



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:39 AM UTC

PDB ID : 4WRO / pdb_00004wro
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

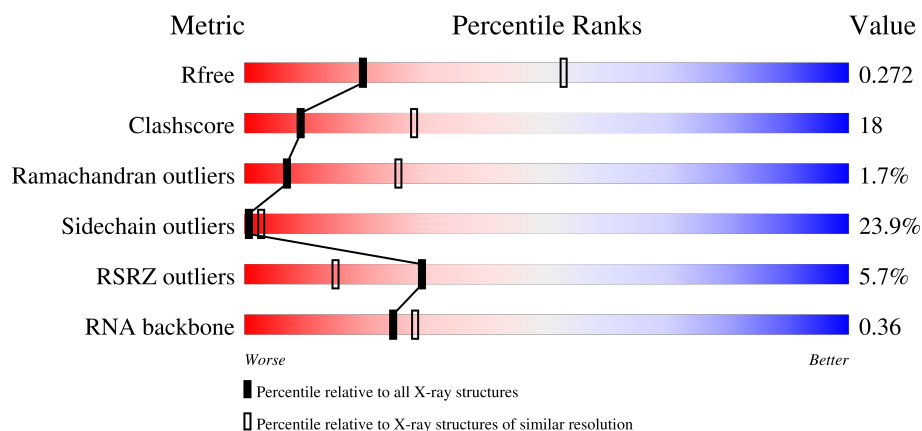
1 Overall quality at a glance

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}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)
RNA backbone	3983	1079 (3.30-2.82)

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

Mol	Chain	Length	Quality of chain
1	13	1522	3% 35% 48% 15% ..
1	1G	1522	5% 36% 46% 16% .
2	1L	76	12% 29% 39% 26% 5%
2	3K	76	20% 18% 43% 34% .

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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	

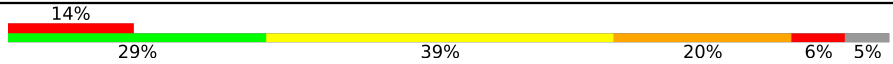
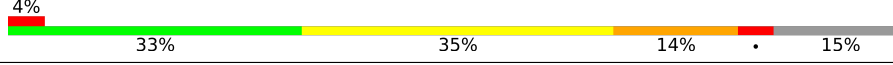
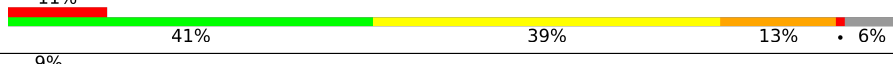
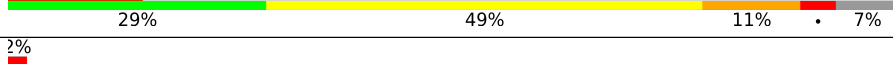
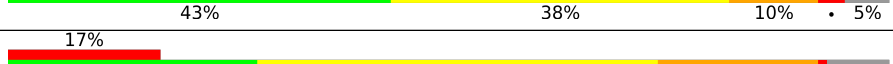
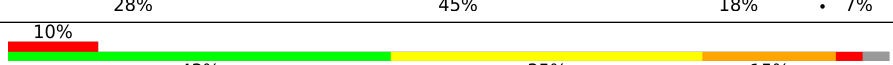
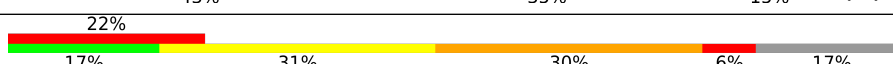
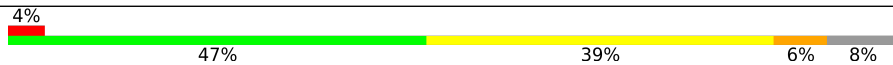
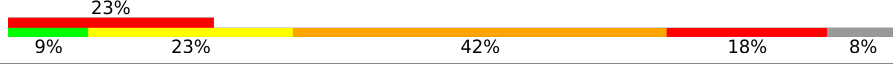
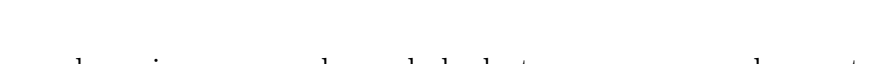
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Mol	Chain	Length	Quality of chain
21	8I	105	
22	9I	88	
23	AI	93	
24	BI	106	
25	1F	27	
26	1K	76	
27	16	122	
27	1J	122	
28	11	276	
29	21	206	
30	31	210	
31	41	182	
32	51	180	
33	61	148	
34	58	140	
35	68	122	
36	78	150	
37	88	141	
38	98	118	
39	A8	112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

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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	1607	-	-	-	X
56	MG	13	1654	-	-	-	X
56	MG	13	1681	-	-	-	X
56	MG	13	1683	-	-	-	X
56	MG	13	1688	-	-	-	X
56	MG	13	1690	-	-	-	X
56	MG	13	1695	-	-	-	X
56	MG	14	3045	-	-	-	X
56	MG	14	3140	-	-	-	X
56	MG	14	3185	-	-	-	X
56	MG	14	3219	-	-	-	X
56	MG	14	3255	-	-	-	X
56	MG	1G	1616	-	-	-	X
56	MG	1G	1621	-	-	-	X
56	MG	1G	1646	-	-	-	X
56	MG	1G	1651	-	-	-	X
56	MG	1H	3105	-	-	-	X
56	MG	1H	3176	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1H	3199	-	-	-	X
56	MG	1H	3203	-	-	-	X
56	MG	1H	3222	-	-	-	X
56	MG	1H	3263	-	-	-	X
56	MG	1H	3277	-	-	-	X
56	MG	1H	3301	-	-	-	X
56	MG	1H	3311	-	-	-	X
56	MG	1H	3315	-	-	-	X
56	MG	2I	302	-	-	-	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
			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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	13	149	Total Mg 149 149	0	0
56	1L	1	Total Mg 1 1	0	0
56	2L	4	Total Mg 4 4	0	0
56	3L	3	Total Mg 3 3	0	0
56	14	421	Total Mg 421 421	0	0
56	3E	2	Total Mg 2 2	0	0
56	5E	1	Total Mg 1 1	0	0
56	3I	1	Total Mg 1 1	0	0
56	5I	1	Total Mg 1 1	0	0
56	1K	2	Total Mg 2 2	0	0
56	2K	8	Total Mg 8 8	0	0
56	1H	537	Total Mg 537 537	0	0
56	1J	7	Total Mg 7 7	0	0
56	16	13	Total Mg 13 13	0	0
56	11	2	Total Mg 2 2	0	0
56	21	2	Total Mg 2 2	0	0
56	41	2	Total Mg 2 2	0	0
56	78	1	Total Mg 1 1	0	0
56	88	2	Total Mg 2 2	0	0
56	I8	1	Total Mg 1 1	0	0
56	J8	1	Total Mg 1 1	0	0
56	L8	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	P8	1	Total 1	Mg 1	0	0
56	1G	96	Total 96	Mg 96	0	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 58 is water.

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

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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

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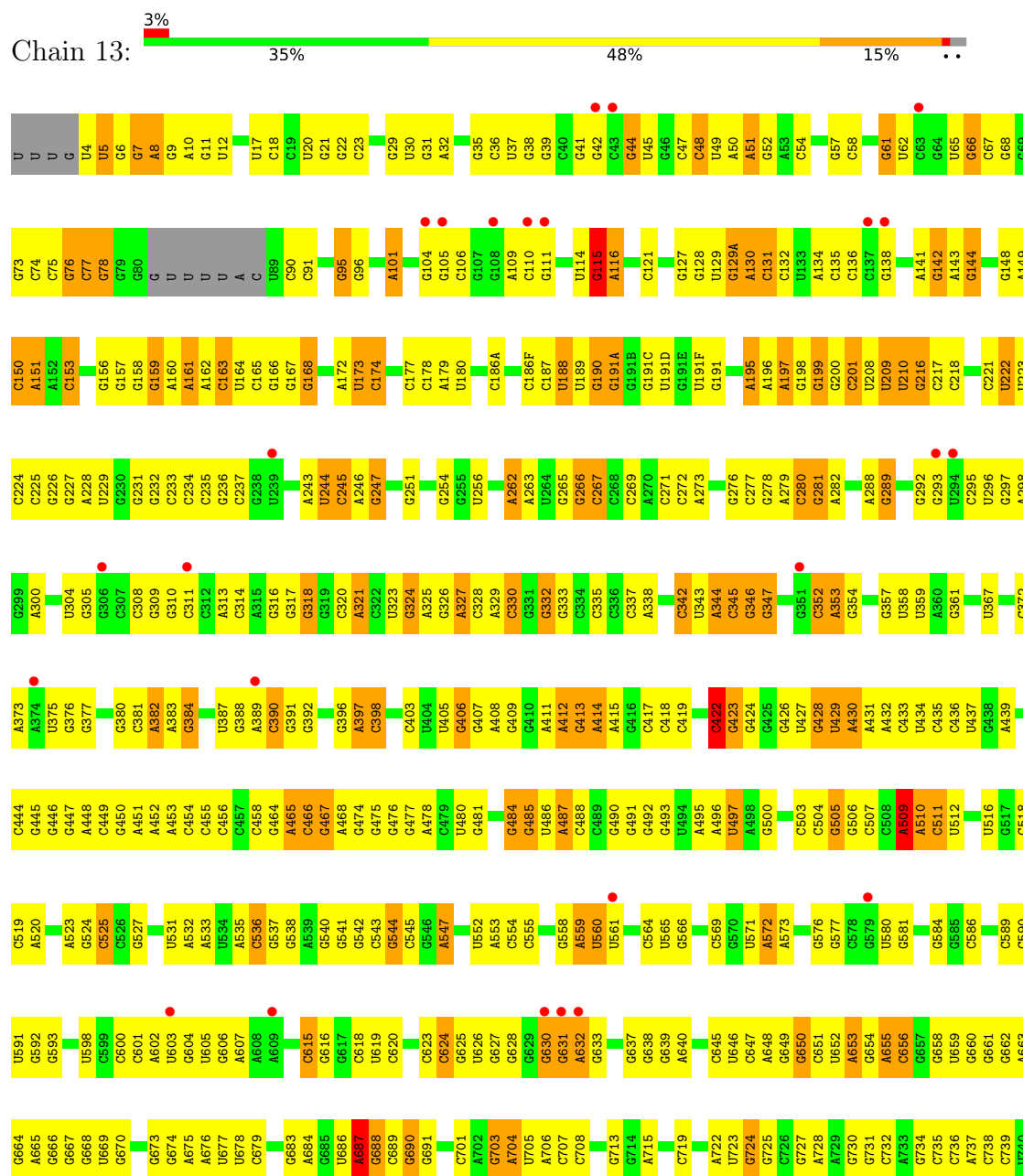
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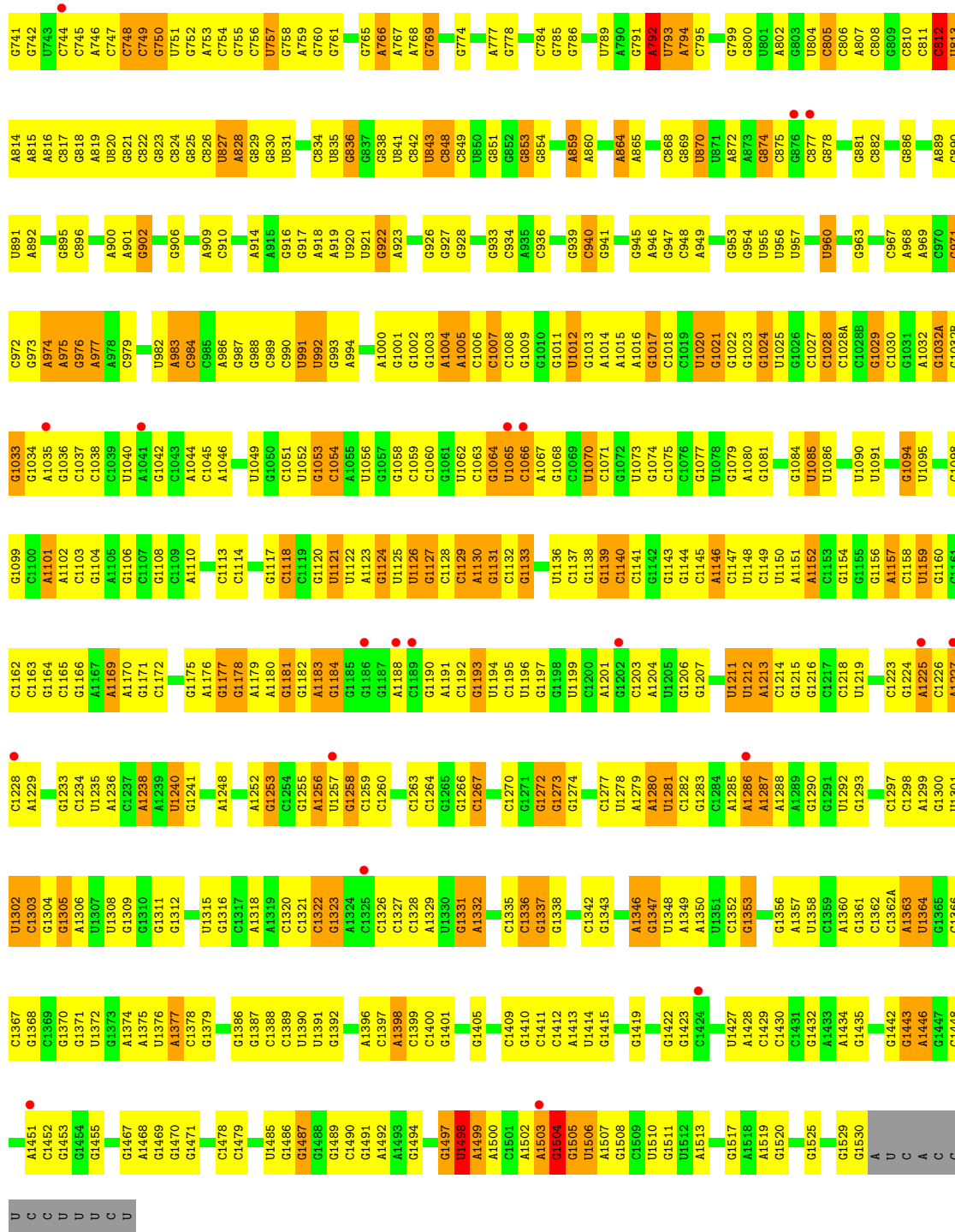
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	F8	2	Total	O	0	0
			2	2		
58	G8	3	Total	O	0	0
			3	3		
58	I8	5	Total	O	0	0
			5	5		
58	J8	1	Total	O	0	0
			1	1		
58	L8	1	Total	O	0	0
			1	1		
58	P8	4	Total	O	0	0
			4	4		
58	Q8	1	Total	O	0	0
			1	1		
58	1G	106	Total	O	0	0
			106	106		

