG	1H	3347	1/1	0.91	0.12	-	54,54,54,54	0
56	MG	14	3179	1/1	0.87	0.09	-	71,71,71,71	0
56	MG	1H	3354	1/1	0.86	0.11	-	106,106,106,106	0
56	MG	11	301	1/1	0.87	0.30	-	78,78,78,78	0
56	MG	14	3028	1/1	0.92	0.23	-	101,101,101,101	0
56	MG	1H	3370	1/1	0.98	0.16	-	67,67,67,67	0
56	MG	14	3044	1/1	0.90	0.25	-	52,52,52,52	0
56	MG	14	3231	1/1	0.79	0.13	-	79,79,79,79	0
56	MG	1H	3157	1/1	0.95	0.29	-	57,57,57,57	0
56	MG	13	1645	1/1	0.86	0.27	-	94,94,94,94	0
56	MG	1H	3495	1/1	0.93	0.15	-	75,75,75,75	0
56	MG	1H	3120	1/1	0.70	0.30	-	89,89,89,89	0
56	MG	14	3310	1/1	0.92	0.10	-	65,65,65,65	0
56	MG	14	3218	1/1	0.69	0.23	-	95,95,95,95	0
56	MG	1H	3512	1/1	0.93	0.13	-	80,80,80,80	0
56	MG	14	3091	1/1	0.95	0.19	-	64,64,64,64	0
56	MG	1H	3508	1/1	0.84	0.10	-	117,117,117,117	0
56	MG	1H	3088	1/1	0.88	0.09	-	71,71,71,71	0
56	MG	1H	3353	1/1	0.81	0.08	-	100,100,100,100	0
56	MG	14	3270	1/1	0.69	0.29	-	98,98,98,98	0
56	MG	1H	3523	1/1	0.79	0.09	-	115,115,115,115	0
56	MG	2K	107	1/1	0.89	0.10	-	86,86,86,86	0
56	MG	1H	3276	1/1	0.71	0.19	-	87,87,87,87	0
56	MG	1H	3321	1/1	0.74	0.30	-	93,93,93,93	0
56	MG	14	3273	1/1	0.91	0.13	-	106,106,106,106	0
56	MG	1H	3029	1/1	0.82	0.22	-	91,91,91,91	0
56	MG	14	3192	1/1	0.94	0.35	-	102,102,102,102	0
56	MG	14	3238	1/1	0.92	0.14	-	94,94,94,94	0
56	MG	1H	3006	1/1	0.97	0.40	-	48,48,48,48	0
56	MG	14	3001	1/1	0.96	0.24	-	62,62,62,62	0
56	MG	1H	3436	1/1	0.85	0.16	-	73,73,73,73	0
56	MG	14	3154	1/1	0.57	0.34	-	59,59,59,59	0
56	MG	1H	3374	1/1	0.95	0.08	-	70,70,70,70	0
56	MG	14	3180	1/1	0.85	0.18	-	104,104,104,104	0
56	MG	14	3364	1/1	0.80	0.09	-	132,132,132,132	0
56	MG	1H	3431	1/1	0.91	0.12	-	71,71,71,71	0
56	MG	14	3332	1/1	0.94	0.05	-	94,94,94,94	0
56	MG	1H	3217	1/1	0.76	0.39	-	96,96,96,96	0
56	MG	1H	3417	1/1	0.86	0.12	-	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3142	1/1	0.81	0.13	-	89,89,89,89	0
56	MG	1H	3241	1/1	0.93	0.20	-	87,87,87,87	0
56	MG	14	3057	1/1	0.98	0.32	-	74,74,74,74	0
56	MG	1G	1633	1/1	0.83	0.34	-	101,101,101,101	0
56	MG	16	207	1/1	0.49	0.34	-	96,96,96,96	0
56	MG	13	1719	1/1	0.93	0.17	-	100,100,100,100	0
56	MG	13	1634	1/1	0.87	0.17	-	76,76,76,76	0
56	MG	14	3018	1/1	0.95	0.15	-	96,96,96,96	0
56	MG	1H	3080	1/1	0.94	0.38	-	76,76,76,76	0
56	MG	1H	3163	1/1	0.71	0.31	-	82,82,82,82	0
56	MG	13	1657	1/1	0.77	0.50	-	84,84,84,84	0
56	MG	1H	3352	1/1	0.83	0.15	-	106,106,106,106	0
56	MG	14	3113	1/1	0.86	0.26	-	57,57,57,57	0
56	MG	1H	3316	1/1	0.35	0.27	-	102,102,102,102	0
56	MG	1H	3090	1/1	0.97	0.30	-	65,65,65,65	0
56	MG	1H	3051	1/1	0.89	0.19	-	71,71,71,71	0
56	MG	13	1668	1/1	0.86	0.09	-	98,98,98,98	0
56	MG	14	3064	1/1	0.91	0.21	-	60,60,60,60	0
56	MG	14	3015	1/1	0.94	0.25	-	83,83,83,83	0
56	MG	1H	3250	1/1	0.91	0.32	-	78,78,78,78	0
56	MG	13	1705	1/1	0.58	0.22	-	82,82,82,82	0
56	MG	1G	1645	1/1	0.91	0.19	-	102,102,102,102	0
56	MG	13	1655	1/1	0.78	0.28	-	68,68,68,68	0
56	MG	1H	3503	1/1	0.95	0.10	-	64,64,64,64	0
56	MG	1H	3319	1/1	0.82	0.29	-	87,87,87,87	0
56	MG	1H	3325	1/1	0.82	0.28	-	96,96,96,96	0
56	MG	1H	3222	1/1	0.76	0.66	-	97,97,97,97	0
56	MG	13	1619	1/1	0.97	0.36	-	71,71,71,71	0
56	MG	1H	3073	1/1	0.92	0.39	-	55,55,55,55	0
56	MG	14	3265	1/1	0.60	0.17	-	96,96,96,96	0
56	MG	14	3355	1/1	0.80	0.09	-	78,78,78,78	0
56	MG	14	3101	1/1	0.53	0.24	-	99,99,99,99	0
56	MG	1H	3099	1/1	0.90	0.30	-	74,74,74,74	0
56	MG	1H	3514	1/1	0.99	0.09	-	96,96,96,96	0
56	MG	13	1695	1/1	0.74	0.40	-	100,100,100,100	0
56	MG	1H	3394	1/1	0.93	0.17	-	58,58,58,58	0
56	MG	1H	3462	1/1	0.96	0.17	-	106,106,106,106	0
56	MG	14	3117	1/1	0.91	0.24	-	69,69,69,69	0
56	MG	14	3356	1/1	0.96	0.03	-	85,85,85,85	0
56	MG	13	1661	1/1	0.89	0.12	-	75,75,75,75	0
56	MG	1H	3304	1/1	0.62	0.38	-	94,94,94,94	0
56	MG	2L	104	1/1	0.76	0.10	-	95,95,95,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	13	1652	1/1	0.91	0.42	-	83,83,83,83	0