3 Residue-property plots

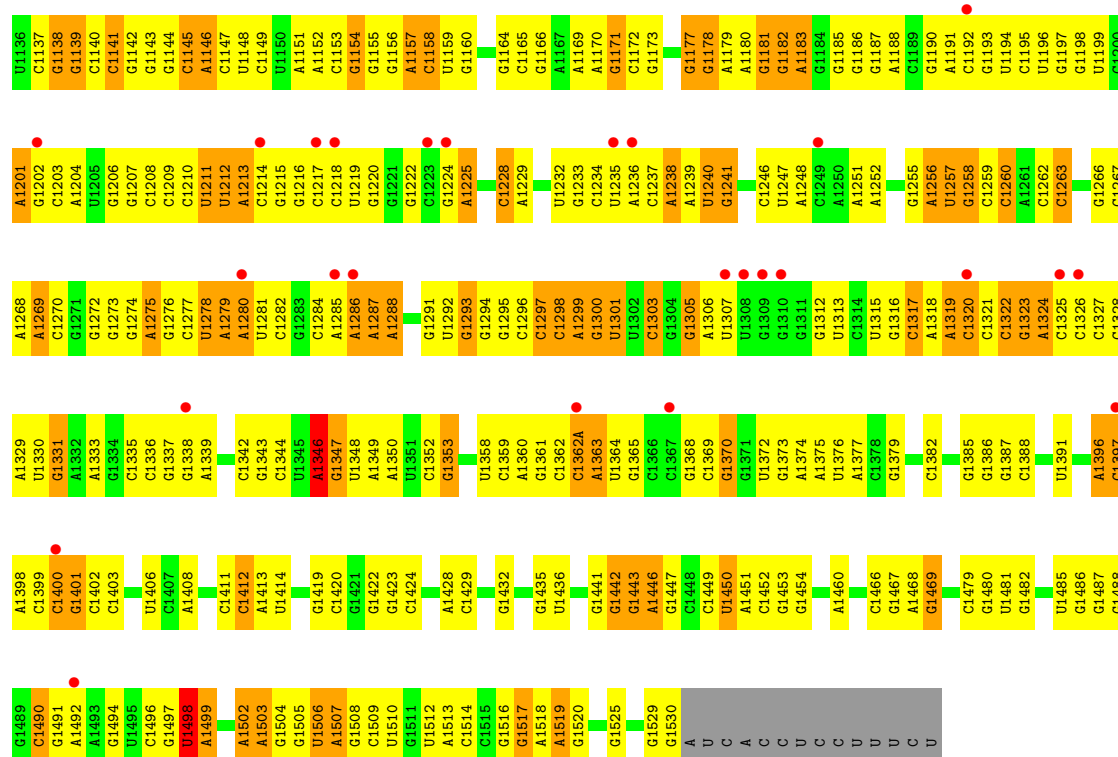
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S ribosomal RNA





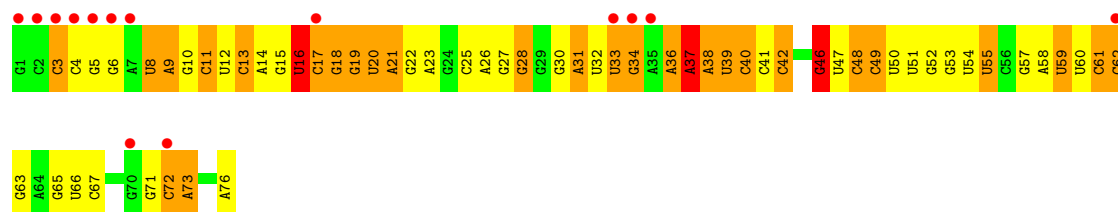
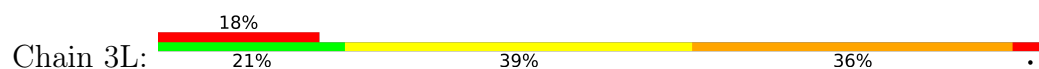




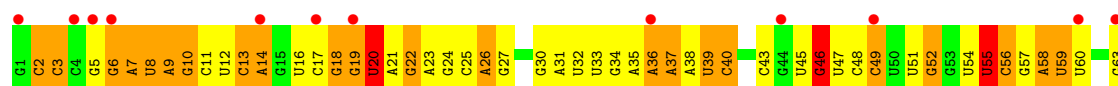
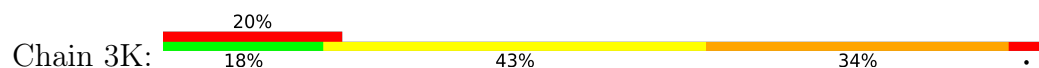
• Molecule 2: tRNA-Phe



• Molecule 2: tRNA-Phe

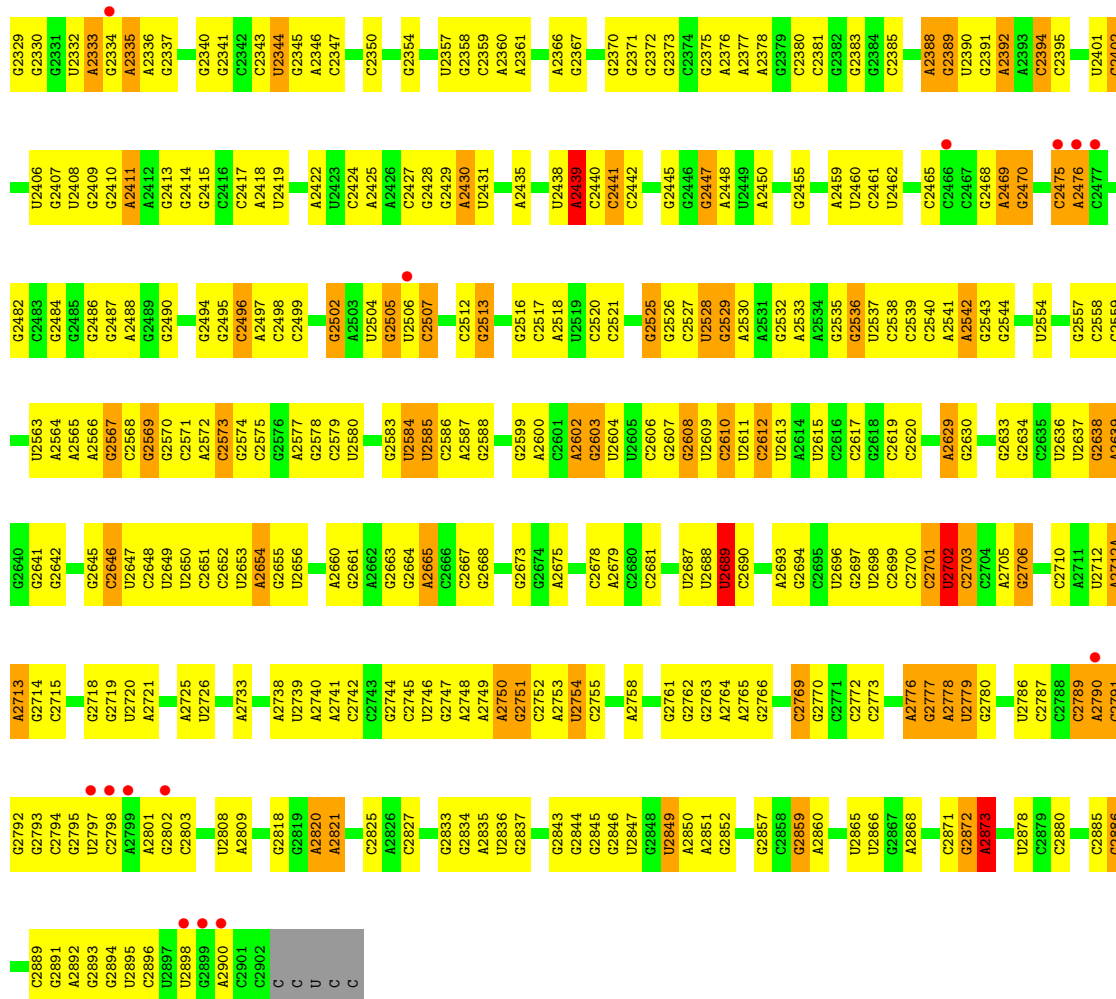


• Molecule 2: tRNA-Phe



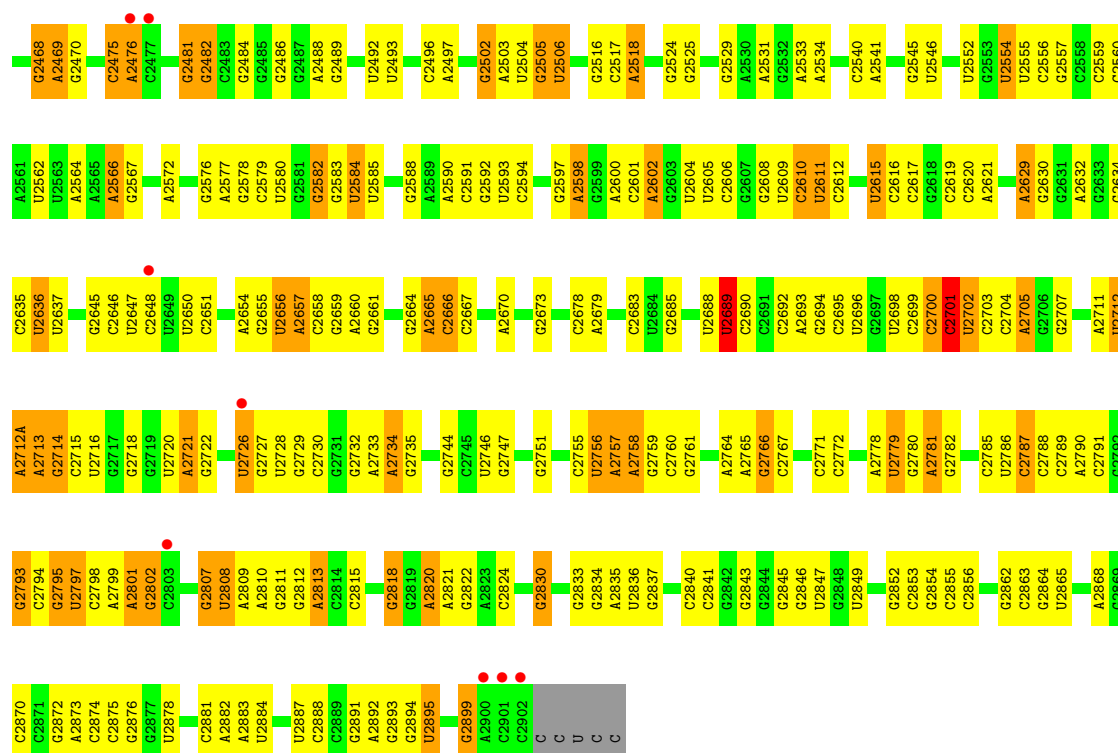
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C1150	A299	C299	G363C	C455	C541	C611	C656	G740	C818	C886	C952	G1018	A1080	C1150
G1151	A300	C300	G363D	C456	C546	U614	C657	G741	A819	A887	A953	U1019	U1081	G1151
C1152	G259	C301	U363E	A457	A546	G617	C658	A746	A820	C888	A954	A1020	U1082	C1152
G1153	G260	C302	A363F	U459	A547	G618	C659	U747	A821	C889	G954	A1021	U1083	G1153
G1154	A265	C303	G372	C460	C548	G619	C660	G748	U822	A890	A957	G1022	A1084	G1154
A1155	G266	C304	U373	C461	A549	G620	C661	G749	G824	G892	A958	U1023	A1085	A1155
U1159	C267	U306	C375	C469	G549	G621	C662	G750	A825	C893	A959	G1024	A1086	U1159
C1160	A270	G307	C376	A470	G552	A621	G663	A751	U827	A896	A960	G1025	A1087	C1160
G1161	G270E	G308	C377	A471	U553	G622	G664	G752	U828	A897	C961	U1026	A1088	G1161
C1162	U270F	G309	G382	A472	U554	G623	A670	G753	A829	C897	G962	A1027	A1028	C1162
G1163	U270G	A310	C386	G473	G556	C624	C671	C754	G830	C898	U963	A1028	A1029	G1163
U1164	G270H	G312	U387	A479	G559	U626	C674	G755	G831	A899	C966	A1032	A1032	U1164
C1166	G270I	G315	G388	A480	C560	U627	A675	G756	A900	A900	C967	U1033	U1033	G1166
G1168	C270J	G316	C388	A481	G561	G628	A676	C758	G836	C901	C968	U1034	U1034	U1168
G1169	C270K	G317	G389	G484	U562	G629	A677	A764	G837	C902	C969	U1035	U1035	G1169
C1170	U270L	C318	U395	C485	C564	G630	C678	G765	C938	C903	C970	U1036	U1036	U1170
G1171	G270M	C319	G396	C486	C565	A631	C679	G766	U839	C904	C971	G1037	G1037	G1171
C1173	G270N	A320	C397	C487	C566	A632	C679	G767	C940	C905	C972	U1038	U1038	C1173
A1174	U270O	G321	C397	G491	U566	A633	C680	G768	C941	G906	A973	G1039	G1039	G1174
U1175	C270P	G322	G400	G492	G570	C634	A685	G769	G843	C908	C974	U1040	U1040	U1175
C1176	C270Q	A322	A401	A493	G571	C635	A686	G771	G844	A909	G977	C1041	C1041	C1176
A1177	G270T	A324	A402	G494	G573	G636	A689	A774	G845	A910	C978	G1042	G1042	C1177
C1178	C270U	G324	U403	G495	C574	G638	C691	G775	U847	A911	C979	C1043	C1043	A1177
G1181	G327	G327	C404	U499	A575	U639	C692	G776	A849	C912	C980	U1044	U1044	U1181
A1182	U328	G329	U405	G500	A576	C640	C693	G777	A853	C915	C982	A1045	A1045	A1182
G1183	A330	A330	A406	A501	A578	C641	U694	U779	G853	C916	C983	G1046	G1046	G1183
C1187	G270V	A332	C407	A502	G579	G642	C695	G780	G854	C917	A984	U1047	U1047	C1187
U1188	U270Z	A333	G408	U504	C580	C645	C696	A781	G855	A918	C985	A1048	A1048	U1188
A1189	C271A	G334	G411	U504	C581	C646	C697	A782	C856	C919	C986	U1049	U1049	G1189
G1192	G271B	C334	U412	A505	G583	G647	C698	A783	C857	C920	C987	G1050	G1050	C1192
C1193	U271C	C335	G413	C509	C584	G648	C699	A784	U858	C921	A988	C1051	C1051	U1192
U1194	G271	C336	C414	A510	G585	C649	C700	G785	G859	C922	G989	A1052	A1052	U1194
G1195	C273C	C337	U415	U511	A586	C650	A706	U787	U860	C923	A990	U1053	U1053	G1195
C1196	U273E	G338	A415	G512	C587	C651	G707	A788	G862	C924	C991	G1054	G1054	C1196
G1197	A340	U339	U421	A513	U588	G654	C715	A789	A864	C925	C992	U1055	U1055	U1197
U1198	G274	A340	U427	A514	C589	A654	A716	G792	C865	C926	C993	G1056	G1056	A1198
C1200	G275	G341	A428	A515	C591	C654A	G717	C796	A866	C927	A996	U1060	U1060	U1199
G1201	A276	G342	C433	U519	G592	C654B	C718	C797	C867	C928	C997	U1061	U1061	C1200
C1202	C277	C344	U434	G521	G597	C654C	C719	G798	U868	C929	C998	G1062	G1062	G1201
G1203	A278	G352	C442	G522	U597	C654E	A722	G799	C869	C930	C999	C1063	C1063	U1202
A1204	C280	G353	A443	G523	G598	C654F	C725	G801	U871	C935	A1000	U1064	U1064	C1203
U1205	G281	C354	C444	C523	G599	C654G	G725	A802	G872	C936	A1001	U1065	U1065	G1204
A1210	C286	G355	A445	U524	G600	C654H	C729	G805	G873	U937	G1002	U1066	U1066	A1205
C1213	C287	C356	C446	U525	C601	C654I	G729	C806	U877	G938	G1003	A1067	A1067	C1213
G1216	C288	G357	C447	C527	G602	A526	C730	C807	U878	C939	G1004	G1068	G1068	U1216
C1217	U358	C358	U447	C527	G604	C654J	C731	U807	A878	G940	C1005	A1069	A1069	C1217
A1220	A289	U359	U448	A529	G605	C654K	C731	G808	G879	A941	G1011	U1070	U1070	A1220
G1220	G290	G360	A449	G530	U606	C654L	A734	G809	G880	G942	U943	C1071	C1071	G1220
C1221	C291	C361	A450	C531	U607	C654M	A735	G812	G881	G943	U944	A1072	A1072	C1221
G1220	U362	C363	C451	A532	C608	C654P	C736	C812	G882	G944	U945	C1073	C1073	G1220
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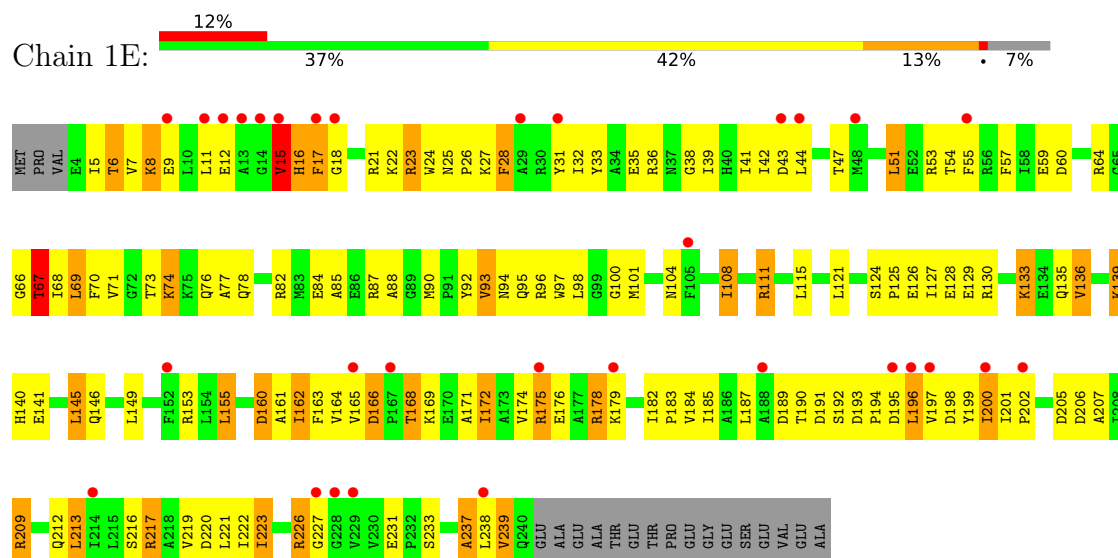


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C1102	A1103	A1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	U1114	C1119	G1120	G1121	C1124	G1125	A1126	A1127	A1128	A1129	U1130	G1131	C1135	G1136	G1137	G1138	U1139	A1140	U1141	U1142	A1143	A1144	C1145	C1150	G1151	C1152	C1153	G1154	A1155	A1156	U1159	G1160	G1163	G1164	U1165	C1166	U1167	G1168	U1240	U1241	G1170	C1171			
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C731	C732	G733	A734	A735	C736	U740	G741	G742	G743	G744	G745	A746	U747	A751	A752	C753	C754	C755	U756	U757	C758	G759	G760	G761	U762	G763	A764	G765	G768	U773	A774	G775	G776	A777	G778	U779	G780	A781	A782	A783	A784	G785	C790	C791	G792	A793	G794	C795	C796	C797	G798	G799	A800	C801		
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A528	A529	A530	C531	A532	A533	U534	C535	G545	G546	A547	A548	G549	G550	G551	G556	U557	G558	U562	G563	C564	C565	U566	A567	U568	U569	A570	A571	A572	C574	A575	U576	U577	A578	C580	C581	G582	G583	C584	G585	A586	C587	U588	C589	G593	G598	G599	G600	C601	G602	A603	G604					
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G363	A363A	G363B	G363C	G363D	U363E	A363F	C364	G365	G370	A371	G372	C376	G381	G382	G386	G389	C392	C393	A394	U395	G396	G397	G398	G399	G400	C404	U405	G406	G407	G411	A412	A415	C416	C420	G425	C426	U427	A428	A429	G430	U431	A432	G438	G439	G442	A443										