56	MG	14	3188	1/1	0.96	0.10	-	83,83,83,83	0
56	MG	14	3072	1/1	0.86	0.17	-	82,82,82,82	0
56	MG	3L	101	1/1	0.90	0.24	-	116,116,116,116	0
56	MG	1H	3192	1/1	0.92	0.33	-	81,81,81,81	0
56	MG	14	3225	1/1	0.74	0.23	-	103,103,103,103	0
56	MG	1H	3193	1/1	0.98	0.30	-	89,89,89,89	0
56	MG	14	3075	1/1	0.93	0.31	-	83,83,83,83	0
56	MG	1G	1689	1/1	0.94	0.08	-	114,114,114,114	0
56	MG	14	3280	1/1	0.95	0.10	-	64,64,64,64	0
56	MG	13	1737	1/1	0.87	0.12	-	116,116,116,116	0
56	MG	2K	106	1/1	0.92	0.07	-	94,94,94,94	0
56	MG	14	3086	1/1	0.97	0.25	-	72,72,72,72	0
56	MG	1H	3290	1/1	0.83	0.37	-	82,82,82,82	0
56	MG	13	1636	1/1	0.95	0.41	-	74,74,74,74	0
56	MG	1H	3310	1/1	0.49	0.38	-	84,84,84,84	0
56	MG	14	3241	1/1	0.43	0.18	-	139,139,139,139	0
56	MG	14	3369	1/1	0.94	0.06	-	73,73,73,73	0
56	MG	14	3206	1/1	0.89	0.17	-	86,86,86,86	0
56	MG	13	1730	1/1	0.82	0.08	-	111,111,111,111	0
56	MG	1H	3402	1/1	0.92	0.04	-	102,102,102,102	0
56	MG	1H	3126	1/1	0.90	0.49	-	96,96,96,96	0
56	MG	14	3053	1/1	0.68	0.36	-	78,78,78,78	0
56	MG	14	3124	1/1	0.79	0.35	-	80,80,80,80	0
56	MG	1G	1612	1/1	0.67	0.14	-	109,109,109,109	0
56	MG	1H	3361	1/1	0.95	0.09	-	103,103,103,103	0
56	MG	1H	3143	1/1	0.92	0.31	-	81,81,81,81	0
56	MG	1H	3506	1/1	0.98	0.15	-	57,57,57,57	0
56	MG	1G	1629	1/1	0.85	0.19	-	75,75,75,75	0
56	MG	16	202	1/1	0.90	0.24	-	68,68,68,68	0
56	MG	13	1729	1/1	0.96	0.10	-	73,73,73,73	0
56	MG	I8	101	1/1	0.90	0.08	-	89,89,89,89	0
56	MG	14	3132	1/1	0.79	0.12	-	84,84,84,84	0
56	MG	1H	3214	1/1	0.93	0.23	-	101,101,101,101	0
56	MG	14	3309	1/1	0.88	0.09	-	53,53,53,53	0
56	MG	21	301	1/1	0.95	0.34	-	56,56,56,56	0
56	MG	13	1681	1/1	0.80	0.50	-	116,116,116,116	0
56	MG	14	3108	1/1	0.96	0.12	-	68,68,68,68	0
56	MG	1H	3246	1/1	0.80	0.28	-	81,81,81,81	0
56	MG	1H	3515	1/1	0.76	0.24	-	107,107,107,107	0
56	MG	14	3024	1/1	0.85	0.20	-	64,64,64,64	0
56	MG	1G	1604	1/1	0.94	0.14	-	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	13	1734	1/1	0.91	0.14	-	79,79,79,79	0
56	MG	1G	1654	1/1	0.94	0.13	-	115,115,115,115	0
56	MG	14	3299	1/1	0.85	0.15	-	68,68,68,68	0
56	MG	1H	3212	1/1	0.63	0.33	-	79,79,79,79	0
56	MG	14	3161	1/1	0.84	0.14	-	100,100,100,100	0
56	MG	1H	3409	1/1	0.95	0.13	-	50,50,50,50	0
56	MG	14	3152	1/1	0.85	0.10	-	67,67,67,67	0
56	MG	1G	1636	1/1	0.89	0.21	-	89,89,89,89	0
56	MG	14	3080	1/1	0.74	0.21	-	96,96,96,96	0
56	MG	14	3373	1/1	0.66	0.04	-	138,138,138,138	0
56	MG	14	3418	1/1	0.73	0.07	-	128,128,128,128	0
56	MG	14	3012	1/1	0.96	0.26	-	54,54,54,54	0
56	MG	14	3338	1/1	0.97	0.10	-	62,62,62,62	0
56	MG	14	3244	1/1	0.36	0.22	-	82,82,82,82	0
56	MG	1H	3224	1/1	0.88	0.26	-	67,67,67,67	0
56	MG	14	3155	1/1	0.85	0.11	-	68,68,68,68	0
56	MG	1H	3270	1/1	0.77	0.26	-	75,75,75,75	0
56	MG	1G	1608	1/1	0.93	0.19	-	86,86,86,86	0
56	MG	1H	3234	1/1	0.86	0.36	-	96,96,96,96	0
56	MG	P8	101	1/1	0.74	0.32	-	76,76,76,76	0
56	MG	1G	1639	1/1	0.89	0.21	-	104,104,104,104	0
56	MG	1G	1632	1/1	0.96	0.34	-	92,92,92,92	0
56	MG	14	3010	1/1	0.99	0.16	-	65,65,65,65	0
56	MG	14	3405	1/1	0.89	0.12	-	93,93,93,93	0
56	MG	14	3070	1/1	0.70	0.43	-	92,92,92,92	0
56	MG	1H	3443	1/1	0.94	0.11	-	111,111,111,111	0
56	MG	14	3226	1/1	0.83	0.21	-	83,83,83,83	0
56	MG	1H	3360	1/1	0.92	0.09	-	94,94,94,94	0
56	MG	1H	3242	1/1	0.57	0.40	-	82,82,82,82	0
56	MG	14	3203	1/1	0.87	0.30	-	103,103,103,103	0
56	MG	1H	3499	1/1	0.96	0.07	-	66,66,66,66	0
56	MG	14	3214	1/1	0.55	0.30	-	88,88,88,88	0
56	MG	1H	3318	1/1	0.66	0.31	-	101,101,101,101	0
56	MG	1J	206	1/1	0.80	0.11	-	106,106,106,106	0
56	MG	1G	1635	1/1	0.52	0.28	-	82,82,82,82	0
56	MG	14	3331	1/1	0.90	0.07	-	73,73,73,73	0
56	MG	1G	1693	1/1	0.93	0.06	-	109,109,109,109	0
56	MG	13	1679	1/1	0.21	0.31	-	94,94,94,94	0
56	MG	1H	3524	1/1	0.70	0.06	-	104,104,104,104	0