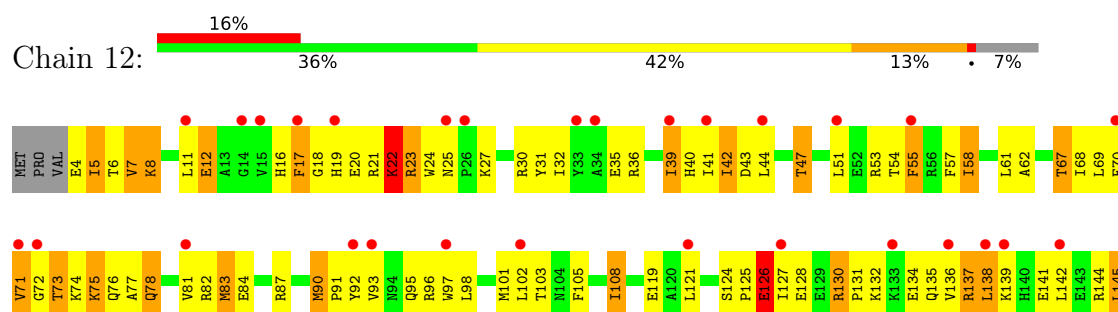
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G2390	A2320	G2256	C2105	G2106	A2021	U1939	A1952	G1776	A1676	U1602	A1536	A1396
G2391	G2321	G2257	A2170	G2107	G2022	U1940	A1853	G1777	A1677	U1603	C1537	U1397
A2392	G2324	C2258	A2171	C2108	G2023	C1942	A1854	U1778	G1678	C1604	G1538	C1398
A2393	G2325	G2259	U2109	G2109	G2027	U1943	G1855	U1779	U1680	G1605	C1539	C1399
C2394	C2326	G2260	C2174	G2110	G2028	U1944	G1856	U1780	G1681	G1606	G1488	G1400
G2395	A2327	G2261	C2175	G2111	U2028	A1952	G1857	A1781	G1682	C1607	U1541	G1401
G2396	A2328	U2262	C2176	G2112	G2029	A1953	G1858	C1782	G1683	A1608	G1470	C1402
G2397	G2329	C2263	C2177	U2113	A2030	G1954	G1860	C1783	A1543	A1609	A1471	C1403
G2398	G2330	C2264	A2114	A2114	A2031	U1955	G1861	A1784	C1684	A1610	A1472	C1404
G2399	G2331	G2267	G2178	G2115	G2032	U1956	A1862	A1785	U1688	G1613	G1473	U1405
G2400	G2332	U2180	U2180	G2116	A2033	C1957	G1862	A1786	A1689	A1614	G1474	U1406
U2401	G2333	G2268	G2181	A2117	U2034	C1958	G1863	G1787	C1547	G1548	G1475	C1407
C2402	A2334	A2268	G2182	A2118	G2035	G1961	A1870	C1790	C1548	C1549	G1478	C1408
C2403	A2335	G2270	C2183	A2119	G2036	G1962	A1871	A1791	C1549	C1550	G1479	A1412
G2404	A2336	G2271	G2184	G2123	G2040	U1963	A1872	U1693	C1694	A1618	G1480	G1413
G2405	G2337	G2272	C2185	G2124	A2041	G1964	C1878	C1695	U1554	U1621	U1482	G1416
U2406	G2338	G2186	G2186	G2125	A2042	G1965	G1883	A1698	G1555	G1622	G1483	C1417
G2407	G2339	G2273	G2187	A2126	C2043	A1966	A1884	G1699	C1556	G1623	A1486	G1418
G2410	G2341	A2274	G2190	G2127	G2049	C1967	A1885	A1700	C1557	G1626	G1487	A1419
G2411	G2342	C2275	G2193	C2128	G2050	U1968	C1886	A1701	A1558	G1530	U1420	G1421
G2413	G2343	G2279	G2194	U2136	A2051	A1970	G1887	G1705	G1559	G1560	G1422	G1422
G2414	U2344	G2280	A2199	G2137	G2052	A1971	G1888	U1706	G1561	G1562	G1423	G1423
G2415	G2345	C2281	C2205	U2138	A2053	A1972	A1889	G1728	C1493	A1494	A1494	G1424
A2418	A2346	G2282	C2206	U2139	G2054	G1973	A1890	A1729	C1508	C1569	U1431	U1431
U2419	U2347	C2283	G2216	C2140	A2055	G1974	G1904	U1730	A1570	C1509	C1432	C1432
A2424	G2348	G2284	G2217	C2141	G2056	G1975	G1905	G1731	A1571	A1510	U1433	U1433
A2425	G2349	C2285	G2218	A2135	G2057	U1976	G1906	A1732	A1511	G1512	A1434	A1434
A2426	C2350	A2287	U2212	C2136	A2058	U1977	U1808	G1726	C1574	G1513	U1438	U1438
G2427	G2351	G2288	G2213	C2137	A2059	G1980	A1809	U1727	C1575	C1513	A1439	A1439
G2428	G2352	G2289	G2214	C2138	A2060	U1981	G1813	G1746	U1576	U1576	G1440	G1440
G2429	G2353	U2291	G2215	C2139	G2061	C1982	G1814	G1747	C1577	C1515	G1441	G1441
A2430	A2360	G2292	G2216	C2140	A2062	C1983	A1815	A1749	A1578	U1516	G1442	G1442
U2431	G2361	G2293	G2217	C2141	C2063	G1984	G1816	C1751	A1580	G1517	G1443	G1443
A2432	G2362	C2294	G2218	U2144	G2064	U1985	G1817	G1756	C1582	U1520	A1444	A1444
A2435	G2363	A2225	C2226	C2145	C2065	G1986	A1819	U1757	A1586	G1521	A1449	A1449
G2436	A2364	A2227	G2227	G2146	C2066	C1987	U1820	G1758	A1587	U1522	G1453	G1453
U2437	G2365	G2228	G2228	G2147	G2067	U1991	A1821	A1762	C1588	U1523	U1454	U1454
U2438	G2366	G2229	G2229	G2148	U2068	G1992	U1915	G1763	C1589	G1524	G1455	G1455
A2439	G2367	G2300	G2300	G2149	G2069	U1993	A1919	C1766	U1590	G1525	G1456	G1456
G2440	G2370	G2301	U2232	U2150	G2070	U1994	C1920	U1767	C1592	A1528	A1457	A1457
G2441	G2371	G2302	U2233	G2151	G2071	U1995	G1921	U1768	G1595	C1529	C1458	C1458
G2442	G2372	G2303	U2234	G2152	U2074	C1996	G1922	G1769	C1598	C1532	G1459	G1459
C2443	G2373	A2304	G2235	G2153	U2075	G1997	U1923	A1847	C1599	C1533	A1460	A1460
G2444	G2374	C2305	G2236	G2154	G2076	G1998	G1924	G1770	C1599	C1534	C1461	C1461
A2375	A2376	C2306	C2237	G2155	U2077	U1999	C1925	G1771	C1599	C1535	C1462	C1462
A2377	A2377	G2307	G2238	G2156	G2080	A2001	U1926	C1772	C1599	C1536	C1463	C1463
A2378	A2378	G2308	G2239	G2157	G2081	G2002	U1927	C1773	C1599	C1537	C1464	C1464
G2445	G2379	A2309	C2240	A2158	U2092	G2003	G1928	A1848	C1774	C1538	C1465	C1465
G2446	G2380	A2310	G2241	G2159	G2093	G2004	G1929	G1775	C1775	C1539	C1466	C1466
A2448	C2381	A2241	G2242	G2160	G2094	G2005	U1930	U1768	C1776	C1540	C1467	C1467
G2449	G2382	U2112	G2243	C2161	G2095	U2010	A1931	U1769	C1777	C1541	C1468	C1468
C2452	G2383	C2313	U2244	C2162	G2096	G2012	G1933	U1770	C1778	C1542	C1469	C1469
A2453	G2384	C2314	U2245	C2163	U2097	A2013	C1934	A1849	C1779	C1543	C1470	C1470
G2454	G2385	G2315	U2246	C2164	G2100	A2014	G1935	C1779	C1779	C1544	C1471	C1471
G2455	G2386	C2316	G2247	G2165	G2101	A2015	A1936	C1779	C1779	C1545	C1472	C1472
G2458	U2387	C2317	C2248	C2166	G2102	A2016	A1937	C1779	C1779	C1546	C1473	C1473

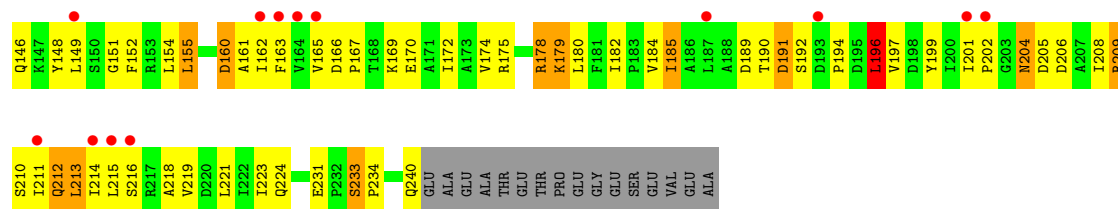


• Molecule 6: 30S ribosomal protein S2

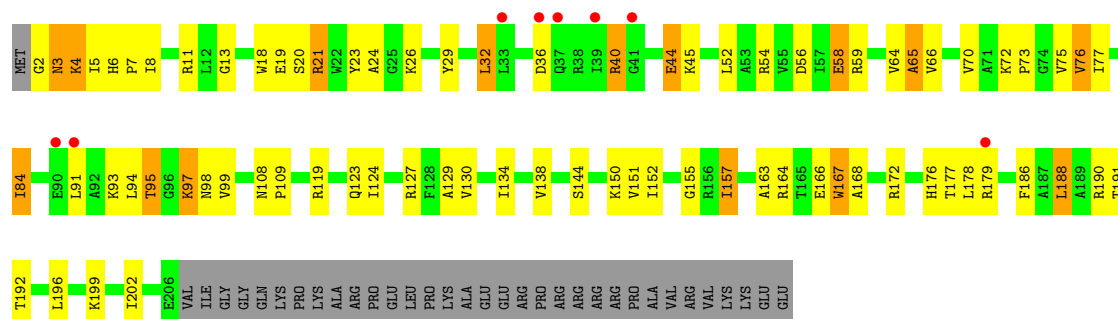


• Molecule 6: 30S ribosomal protein S2

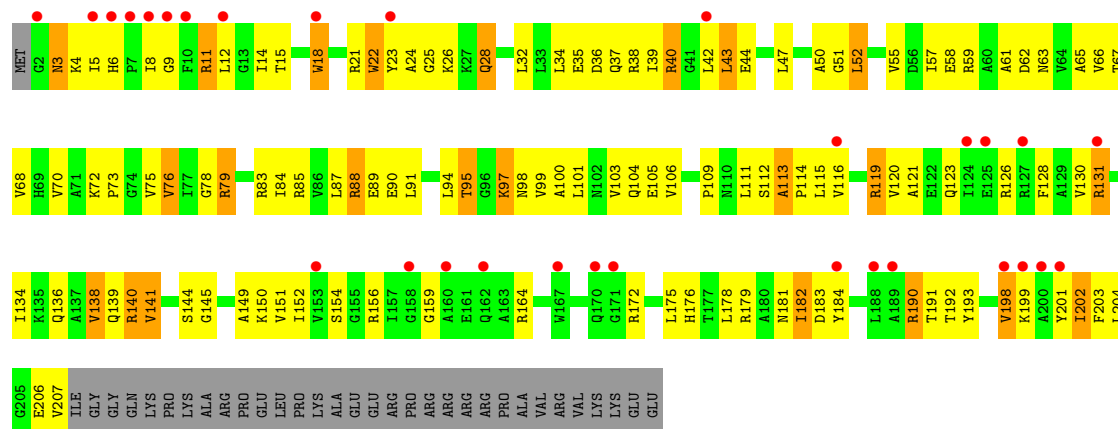




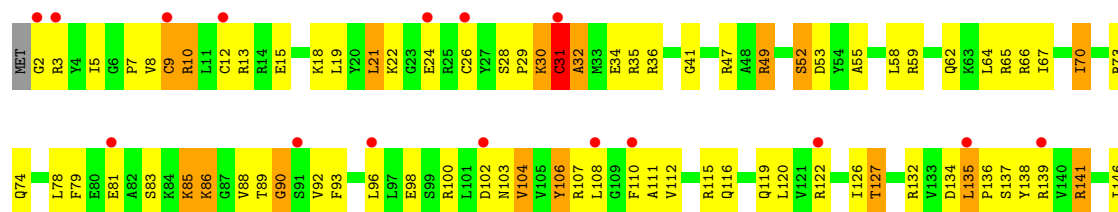
• Molecule 7: 30S ribosomal protein S3



• Molecule 7: 30S ribosomal protein S3

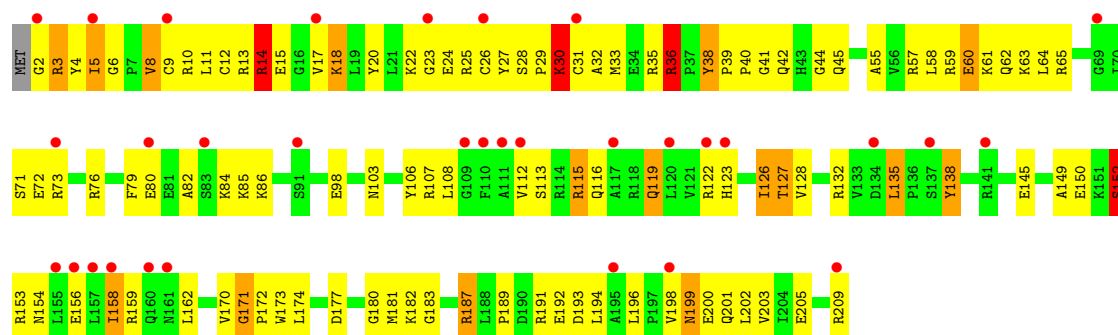


• Molecule 8: 30S ribosomal protein S4

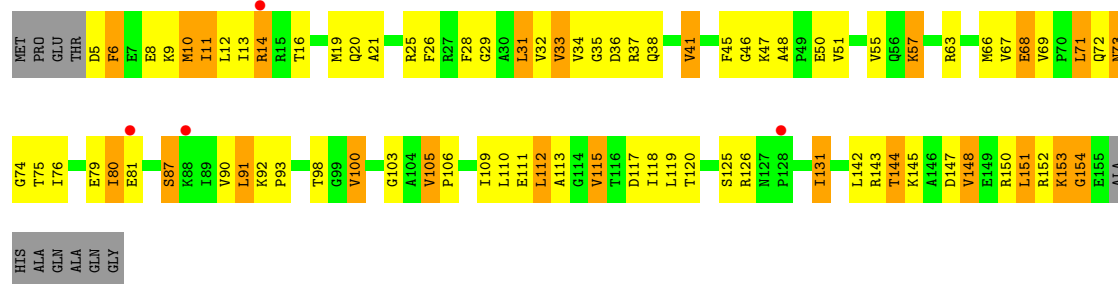
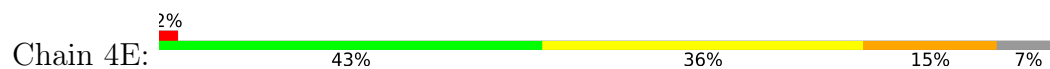




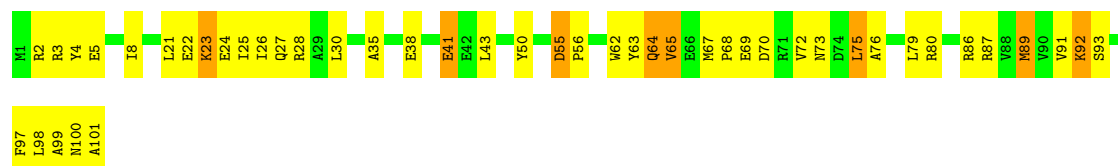
• Molecule 8: 30S ribosomal protein S4



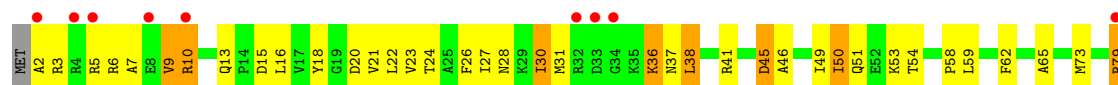
• Molecule 9: 30S ribosomal protein S5

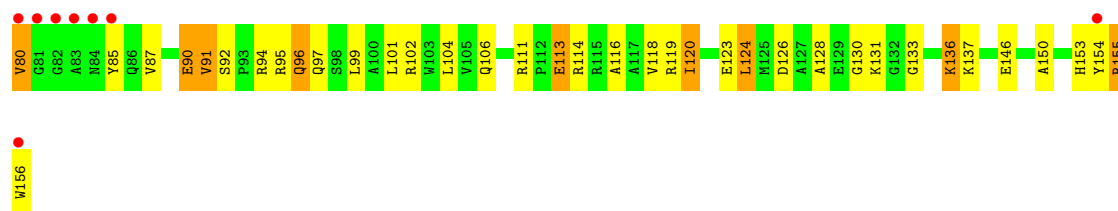


• Molecule 10: 30S ribosomal protein S6

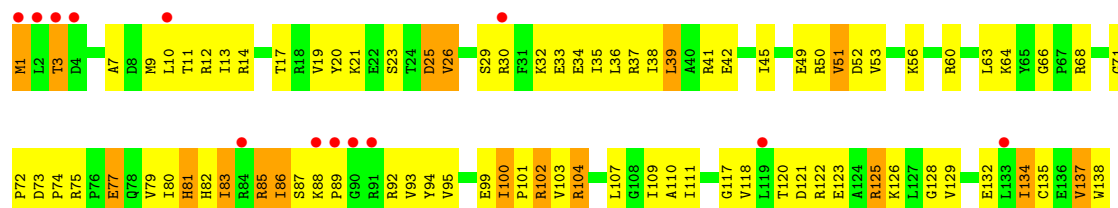


• Molecule 11: 30S ribosomal protein S7

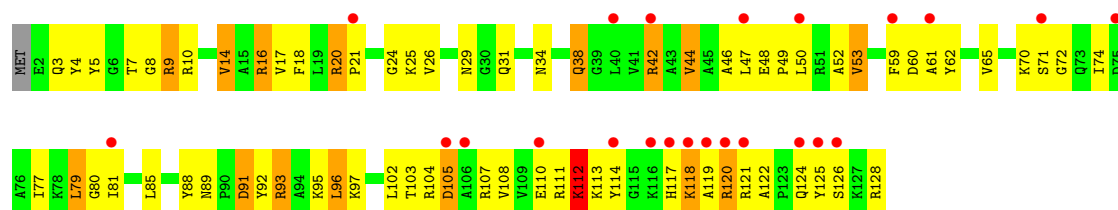
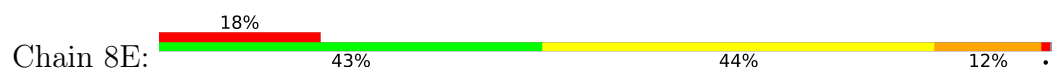




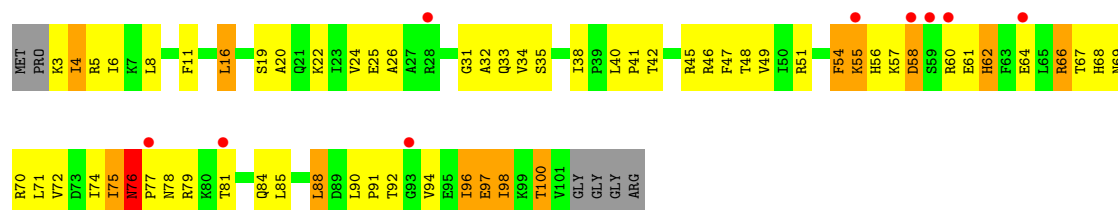
• Molecule 12: 30S ribosomal protein S8



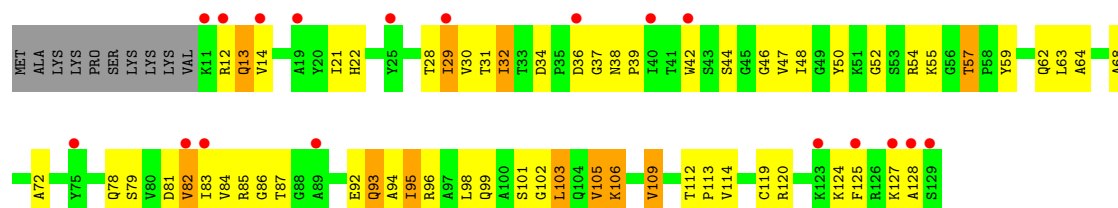
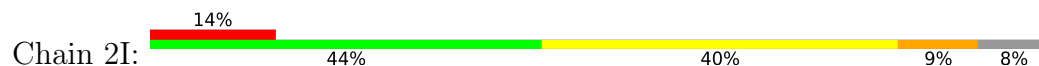
• Molecule 13: 30S ribosomal protein S9



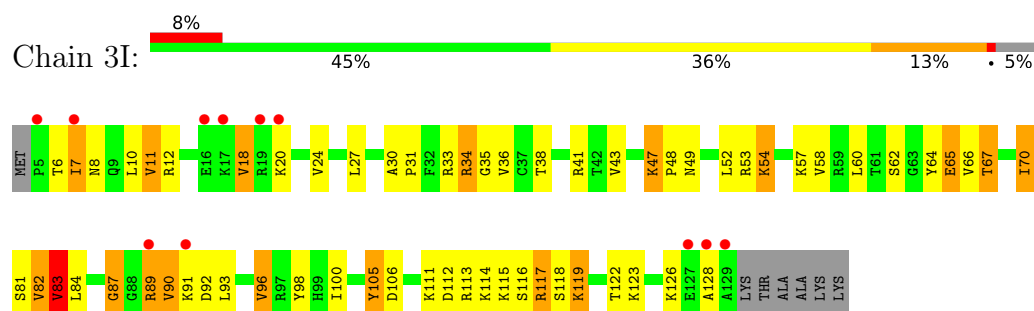
• Molecule 14: 30S ribosomal protein S10



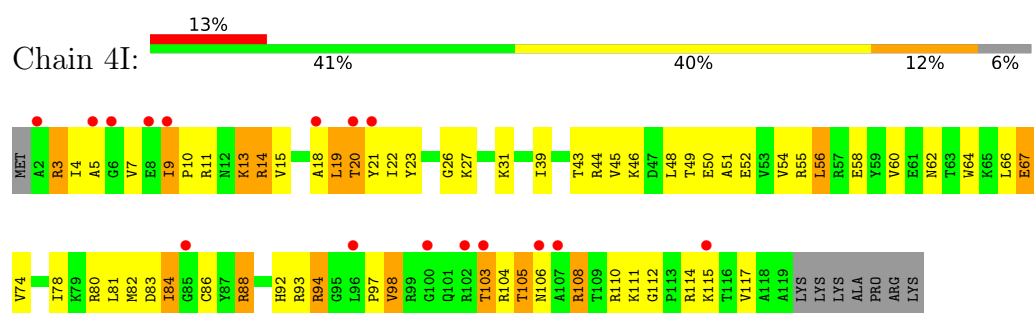
• Molecule 15: 30S ribosomal protein S11



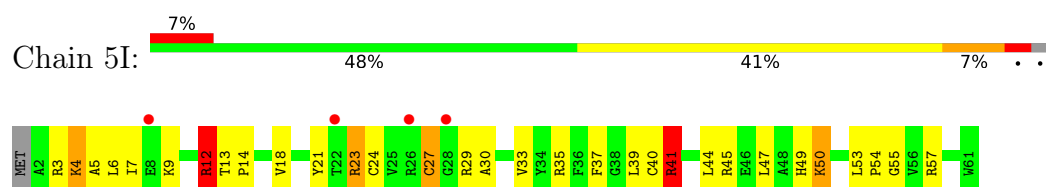
- Molecule 16: 30S ribosomal protein S12



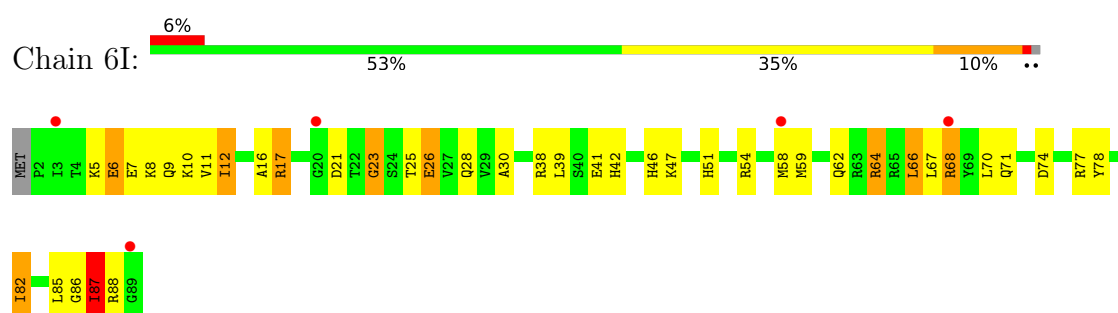
- Molecule 17: 30S ribosomal protein S13