56	MG	1G	1650	1/1	0.85	0.20	-	91,91,91,91	0
56	MG	1H	3475	1/1	0.82	0.19	-	114,114,114,114	0
56	MG	1H	3439	1/1	0.73	0.11	-	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3487	1/1	0.83	0.12	-	101,101,101,101	0
56	MG	1H	3172	1/1	0.96	0.26	-	60,60,60,60	0
56	MG	14	3254	1/1	0.80	0.18	-	91,91,91,91	0
56	MG	1H	3486	1/1	0.85	0.09	-	97,97,97,97	0
56	MG	13	1716	1/1	0.97	0.13	-	58,58,58,58	0
56	MG	1H	3225	1/1	0.75	0.42	-	87,87,87,87	0
56	MG	14	3404	1/1	0.74	0.05	-	97,97,97,97	0
56	MG	1G	1630	1/1	0.86	0.37	-	92,92,92,92	0
56	MG	1H	3100	1/1	0.97	0.17	-	48,48,48,48	0
56	MG	13	1702	1/1	0.66	0.41	-	109,109,109,109	0
56	MG	14	3026	1/1	0.87	0.13	-	55,55,55,55	0
56	MG	14	3178	1/1	0.97	0.12	-	86,86,86,86	0
56	MG	1H	3531	1/1	0.60	0.09	-	109,109,109,109	0
56	MG	1H	3156	1/1	0.95	0.40	-	85,85,85,85	0
56	MG	14	3344	1/1	0.89	0.12	-	100,100,100,100	0
56	MG	1H	3018	1/1	0.98	0.26	-	67,67,67,67	0
56	MG	14	3311	1/1	0.93	0.11	-	62,62,62,62	0
56	MG	13	1610	1/1	0.88	0.32	-	86,86,86,86	0
56	MG	1H	3415	1/1	0.75	0.06	-	94,94,94,94	0
56	MG	13	1732	1/1	0.92	0.13	-	99,99,99,99	0
56	MG	1H	3053	1/1	0.92	0.31	-	56,56,56,56	0
56	MG	1G	1614	1/1	0.91	0.18	-	92,92,92,92	0
56	MG	14	3284	1/1	0.75	0.08	-	104,104,104,104	0
56	MG	14	3220	1/1	0.72	0.53	-	108,108,108,108	0
56	MG	1H	3158	1/1	0.94	0.27	-	64,64,64,64	0
56	MG	14	3059	1/1	0.94	0.35	-	83,83,83,83	0
56	MG	1H	3386	1/1	0.88	0.12	-	58,58,58,58	0
56	MG	14	3346	1/1	0.96	0.07	-	88,88,88,88	0
56	MG	14	3006	1/1	0.98	0.33	-	68,68,68,68	0
56	MG	88	202	1/1	0.69	0.32	-	60,60,60,60	0
56	MG	14	3281	1/1	0.96	0.10	-	74,74,74,74	0
56	MG	14	3087	1/1	0.90	0.31	-	89,89,89,89	0
56	MG	1G	1627	1/1	0.90	0.24	-	83,83,83,83	0
56	MG	1H	3220	1/1	0.53	0.37	-	82,82,82,82	0
56	MG	1H	3293	1/1	0.76	0.35	-	95,95,95,95	0
56	MG	14	3391	1/1	0.94	0.05	-	96,96,96,96	0
56	MG	14	3061	1/1	0.94	0.27	-	49,49,49,49	0
56	MG	1H	3084	1/1	0.97	0.36	-	64,64,64,64	0
56	MG	14	3337	1/1	0.91	0.05	-	90,90,90,90	0
56	MG	14	3145	1/1	0.72	0.20	-	57,57,57,57	0
56	MG	1H	3472	1/1	0.86	0.11	-	95,95,95,95	0
56	MG	14	3301	1/1	0.95	0.09	-	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3400	1/1	0.92	0.11	-	112,112,112,112	0
56	MG	1H	3480	1/1	0.89	0.10	-	100,100,100,100	0
56	MG	1G	1628	1/1	0.78	0.46	-	83,83,83,83	0
56	MG	1H	3287	1/1	0.82	0.27	-	88,88,88,88	0
56	MG	14	3016	1/1	0.80	0.32	-	65,65,65,65	0
56	MG	14	3376	1/1	0.77	0.24	-	122,122,122,122	0
56	MG	1H	3497	1/1	0.96	0.07	-	64,64,64,64	0
56	MG	1G	1696	1/1	0.52	0.12	-	113,113,113,113	0
56	MG	1H	3364	1/1	0.93	0.07	-	71,71,71,71	0
56	MG	14	3133	1/1	0.81	0.36	-	82,82,82,82	0
56	MG	13	1685	1/1	0.64	0.34	-	91,91,91,91	0
56	MG	13	1699	1/1	0.44	0.19	-	146,146,146,146	0
56	MG	14	3186	1/1	0.89	0.30	-	84,84,84,84	0
56	MG	1H	3420	1/1	0.79	0.09	-	114,114,114,114	0
56	MG	14	3296	1/1	0.85	0.07	-	97,97,97,97	0
56	MG	13	1714	1/1	0.98	0.08	-	79,79,79,79	0
56	MG	1H	3168	1/1	0.77	0.39	-	77,77,77,77	0
56	MG	1G	1671	1/1	0.86	0.11	-	92,92,92,92	0
56	MG	1H	3371	1/1	0.97	0.09	-	73,73,73,73	0
56	MG	14	3234	1/1	0.94	0.28	-	81,81,81,81	0
56	MG	1H	3119	1/1	0.89	0.48	-	70,70,70,70	0
56	MG	13	1660	1/1	0.92	0.40	-	76,76,76,76	0
56	MG	14	3176	1/1	0.96	0.17	-	88,88,88,88	0
56	MG	1H	3507	1/1	0.85	0.08	-	101,101,101,101	0
56	MG	14	3003	1/1	0.99	0.21	-	49,49,49,49	0
56	MG	1H	3253	1/1	0.76	0.49	-	87,87,87,87	0
56	MG	14	3098	1/1	0.82	0.13	-	53,53,53,53	0
56	MG	1H	3322	1/1	0.94	0.23	-	77,77,77,77	0
56	MG	13	1742	1/1	0.70	0.09	-	124,124,124,124	0
56	MG	1H	3005	1/1	0.89	0.28	-	51,51,51,51	0
56	MG	1H	3125	1/1	0.57	0.19	-	97,97,97,97	0
56	MG	1G	1690	1/1	0.88	0.14	-	120,120,120,120	0
56	MG	1H	3400	1/1	0.96	0.11	-	72,72,72,72	0
56	MG	14	3403	1/1	0.91	0.11	-	70,70,70,70	0
56	MG	1H	3257	1/1	0.60	0.27	-	85,85,85,85	0