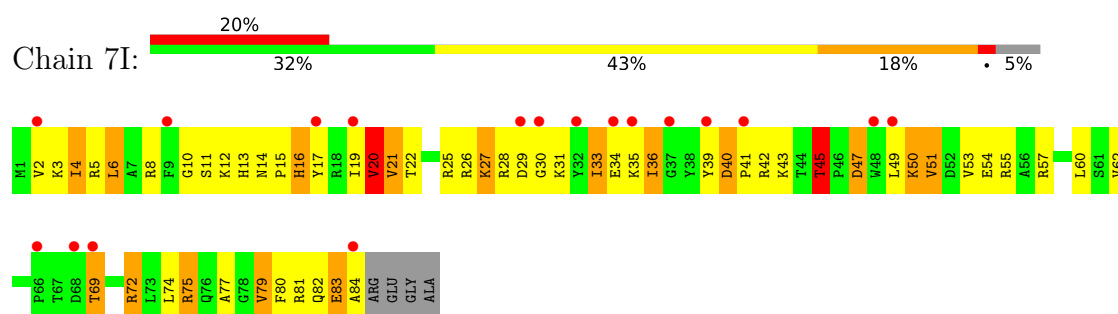
- Molecule 18: 30S ribosomal protein S14 type Z



- Molecule 19: 30S ribosomal protein S15

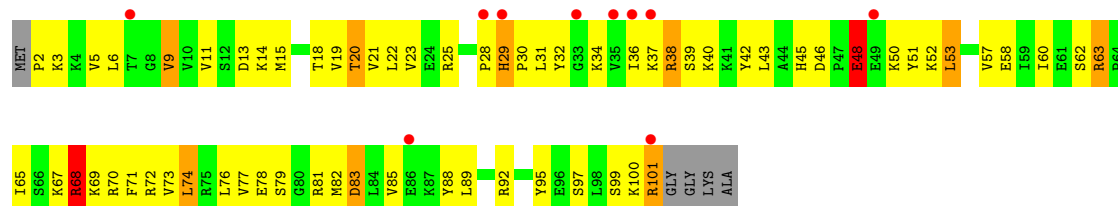


- Molecule 20: 30S ribosomal protein S16



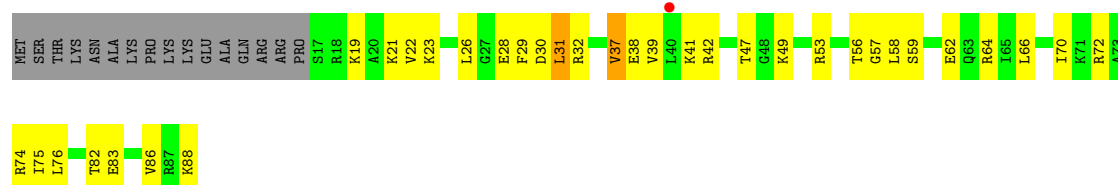
- Molecule 21: 30S ribosomal protein S17

Chain 8I: 

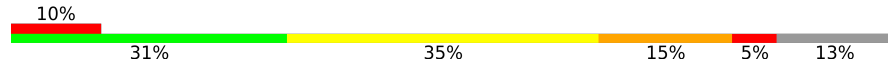


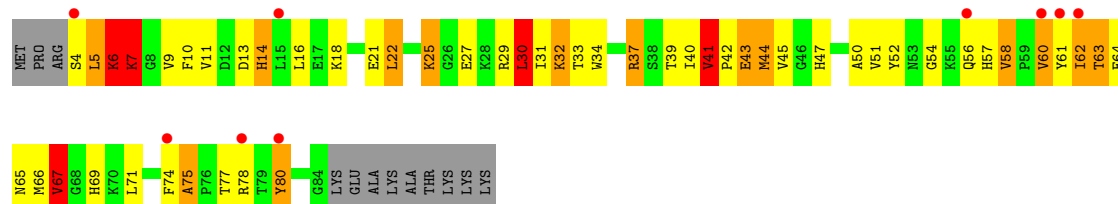
- Molecule 22: 30S ribosomal protein S18

Chain 9I: 



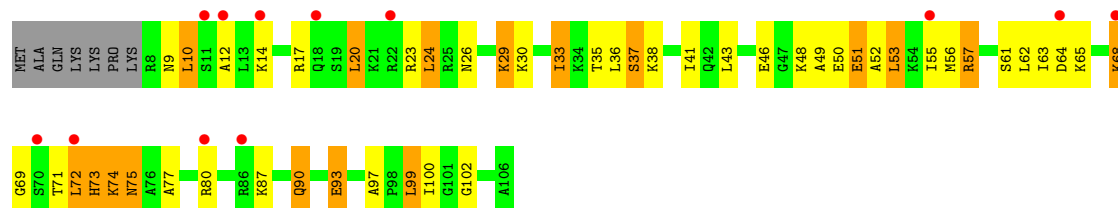
- Molecule 23: 30S ribosomal protein S19

Chain AI: 



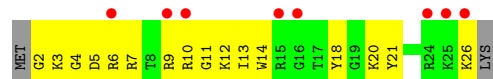
- Molecule 24: 30S ribosomal protein S20

Chain BI: 

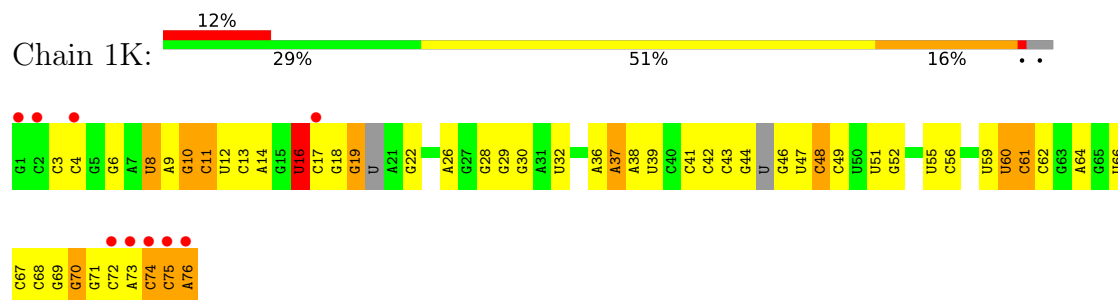


- Molecule 25: 30S ribosomal protein Thx

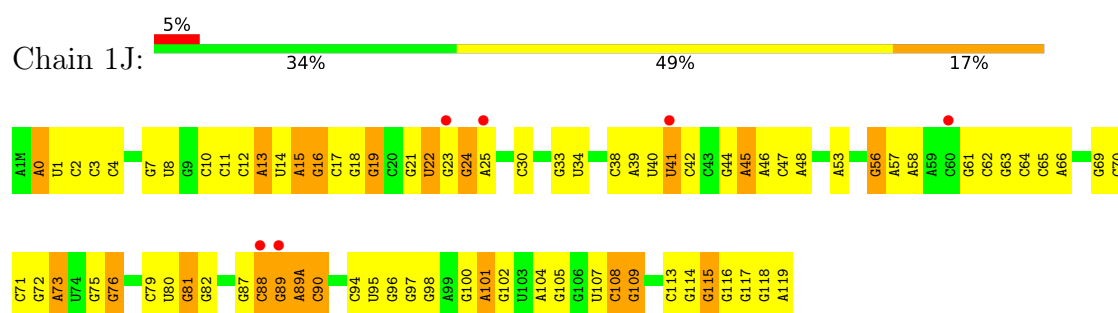
Chain 1F: 



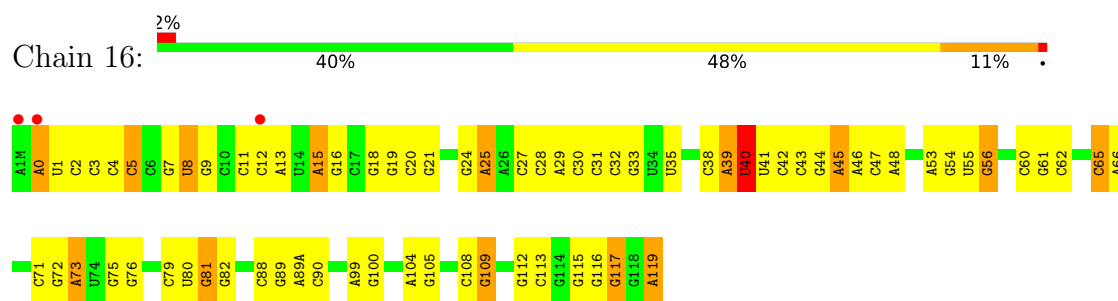
- Molecule 26: tRNA-Phe



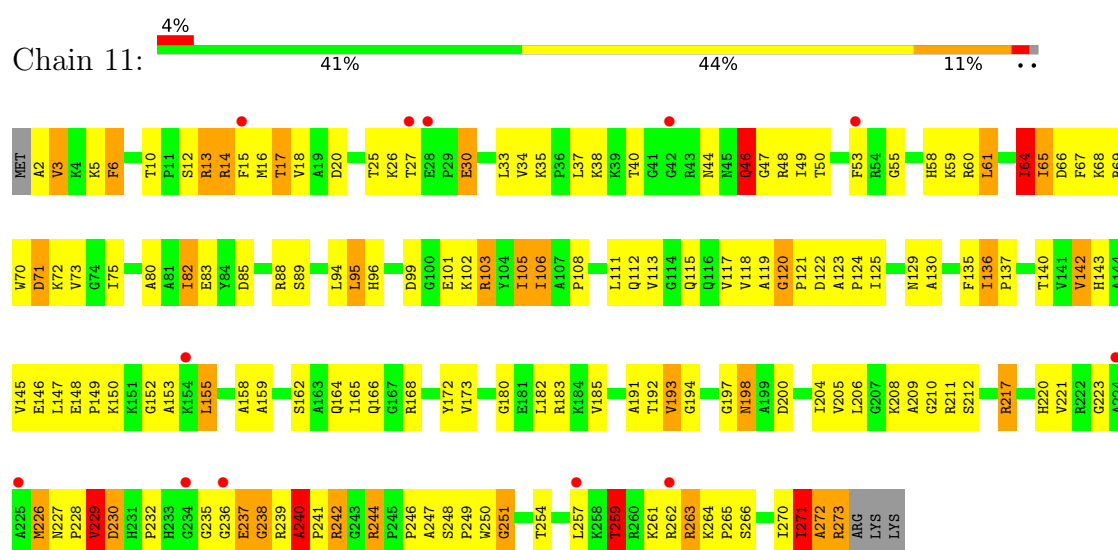
- Molecule 27: 5S ribosomal RNA



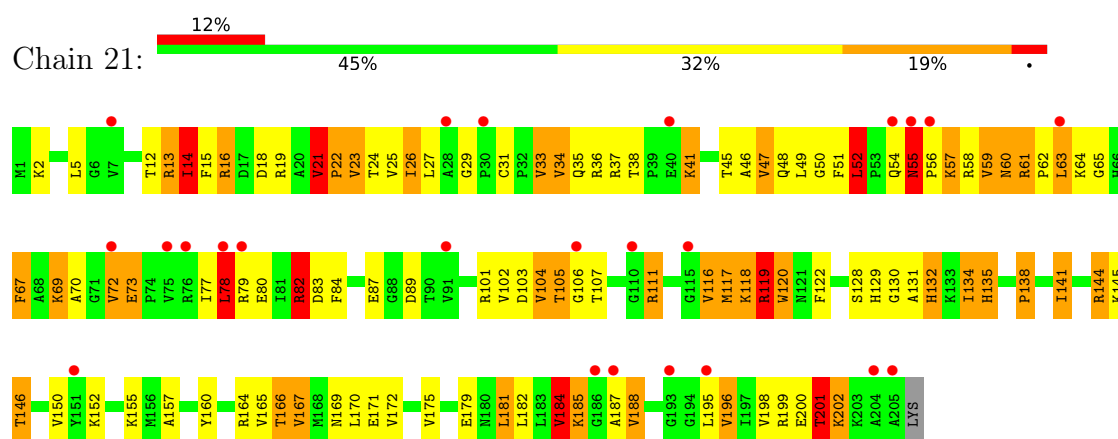
- Molecule 27: 5S ribosomal RNA



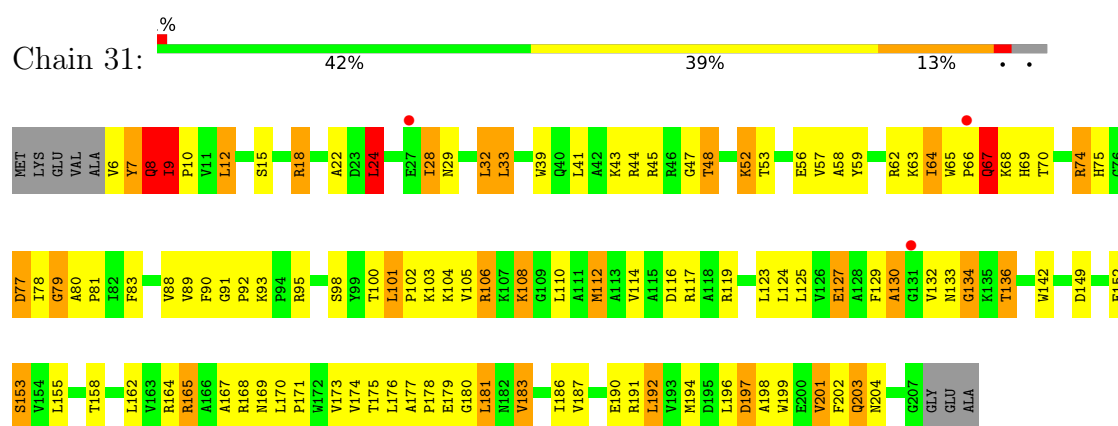
- Molecule 28: 50S ribosomal protein L2



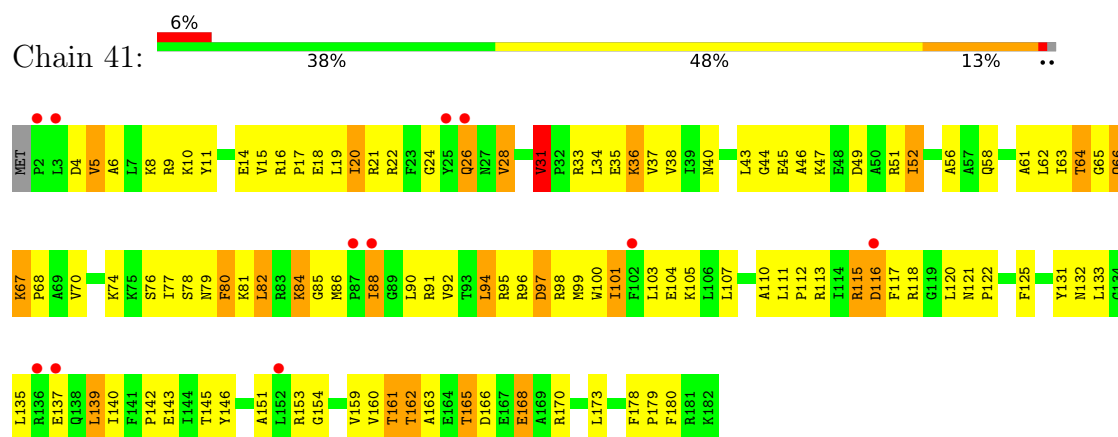
- Molecule 29: 50S ribosomal protein L3



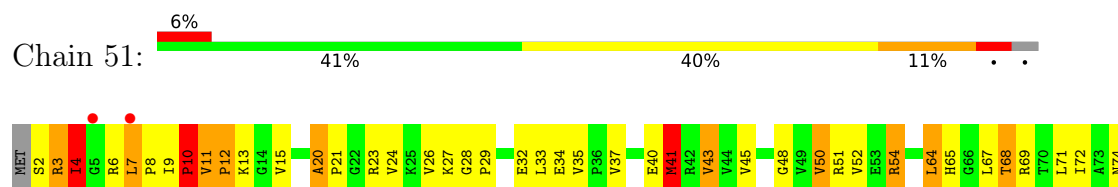
• Molecule 30: 50S ribosomal protein L4

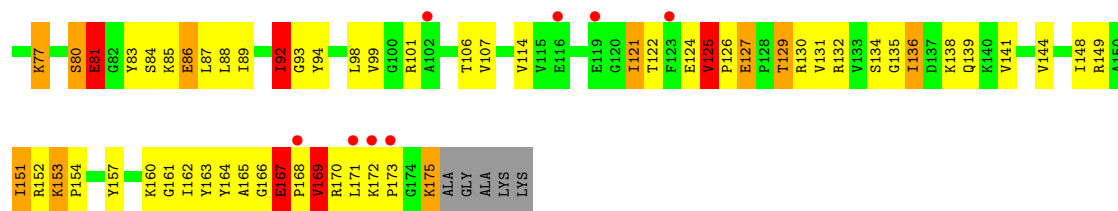


• Molecule 31: 50S ribosomal protein L5

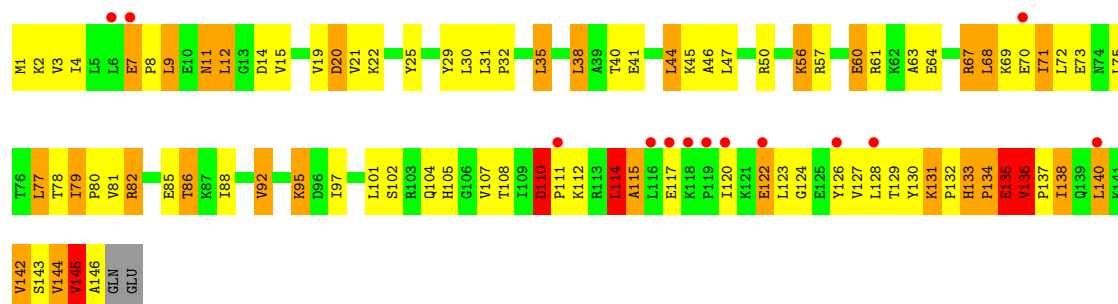


• Molecule 32: 50S ribosomal protein L6

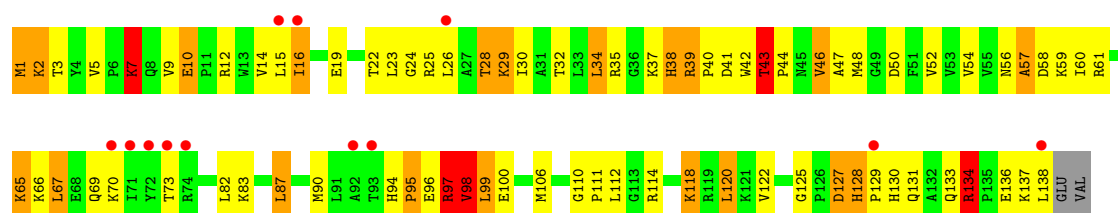




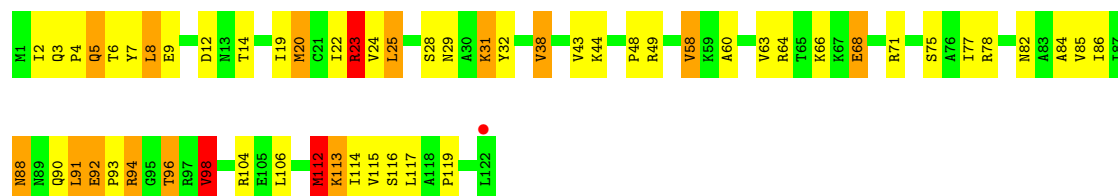
• Molecule 33: 50S ribosomal protein L9



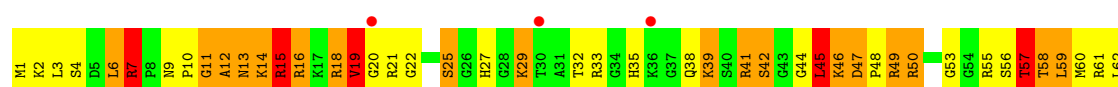
• Molecule 34: 50S ribosomal protein L13

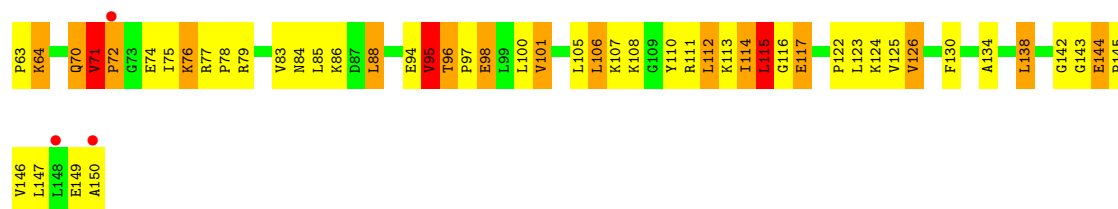


• Molecule 35: 50S ribosomal protein L14

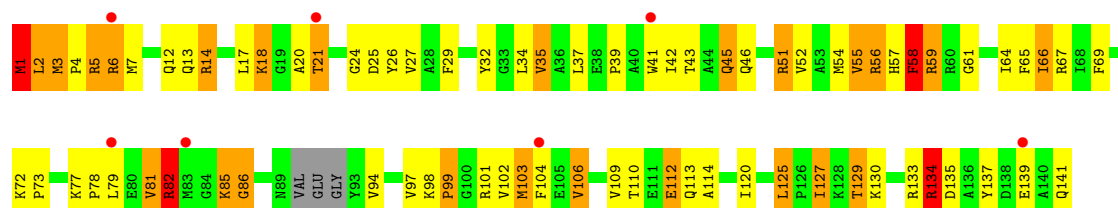
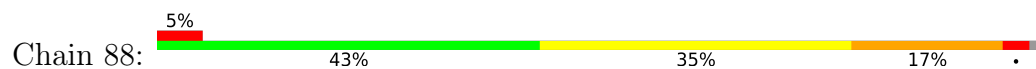


• Molecule 36: 50S ribosomal protein L15

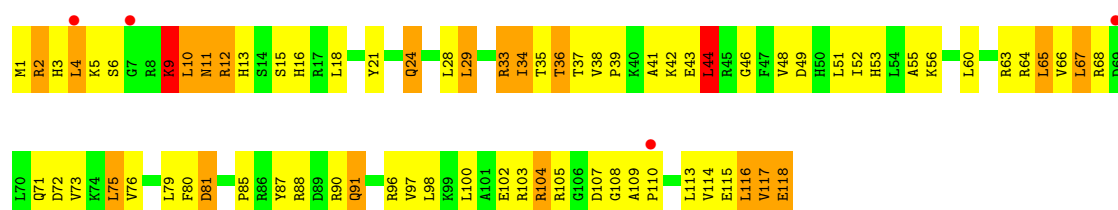




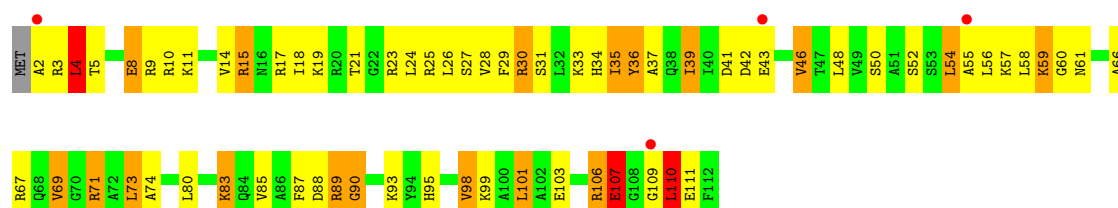
• Molecule 37: 50S ribosomal protein L16



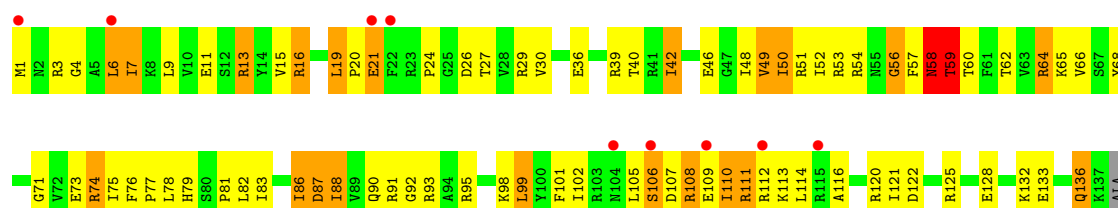
• Molecule 38: 50S ribosomal protein L17



• Molecule 39: 50S ribosomal protein L18



• Molecule 40: 50S ribosomal protein L19



GLN
GLU
PRO
LYS
ALA
SER
GLN
GLU

• Molecule 41: 50S ribosomal protein L20

Chain C8:  8% 38% 50% 10% ..