56	MG	1H	3429	1/1	0.91	0.12	-	64,64,64,64	0
56	MG	13	1629	1/1	0.89	0.34	-	84,84,84,84	0
56	MG	1H	3461	1/1	0.95	0.06	-	89,89,89,89	0
56	MG	13	1623	1/1	0.87	0.38	-	98,98,98,98	0
56	MG	1G	1681	1/1	0.94	0.10	-	93,93,93,93	0
56	MG	1G	1676	1/1	0.60	0.24	-	113,113,113,113	0
56	MG	14	3417	1/1	0.94	0.07	-	118,118,118,118	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3406	1/1	0.95	0.12	-	76,76,76,76	0
56	MG	1H	3215	1/1	0.79	0.32	-	88,88,88,88	0
56	MG	14	3348	1/1	0.84	0.07	-	111,111,111,111	0
56	MG	1H	3375	1/1	0.82	0.08	-	103,103,103,103	0
56	MG	1H	3423	1/1	0.93	0.13	-	77,77,77,77	0
56	MG	1H	3161	1/1	0.53	0.29	-	101,101,101,101	0
56	MG	14	3164	1/1	0.52	0.12	-	76,76,76,76	0
56	MG	14	3103	1/1	0.74	0.28	-	84,84,84,84	0
56	MG	1H	3282	1/1	0.85	0.23	-	60,60,60,60	0
56	MG	14	3106	1/1	0.67	0.28	-	93,93,93,93	0
56	MG	1H	3121	1/1	0.92	0.26	-	59,59,59,59	0
56	MG	14	3312	1/1	0.96	0.04	-	93,93,93,93	0
56	MG	1H	3130	1/1	0.68	0.21	-	83,83,83,83	0
56	MG	14	3362	1/1	0.91	0.10	-	101,101,101,101	0
56	MG	14	3063	1/1	0.96	0.31	-	70,70,70,70	0
56	MG	1H	3060	1/1	0.95	0.12	-	56,56,56,56	0
56	MG	13	1718	1/1	0.79	0.07	-	108,108,108,108	0
56	MG	1H	3077	1/1	0.82	0.48	-	81,81,81,81	0
56	MG	1H	3256	1/1	0.81	0.13	-	83,83,83,83	0
56	MG	14	3077	1/1	0.97	0.11	-	68,68,68,68	0
56	MG	1H	3211	1/1	0.88	0.38	-	69,69,69,69	0
56	MG	14	3288	1/1	0.93	0.06	-	78,78,78,78	0
56	MG	14	3143	1/1	0.86	0.35	-	88,88,88,88	0
56	MG	1H	3522	1/1	0.92	0.25	-	74,74,74,74	0
56	MG	1H	3231	1/1	0.86	0.33	-	92,92,92,92	0
56	MG	14	3399	1/1	0.86	0.09	-	116,116,116,116	0
56	MG	1H	3440	1/1	0.94	0.06	-	98,98,98,98	0
56	MG	1H	3288	1/1	0.67	0.45	-	73,73,73,73	0
56	MG	1H	3492	1/1	0.97	0.06	-	90,90,90,90	0
56	MG	1H	3277	1/1	0.73	0.60	-	98,98,98,98	0
56	MG	1H	3007	1/1	0.82	0.29	-	58,58,58,58	0
56	MG	1H	3469	1/1	0.94	0.06	-	95,95,95,95	0
57	ZN	1G	1697	1/1	0.90	0.35	-	149,149,149,149	0
56	MG	13	1733	1/1	0.84	0.06	-	102,102,102,102	0
56	MG	1G	1622	1/1	0.85	0.17	-	128,128,128,128	0
56	MG	14	3419	1/1	0.85	0.14	-	135,135,135,135	0
56	MG	1L	101	1/1	0.94	0.08	-	94,94,94,94	0
56	MG	1H	3227	1/1	0.66	0.33	-	77,77,77,77	0
56	MG	1H	3139	1/1	0.54	0.23	-	70,70,70,70	0
56	MG	1H	3490	1/1	0.74	0.07	-	147,147,147,147	0
56	MG	1G	1679	1/1	0.98	0.08	-	109,109,109,109	0
56	MG	14	3104	1/1	0.76	0.12	-	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3298	1/1	0.82	0.07	-	79,79,79,79	0
56	MG	14	3370	1/1	0.86	0.08	-	90,90,90,90	0
56	MG	13	1748	1/1	0.95	0.03	-	96,96,96,96	0
56	MG	1H	3446	1/1	0.92	0.17	-	87,87,87,87	0
56	MG	14	3081	1/1	0.95	0.32	-	90,90,90,90	0
56	MG	14	3045	1/1	0.86	0.20	-	82,82,82,82	0
56	MG	14	3111	1/1	0.69	0.39	-	98,98,98,98	0
56	MG	14	3382	1/1	0.78	0.19	-	94,94,94,94	0
56	MG	1G	1660	1/1	0.97	0.27	-	105,105,105,105	0
56	MG	1H	3303	1/1	0.91	0.25	-	84,84,84,84	0
56	MG	1G	1694	1/1	0.75	0.13	-	105,105,105,105	0
56	MG	13	1672	1/1	0.88	0.26	-	103,103,103,103	0
56	MG	14	3384	1/1	0.96	0.10	-	98,98,98,98	0
56	MG	14	3341	1/1	0.96	0.12	-	65,65,65,65	0
56	MG	1H	3141	1/1	0.88	0.42	-	78,78,78,78	0
56	MG	13	1731	1/1	0.62	0.11	-	115,115,115,115	0
56	MG	1H	3183	1/1	0.78	0.15	-	61,61,61,61	0
56	MG	1H	3216	1/1	0.81	0.32	-	87,87,87,87	0
56	MG	14	3402	1/1	0.65	0.08	-	105,105,105,105	0
56	MG	1G	1659	1/1	0.92	0.07	-	150,150,150,150	0
56	MG	14	3038	1/1	0.89	0.20	-	96,96,96,96	0
56	MG	1G	1655	1/1	0.96	0.12	-	127,127,127,127	0
56	MG	1H	3296	1/1	0.88	0.22	-	71,71,71,71	0
56	MG	14	3258	1/1	0.63	0.23	-	80,80,80,80	0
56	MG	14	3413	1/1	0.84	0.07	-	100,100,100,100	0
56	MG	1H	3520	1/1	0.97	0.22	-	91,91,91,91	0
56	MG	2L	102	1/1	0.74	0.38	-	85,85,85,85	0
56	MG	1H	3344	1/1	0.95	0.14	-	69,69,69,69	0
56	MG	14	3008	1/1	0.97	0.36	-	61,61,61,61	0
56	MG	14	3350	1/1	0.98	0.07	-	64,64,64,64	0
56	MG	1H	3306	1/1	0.61	0.28	-	81,81,81,81	0
56	MG	14	3141	1/1	0.86	0.30	-	72,72,72,72	0
56	MG	13	1745	1/1	0.97	0.05	-	104,104,104,104	0
56	MG	1H	3458	1/1	0.56	0.23	-	126,126,126,126	0
56	MG	1G	1684	1/1	0.94	0.07	-	121,121,121,121	0
56	MG	1H	3301	1/1	0.89	0.50	-	110,110,110,110	0
56	MG	14	3266	1/1	0.76	0.23	-	107,107,107,107	0
56	MG	14	3237	1/1	0.90	0.28	-	85,85,85,85	0
56	MG	1H	3094	1/1	0.97	0.14	-	65,65,65,65	0
56	MG	1H	3500	1/1	0.96	0.07	-	82,82,82,82	0
56	MG	1H	3115	1/1	0.75	0.25	-	78,78,78,78	0
56	MG	1H	3478	1/1	0.94	0.11	-	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3138	1/1	0.93	0.14	-	71,71,71,71	0
56	MG	1G	1641	1/1	0.90	0.28	-	92,92,92,92	0
56	MG	1H	3433	1/1	0.79	0.21	-	92,92,92,92	0
56	MG	1H	3279	1/1	0.84	0.19	-	80,80,80,80	0
56	MG	1G	1643	1/1	0.94	0.14	-	147,147,147,147	0
56	MG	14	3410	1/1	0.73	0.23	-	112,112,112,112	0
56	MG	1G	1673	1/1	0.61	0.18	-	93,93,93,93	0
56	MG	1H	3314	1/1	0.91	0.09	-	81,81,81,81	0
56	MG	14	3119	1/1	0.47	0.23	-	97,97,97,97	0
56	MG	14	3005	1/1	0.96	0.20	-	59,59,59,59	0
56	MG	14	3228	1/1	0.87	0.30	-	109,109,109,109	0
56	MG	14	3313	1/1	0.95	0.12	-	65,65,65,65	0
56	MG	13	1687	1/1	0.65	0.35	-	94,94,94,94	0
56	MG	1H	3459	1/1	0.89	0.10	-	101,101,101,101	0
56	MG	1H	3105	1/1	0.91	0.42	-	89,89,89,89	0
56	MG	1H	3335	1/1	0.97	0.10	-	45,45,45,45	0
56	MG	14	3339	1/1	0.93	0.11	-	56,56,56,56	0
56	MG	1H	3505	1/1	0.98	0.10	-	78,78,78,78	0
56	MG	1H	3285	1/1	0.96	0.23	-	82,82,82,82	0
56	MG	1G	1691	1/1	0.95	0.08	-	98,98,98,98	0
56	MG	14	3058	1/1	0.96	0.25	-	89,89,89,89	0
56	MG	14	3302	1/1	0.88	0.14	-	76,76,76,76	0
56	MG	13	1674	1/1	0.74	0.24	-	83,83,83,83	0
56	MG	1H	3070	1/1	0.96	0.41	-	61,61,61,61	0
56	MG	1H	3298	1/1	0.81	0.18	-	71,71,71,71	0
56	MG	1H	3273	1/1	0.48	0.52	-	101,101,101,101	0
56	MG	14	3223	1/1	0.91	0.23	-	60,60,60,60	0
56	MG	14	3166	1/1	0.94	0.29	-	85,85,85,85	0
56	MG	1H	3002	1/1	0.89	0.34	-	43,43,43,43	0
56	MG	1G	1611	1/1	0.93	0.10	-	89,89,89,89	0
56	MG	1H	3445	1/1	0.85	0.12	-	81,81,81,81	0
56	MG	14	3380	1/1	0.96	0.07	-	87,87,87,87	0
56	MG	14	3421	1/1	0.90	0.09	-	136,136,136,136	0
56	MG	14	3401	1/1	0.93	0.07	-	90,90,90,90	0
56	MG	14	3255	1/1	0.02	0.27	-	102,102,102,102	0
56	MG	1H	3086	1/1	0.81	0.17	-	75,75,75,75	0
56	MG	1H	3460	1/1	0.95	0.09	-	81,81,81,81	0
56	MG	14	3291	1/1	0.97	0.11	-	52,52,52,52	0
56	MG	1H	3261	1/1	0.58	0.32	-	98,98,98,98	0
56	MG	1H	3424	1/1	0.97	0.13	-	92,92,92,92	0
56	MG	1G	1662	1/1	0.91	0.14	-	81,81,81,81	0
56	MG	1G	1619	1/1	0.97	0.27	-	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3165	1/1	0.88	0.13	-	69,69,69,69	0
56	MG	1H	3463	1/1	0.83	0.10	-	81,81,81,81	0
56	MG	14	3347	1/1	0.94	0.09	-	88,88,88,88	0
56	MG	1H	3137	1/1	0.75	0.37	-	87,87,87,87	0
56	MG	1H	3467	1/1	0.95	0.09	-	57,57,57,57	0
56	MG	14	3330	1/1	0.97	0.11	-	50,50,50,50	0
56	MG	1G	1624	1/1	0.95	0.16	-	88,88,88,88	0
56	MG	1H	3013	1/1	0.97	0.34	-	59,59,59,59	0
56	MG	1H	3444	1/1	0.71	0.15	-	119,119,119,119	0
56	MG	14	3229	1/1	0.85	0.25	-	107,107,107,107	0
56	MG	1H	3254	1/1	0.58	0.37	-	90,90,90,90	0
56	MG	14	3232	1/1	0.93	0.10	-	100,100,100,100	0
56	MG	1G	1666	1/1	0.76	0.12	-	101,101,101,101	0
56	MG	1H	3373	1/1	0.84	0.07	-	75,75,75,75	0
56	MG	13	1697	1/1	0.52	0.16	-	92,92,92,92	0
56	MG	1H	3131	1/1	0.94	0.13	-	71,71,71,71	0
56	MG	1G	1661	1/1	0.78	0.16	-	104,104,104,104	0
56	MG	1H	3471	1/1	0.87	0.11	-	91,91,91,91	0
56	MG	1H	3180	1/1	0.88	0.20	-	63,63,63,63	0
56	MG	1H	3427	1/1	0.98	0.16	-	56,56,56,56	0
56	MG	13	1723	1/1	0.88	0.12	-	85,85,85,85	0
56	MG	14	3123	1/1	0.65	0.28	-	93,93,93,93	0
56	MG	13	1622	1/1	0.95	0.26	-	99,99,99,99	0
56	MG	1H	3046	1/1	0.93	0.21	-	46,46,46,46	0
56	MG	14	3349	1/1	0.93	0.26	-	82,82,82,82	0
56	MG	14	3211	1/1	0.95	0.10	-	94,94,94,94	0
56	MG	13	1635	1/1	0.60	0.32	-	85,85,85,85	0
56	MG	1H	3034	1/1	0.95	0.30	-	46,46,46,46	0
56	MG	16	212	1/1	0.95	0.07	-	84,84,84,84	0
56	MG	13	1743	1/1	0.87	0.09	-	125,125,125,125	0
56	MG	14	3256	1/1	0.81	0.18	-	86,86,86,86	0
56	MG	1H	3160	1/1	0.65	0.27	-	81,81,81,81	0
56	MG	14	3051	1/1	0.84	0.31	-	83,83,83,83	0
56	MG	1H	3274	1/1	0.69	0.36	-	87,87,87,87	0
56	MG	1H	3075	1/1	0.96	0.35	-	52,52,52,52	0
56	MG	14	3366	1/1	0.83	0.11	-	90,90,90,90	0
56	MG	14	3197	1/1	0.70	0.19	-	83,83,83,83	0
56	MG	13	1683	1/1	0.93	0.40	-	101,101,101,101	0
56	MG	14	3216	1/1	0.68	0.24	-	106,106,106,106	0
56	MG	14	3144	1/1	0.94	0.21	-	83,83,83,83	0
56	MG	1H	3338	1/1	0.98	0.11	-	64,64,64,64	0
56	MG	1H	3275	1/1	0.71	0.26	-	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1G	1638	1/1	0.96	0.14	-	89,89,89,89	0
56	MG	1H	3229	1/1	0.90	0.32	-	82,82,82,82	0
56	MG	1H	3362	1/1	0.98	0.05	-	68,68,68,68	0
56	MG	14	3334	1/1	0.97	0.06	-	111,111,111,111	0
56	MG	14	3109	1/1	0.64	0.17	-	67,67,67,67	0
56	MG	1H	3154	1/1	0.97	0.36	-	77,77,77,77	0
56	MG	16	203	1/1	0.72	0.33	-	82,82,82,82	0
56	MG	1H	3012	1/1	0.99	0.20	-	52,52,52,52	0
56	MG	1H	3477	1/1	0.93	0.10	-	114,114,114,114	0
56	MG	14	3398	1/1	0.95	0.08	-	76,76,76,76	0
56	MG	14	3207	1/1	0.95	0.10	-	72,72,72,72	0
56	MG	1H	3530	1/1	0.69	0.06	-	111,111,111,111	0
56	MG	14	3079	1/1	0.95	0.26	-	83,83,83,83	0
56	MG	1H	3184	1/1	0.92	0.51	-	73,73,73,73	0
56	MG	13	1617	1/1	0.72	0.29	-	85,85,85,85	0
56	MG	1H	3454	1/1	0.97	0.15	-	87,87,87,87	0
56	MG	1G	1678	1/1	0.76	0.12	-	98,98,98,98	0
56	MG	13	1607	1/1	0.94	0.39	-	88,88,88,88	0
56	MG	14	3316	1/1	0.97	0.09	-	57,57,57,57	0
56	MG	14	3099	1/1	0.96	0.33	-	82,82,82,82	0
56	MG	1H	3283	1/1	0.64	0.27	-	103,103,103,103	0
56	MG	14	3205	1/1	0.98	0.22	-	99,99,99,99	0
56	MG	1J	203	1/1	0.92	0.14	-	96,96,96,96	0
56	MG	14	3201	1/1	0.82	0.17	-	86,86,86,86	0
56	MG	1H	3382	1/1	0.97	0.08	-	55,55,55,55	0
56	MG	14	3140	1/1	-0.06	0.39	-	113,113,113,113	0
56	MG	2K	104	1/1	0.92	0.25	-	88,88,88,88	0
56	MG	13	1642	1/1	0.82	0.41	-	76,76,76,76	0
56	MG	1H	3213	1/1	0.96	0.28	-	78,78,78,78	0
56	MG	14	3340	1/1	0.90	0.08	-	104,104,104,104	0
56	MG	1H	3401	1/1	0.91	0.07	-	87,87,87,87	0
56	MG	1H	3534	1/1	0.86	0.17	-	101,101,101,101	0
56	MG	13	1698	1/1	0.50	0.28	-	91,91,91,91	0
56	MG	1G	1606	1/1	0.89	0.15	-	102,102,102,102	0
56	MG	1H	3079	1/1	0.98	0.18	-	46,46,46,46	0
56	MG	1H	3150	1/1	0.94	0.44	-	86,86,86,86	0
56	MG	14	3131	1/1	0.84	0.35	-	89,89,89,89	0
56	MG	14	3196	1/1	0.83	0.12	-	69,69,69,69	0
56	MG	16	208	1/1	0.84	0.48	-	88,88,88,88	0
56	MG	14	3361	1/1	0.88	0.07	-	119,119,119,119	0
56	MG	14	3352	1/1	0.89	0.07	-	91,91,91,91	0
56	MG	1H	3372	1/1	0.90	0.10	-	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1H	3198	1/1	0.86	0.39	-	82,82,82,82	0
56	MG	1H	3003	1/1	0.94	0.25	-	60,60,60,60	0
56	MG	1H	3464	1/1	0.84	0.13	-	90,90,90,90	0
56	MG	1H	3022	1/1	0.90	0.33	-	89,89,89,89	0
56	MG	1G	1647	1/1	0.91	0.31	-	102,102,102,102	0
56	MG	13	1665	1/1	0.86	0.18	-	90,90,90,90	0
56	MG	1H	3030	1/1	0.63	0.31	-	87,87,87,87	0
56	MG	1H	3260	1/1	0.87	0.27	-	93,93,93,93	0
56	MG	14	3151	1/1	0.96	0.09	-	56,56,56,56	0
56	MG	14	3017	1/1	0.98	0.24	-	70,70,70,70	0
56	MG	1H	3393	1/1	0.92	0.13	-	51,51,51,51	0
56	MG	2K	102	1/1	0.91	0.16	-	92,92,92,92	0
56	MG	1J	207	1/1	0.77	0.05	-	100,100,100,100	0
56	MG	1H	3201	1/1	0.90	0.20	-	68,68,68,68	0
56	MG	1H	3438	1/1	0.97	0.09	-	63,63,63,63	0
56	MG	14	3415	1/1	0.91	0.05	-	121,121,121,121	0
56	MG	1H	3096	1/1	0.89	0.32	-	66,66,66,66	0
56	MG	1H	3489	1/1	0.97	0.05	-	89,89,89,89	0
56	MG	2K	105	1/1	0.55	0.29	-	102,102,102,102	0
56	MG	14	3105	1/1	0.77	0.35	-	60,60,60,60	0
56	MG	14	3050	1/1	0.73	0.24	-	74,74,74,74	0
56	MG	1G	1649	1/1	0.64	0.25	-	84,84,84,84	0
56	MG	14	3304	1/1	0.97	0.06	-	89,89,89,89	0
56	MG	1H	3481	1/1	0.84	0.07	-	76,76,76,76	0
56	MG	1H	3289	1/1	0.81	0.20	-	79,79,79,79	0
56	MG	1H	3346	1/1	0.96	0.12	-	58,58,58,58	0
56	MG	14	3282	1/1	0.91	0.08	-	76,76,76,76	0
56	MG	1H	3300	1/1	0.36	0.52	-	102,102,102,102	0
56	MG	13	1689	1/1	0.90	0.50	-	92,92,92,92	0
56	MG	1H	3017	1/1	0.95	0.13	-	63,63,63,63	0
56	MG	1G	1625	1/1	0.42	0.31	-	108,108,108,108	0
56	MG	14	3269	1/1	0.73	0.14	-	84,84,84,84	0
56	MG	1H	3173	1/1	0.70	0.22	-	73,73,73,73	0
56	MG	14	3367	1/1	0.79	0.05	-	115,115,115,115	0
56	MG	1H	3525	1/1	0.89	0.13	-	113,113,113,113	0
56	MG	14	3185	1/1	0.77	0.28	-	80,80,80,80	0
56	MG	14	3397	1/1	0.79	0.11	-	94,94,94,94	0
56	MG	14	3416	1/1	0.61	0.15	-	116,116,116,116	0
56	MG	14	3200	1/1	0.48	0.30	-	94,94,94,94	0
56	MG	1H	3476	1/1	0.73	0.06	-	95,95,95,95	0
56	MG	1H	3491	1/1	0.81	0.05	-	99,99,99,99	0
56	MG	1H	3237	1/1	0.78	0.30	-	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1G	1674	1/1	0.70	0.20	-	92,92,92,92	0
56	MG	1G	1677	1/1	0.77	0.27	-	96,96,96,96	0
56	MG	14	3066	1/1	0.94	0.12	-	62,62,62,62	0
56	MG	1H	3426	1/1	0.96	0.15	-	59,59,59,59	0
56	MG	3E	302	1/1	0.79	0.24	-	121,121,121,121	0
56	MG	1H	3517	1/1	0.76	0.10	-	105,105,105,105	0
56	MG	1G	1653	1/1	0.93	0.12	-	99,99,99,99	0
56	MG	1H	3197	1/1	0.82	0.50	-	101,101,101,101	0
56	MG	1H	3194	1/1	0.85	0.14	-	83,83,83,83	0
56	MG	1H	3269	1/1	0.68	0.33	-	78,78,78,78	0
56	MG	14	3236	1/1	0.89	0.42	-	92,92,92,92	0
56	MG	1H	3324	1/1	0.91	0.09	-	81,81,81,81	0
56	MG	13	1614	1/1	0.88	0.21	-	98,98,98,98	0
56	MG	L8	101	1/1	0.70	0.40	-	81,81,81,81	0
56	MG	14	3279	1/1	0.91	0.03	-	115,115,115,115	0
56	MG	1H	3056	1/1	0.82	0.26	-	74,74,74,74	0
56	MG	14	3134	1/1	0.96	0.23	-	82,82,82,82	0
56	MG	1H	3411	1/1	0.76	0.12	-	80,80,80,80	0
56	MG	13	1658	1/1	0.93	0.41	-	79,79,79,79	0
56	MG	1H	3527	1/1	0.58	0.11	-	103,103,103,103	0
56	MG	1H	3195	1/1	0.87	0.20	-	91,91,91,91	0
56	MG	14	3039	1/1	0.89	0.19	-	81,81,81,81	0
56	MG	1H	3031	1/1	0.93	0.30	-	58,58,58,58	0
56	MG	14	3222	1/1	0.97	0.12	-	62,62,62,62	0
56	MG	14	3043	1/1	0.95	0.23	-	52,52,52,52	0
56	MG	14	3233	1/1	0.40	0.19	-	77,77,77,77	0
56	MG	14	3335	1/1	0.99	0.12	-	89,89,89,89	0
56	MG	1H	3473	1/1	0.93	0.08	-	109,109,109,109	0
56	MG	1H	3016	1/1	0.94	0.30	-	61,61,61,61	0
56	MG	1H	3159	1/1	0.96	0.15	-	53,53,53,53	0
56	MG	1H	3114	1/1	0.92	0.29	-	75,75,75,75	0
56	MG	14	3414	1/1	0.74	0.06	-	99,99,99,99	0
56	MG	1H	3519	1/1	0.79	0.10	-	93,93,93,93	0
56	MG	14	3396	1/1	0.90	0.26	-	101,101,101,101	0
56	MG	1H	3210	1/1	0.82	0.17	-	71,71,71,71	0
56	MG	1H	3291	1/1	0.84	0.15	-	93,93,93,93	0
56	MG	14	3274	1/1	0.94	0.14	-	69,69,69,69	0
56	MG	14	3261	1/1	0.64	0.21	-	91,91,91,91	0
56	MG	1H	3014	1/1	0.97	0.36	-	62,62,62,62	0
56	MG	14	3271	1/1	0.90	0.15	-	99,99,99,99	0
56	MG	1H	3457	1/1	0.94	0.08	-	81,81,81,81	0
56	MG	13	1747	1/1	0.60	0.08	-	107,107,107,107	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3363	1/1	0.71	0.06	-	120,120,120,120	0
56	MG	13	1650	1/1	0.83	0.22	-	105,105,105,105	0
56	MG	1H	3308	1/1	0.93	0.20	-	85,85,85,85	0
56	MG	1H	3248	1/1	0.74	0.37	-	82,82,82,82	0
56	MG	1H	3529	1/1	0.60	0.09	-	113,113,113,113	0
56	MG	1H	3255	1/1	0.49	0.33	-	110,110,110,110	0
56	MG	1H	3069	1/1	0.97	0.34	-	53,53,53,53	0
56	MG	1H	3134	1/1	0.82	0.29	-	90,90,90,90	0
56	MG	14	3137	1/1	0.86	0.15	-	96,96,96,96	0
56	MG	14	3213	1/1	0.76	0.27	-	76,76,76,76	0
56	MG	1H	3403	1/1	0.79	0.12	-	78,78,78,78	0
56	MG	1H	3113	1/1	0.94	0.32	-	84,84,84,84	0
56	MG	14	3129	1/1	0.57	0.17	-	89,89,89,89	0
56	MG	14	3085	1/1	0.97	0.17	-	70,70,70,70	0
56	MG	13	1693	1/1	0.41	0.24	-	86,86,86,86	0
56	MG	14	3163	1/1	0.81	0.15	-	109,109,109,109	0
56	MG	13	1688	1/1	0.77	0.56	-	106,106,106,106	0
56	MG	14	3293	1/1	0.95	0.11	-	73,73,73,73	0
56	MG	1G	1695	1/1	0.85	0.07	-	94,94,94,94	0
56	MG	1H	3453	1/1	0.91	0.06	-	83,83,83,83	0
56	MG	14	3209	1/1	0.92	0.13	-	71,71,71,71	0
56	MG	14	3100	1/1	0.83	0.31	-	69,69,69,69	0
56	MG	1H	3238	1/1	0.82	0.15	-	98,98,98,98	0
56	MG	13	1656	1/1	0.88	0.23	-	84,84,84,84	0
56	MG	1H	3320	1/1	0.82	0.16	-	95,95,95,95	0
56	MG	14	3148	1/1	0.34	0.19	-	96,96,96,96	0
56	MG	14	3345	1/1	0.96	0.05	-	82,82,82,82	0
56	MG	1H	3410	1/1	0.96	0.05	-	66,66,66,66	0
56	MG	14	3181	1/1	0.85	0.14	-	84,84,84,84	0
56	MG	14	3168	1/1	0.93	0.20	-	58,58,58,58	0
56	MG	14	3375	1/1	0.88	0.09	-	92,92,92,92	0
56	MG	1H	3218	1/1	0.82	0.20	-	91,91,91,91	0
56	MG	1G	1687	1/1	0.91	0.10	-	134,134,134,134	0
56	MG	1H	3418	1/1	0.96	0.10	-	77,77,77,77	0
56	MG	13	1744	1/1	0.80	0.09	-	112,112,112,112	0
56	MG	1H	3465	1/1	0.89	0.06	-	85,85,85,85	0
56	MG	1H	3336	1/1	0.92	0.11	-	53,53,53,53	0
56	MG	13	1624	1/1	0.83	0.37	-	89,89,89,89	0
56	MG	14	3120	1/1	0.89	0.12	-	82,82,82,82	0
56	MG	1H	3171	1/1	0.83	0.27	-	65,65,65,65	0
56	MG	14	3158	1/1	0.86	0.41	-	83,83,83,83	0
56	MG	14	3078	1/1	0.90	0.21	-	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3372	1/1	0.29	0.21	-	114,114,114,114	0
56	MG	13	1708	1/1	0.07	0.42	-	112,112,112,112	0
56	MG	13	1669	1/1	0.75	0.36	-	78,78,78,78	0
56	MG	13	1612	1/1	0.93	0.32	-	68,68,68,68	0
56	MG	1H	3123	1/1	0.94	0.34	-	90,90,90,90	0
56	MG	1H	3267	1/1	0.96	0.18	-	96,96,96,96	0
56	MG	1G	1613	1/1	0.92	0.18	-	98,98,98,98	0
56	MG	13	1602	1/1	0.98	0.25	-	70,70,70,70	0
56	MG	1H	3485	1/1	0.93	0.10	-	105,105,105,105	0
56	MG	14	3118	1/1	0.67	0.36	-	110,110,110,110	0
56	MG	14	3009	1/1	0.97	0.17	-	73,73,73,73	0
56	MG	14	3408	1/1	0.90	0.07	-	96,96,96,96	0
56	MG	1H	3535	1/1	0.59	0.08	-	115,115,115,115	0
56	MG	16	211	1/1	0.96	0.13	-	80,80,80,80	0
56	MG	14	3260	1/1	0.90	0.12	-	112,112,112,112	0
56	MG	1H	3421	1/1	0.95	0.08	-	74,74,74,74	0
56	MG	14	3297	1/1	0.95	0.06	-	80,80,80,80	0
56	MG	14	3329	1/1	0.82	0.06	-	88,88,88,88	0
56	MG	1H	3165	1/1	0.85	0.18	-	45,45,45,45	0
56	MG	14	3247	1/1	0.71	0.20	-	89,89,89,89	0
56	MG	1H	3223	1/1	0.88	0.12	-	88,88,88,88	0
56	MG	1G	1680	1/1	0.84	0.05	-	126,126,126,126	0
56	MG	1K	101	1/1	0.98	0.22	-	91,91,91,91	0
56	MG	1G	1656	1/1	0.78	0.16	-	112,112,112,112	0
56	MG	14	3208	1/1	0.89	0.09	-	69,69,69,69	0
56	MG	1H	3309	1/1	0.79	0.38	-	94,94,94,94	0
56	MG	14	3215	1/1	0.87	0.18	-	91,91,91,91	0
56	MG	1G	1623	1/1	0.87	0.45	-	108,108,108,108	0
56	MG	1H	3247	1/1	0.65	0.39	-	105,105,105,105	0
56	MG	1H	3196	1/1	0.94	0.21	-	56,56,56,56	0
56	MG	1H	3281	1/1	0.97	0.38	-	85,85,85,85	0
56	MG	1H	3205	1/1	0.71	0.38	-	78,78,78,78	0
56	MG	1H	3244	1/1	0.72	0.35	-	85,85,85,85	0
56	MG	13	1690	1/1	0.54	0.48	-	109,109,109,109	0
56	MG	14	3325	1/1	0.86	0.08	-	110,110,110,110	0
56	MG	13	1649	1/1	0.81	0.32	-	102,102,102,102	0
56	MG	1H	3501	1/1	0.83	0.14	-	81,81,81,81	0
56	MG	14	3212	1/1	0.77	0.17	-	85,85,85,85	0
56	MG	13	1738	1/1	0.87	0.10	-	109,109,109,109	0
56	MG	1H	3265	1/1	0.68	0.36	-	94,94,94,94	0
56	MG	1H	3488	1/1	0.51	0.12	-	134,134,134,134	0
56	MG	14	3317	1/1	0.98	0.12	-	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	14	3054	1/1	0.79	0.26	-	70,70,70,70	0
56	MG	14	3094	1/1	0.84	0.19	-	89,89,89,89	0
56	MG	1H	3187	1/1	0.92	0.41	-	72,72,72,72	0
56	MG	14	3136	1/1	0.89	0.13	-	92,92,92,92	0
56	MG	1H	3434	1/1	0.94	0.06	-	107,107,107,107	0
56	MG	1G	1668	1/1	0.98	0.26	-	90,90,90,90	0
56	MG	1H	3466	1/1	0.79	0.08	-	105,105,105,105	0
56	MG	1H	3428	1/1	0.96	0.15	-	56,56,56,56	0
56	MG	14	3046	1/1	0.96	0.17	-	70,70,70,70	0
56	MG	14	3374	1/1	0.80	0.12	-	131,131,131,131	0
56	MG	14	3033	1/1	0.96	0.18	-	63,63,63,63	0
56	MG	13	1646	1/1	0.78	0.23	-	80,80,80,80	0
56	MG	1H	3148	1/1	0.82	0.30	-	65,65,65,65	0
56	MG	13	1703	1/1	0.45	0.41	-	105,105,105,105	0
56	MG	1G	1631	1/1	0.86	0.22	-	88,88,88,88	0
57	ZN	14	3422	1/1	0.41	0.19	-	181,181,181,181	0

6.5 Other polymers

There are no such residues in this entry.