MET P2 R3 A4 LYS T6 G7 V8 V9 R10 R11 R12 R13 K14 K15 K16 I17 K18 K19 K22 G23 Y24 Y25 G26 L27 R28 S29 K30 R33 K34 A35 T38 L39 F40 A41 A42 Y47 A48 H49 R50 K51 R52 R53 K54 R58 R59 L60 W61 I62 V63 R64 I65 N66 A67 A68

C69 R70 L74 N75 Y76 S77 T78 F79 H80 H81 K85 A86 G87 T88 E89 V90 P91 R92 R93 N94 L95 A96 G97 L98 A99 V100 R101 P102 P103 Q104 V105 F106 A107 E108 L109 V110 R111 R112 A113 K114 A115 A116 Q117 G118

• Molecule 42: 50S ribosomal protein L21

Chain D8:  11% 48% 40% 10% .

M1 F2 A3 I4 V5 K6 T7 G8 G9 R10 Q11 Q12 Y13 R14 L18 L19 L20 L21 V22 E23 L24 L25 E34 L36 P36 V37 L38 L39 L40 G41 G42 E43 K44 T45 V46 V47 G48 T49 P50 E53 G54 L62 G65 R66 G67 T70 L71 V72 V73 S74 R75 F76 K78

V79 R82 R83 K84 R88 Y91 T92 E93 L94 L95 G101

• Molecule 43: 50S ribosomal protein L22

Chain E8:  2% 55% 35% 9% .

M1 R11 I12 I13 S14 S15 R18 L19 V20 L23 T24 K27 E30 E31 E32 R33 L36 R37 Y38 T39 N40 K41 L51 E52 N57 A58 N61 R62 D63 R64 L65 E66 E67 R68 L69 Y70 V71 V76 D77 E78 G79 L82 K83 R84 R85 L86 R87 R88 A89

R90 G91 R92 I96 K97 K98 R99 T100 I103 L107 K110 H111 G112 K113

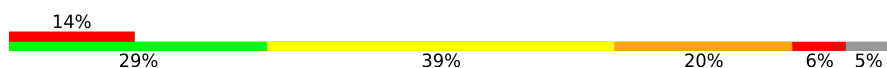
• Molecule 44: 50S ribosomal protein L23

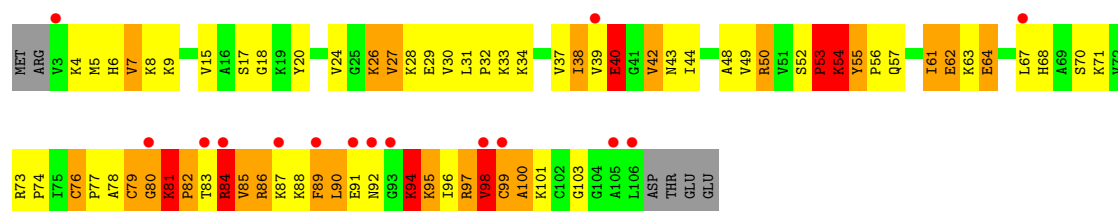
Chain F8:  2% 43% 40% 15% ..

M1 K2 T3 A4 Y5 D6 P11 V12 L13 S14 E15 K16 A17 Y18 A19 G20 G21 A22 E23 G24 K25 Y26 T27 H31 P32 K33 A34 A35 K36 T37 T38 I39 K40 N41 E44 T45 V49 K50 V51 V54 L57 R60 G61 R65 L66 G67 R68 Y69 P74 D75 R76

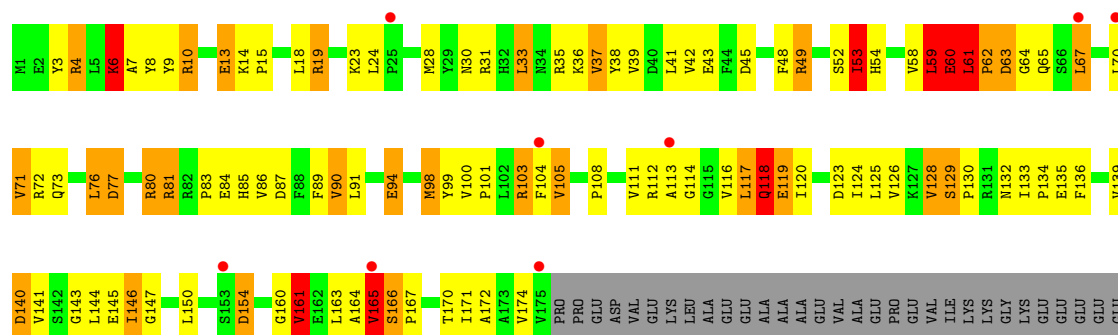
I80 V81 Q82 V83 Q87 K88 R89 L92 E93 G94 LEU ILE

• Molecule 45: 50S ribosomal protein L24

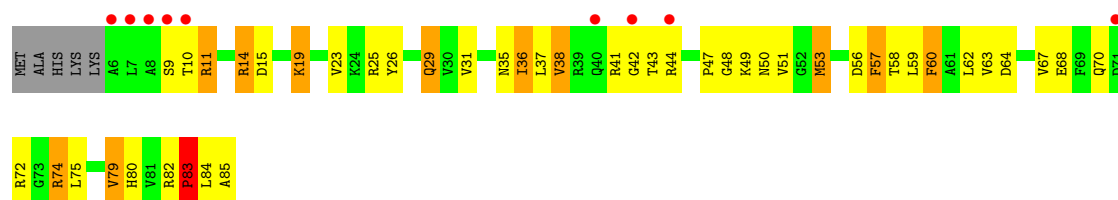
Chain G8:  14% 29% 39% 20% 6% 5%



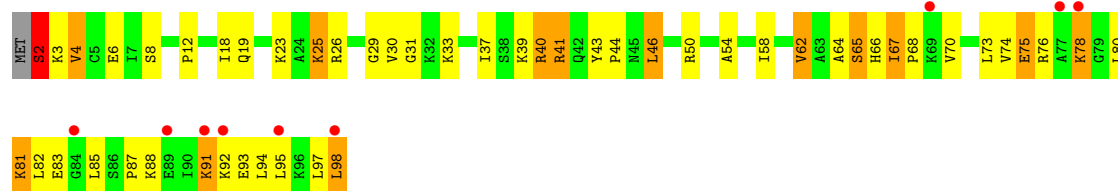
• Molecule 46: 50S ribosomal protein L25



• Molecule 47: 50S ribosomal protein L27



• Molecule 48: 50S ribosomal protein L28

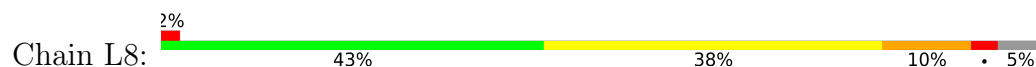


• Molecule 49: 50S ribosomal protein L29

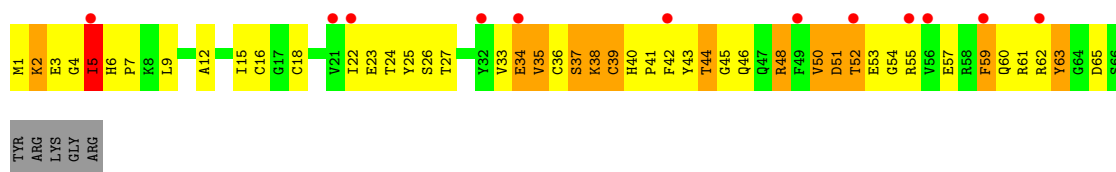




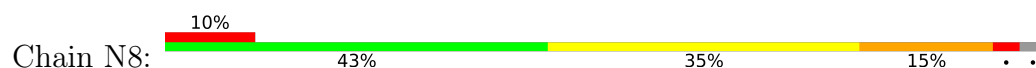
- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L32



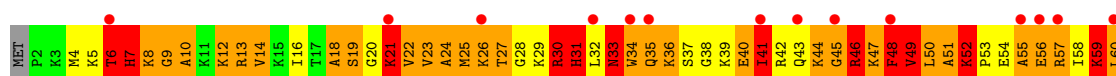
- Molecule 53: 50S ribosomal protein L33



- Molecule 54: 50S ribosomal protein L34



- Molecule 55: 50S ribosomal protein L35



LEU
PRO
TYR
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.40Å 447.70Å 619.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.96 – 3.05 151.96 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (151.96-3.05) 92.8 (151.96-3.05)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.193 , 0.231 0.249 , 0.272	Depositor DCC
R_{free} test set	2000 reflections (0.18%)	wwPDB-VP
Wilson B-factor (Å ²)	89.4	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	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 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 7MG, 4SU, OMC, MG, H2U, ZN, PSU, MIA

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	0.48	0/36028	0.75	14/56231 (0.0%)
1	1G	0.42	0/36025	0.68	9/56227 (0.0%)
2	1L	0.31	1/1625 (0.1%)	0.46	0/2531
2	3K	0.38	1/1625 (0.1%)	0.58	0/2531
2	3L	0.39	1/1625 (0.1%)	0.53	0/2531
3	2K	0.57	1/1721 (0.1%)	0.80	0/2682
3	2L	0.44	0/1721	0.71	0/2682
4	4K	0.53	0/313	0.63	0/485
4	4L	0.75	0/213	0.96	0/329
5	14	0.54	0/70167	0.80	20/109541 (0.0%)
5	1H	0.66	0/70233	0.89	57/109643 (0.1%)
6	12	0.56	0/1959	1.11	13/2642 (0.5%)
6	1E	0.61	0/1959	1.11	6/2642 (0.2%)
7	22	0.59	0/1636	1.07	8/2205 (0.4%)
7	2E	0.73	0/1629	1.10	3/2195 (0.1%)
8	32	0.66	0/1732	1.21	18/2318 (0.8%)
8	3E	0.75	0/1732	1.18	10/2318 (0.4%)
9	4E	0.79	0/1171	1.18	8/1576 (0.5%)
10	5E	0.78	0/855	1.13	1/1154 (0.1%)
11	6E	0.68	0/1275	1.07	4/1709 (0.2%)
12	7E	0.72	0/1135	1.26	11/1527 (0.7%)
13	8E	0.66	0/1028	1.11	3/1379 (0.2%)
14	1I	0.77	0/814	1.16	9/1095 (0.8%)
15	2I	0.85	0/899	1.33	8/1213 (0.7%)
16	3I	1.00	0/991	1.41	7/1327 (0.5%)
17	4I	0.74	0/948	1.11	1/1272 (0.1%)
18	5I	0.87	1/500 (0.2%)	1.23	4/664 (0.6%)
19	6I	0.80	0/744	1.19	2/992 (0.2%)
20	7I	0.72	0/721	1.15	6/970 (0.6%)
21	8I	0.71	0/847	1.21	7/1131 (0.6%)
22	9I	0.71	0/595	1.12	3/790 (0.4%)
23	AI	0.73	1/661 (0.2%)	1.28	13/890 (1.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
24	BI	0.59	0/764	1.11	4/1007 (0.4%)
25	1F	0.58	0/221	1.12	0/288
26	1K	0.34	0/1602	0.52	0/2493
27	16	0.53	0/2928	0.87	1/4568 (0.0%)
27	1J	0.44	0/2928	0.71	0/4568
28	11	1.18	5/2165 (0.2%)	1.56	43/2919 (1.5%)
29	21	0.95	1/1601 (0.1%)	1.53	29/2160 (1.3%)
30	31	1.07	1/1620 (0.1%)	1.39	20/2194 (0.9%)
31	41	0.79	1/1498 (0.1%)	1.25	10/2016 (0.5%)
32	51	0.86	1/1362 (0.1%)	1.42	18/1841 (1.0%)
33	61	0.79	0/1151	1.24	10/1558 (0.6%)
34	58	0.86	0/1131	1.30	12/1525 (0.8%)
35	68	0.92	0/942	1.24	7/1269 (0.6%)
36	78	1.04	2/1161 (0.2%)	1.54	25/1544 (1.6%)
37	88	1.20	5/1106 (0.5%)	1.60	26/1478 (1.8%)
38	98	0.89	0/981	1.30	7/1312 (0.5%)
39	A8	0.87	0/891	1.41	9/1187 (0.8%)
40	B8	0.93	0/1155	1.32	9/1542 (0.6%)
41	C8	1.00	1/981 (0.1%)	1.20	3/1306 (0.2%)
42	D8	0.83	0/789	1.34	7/1057 (0.7%)
43	E8	1.03	0/910	1.30	2/1220 (0.2%)
44	F8	1.10	0/756	1.36	5/1014 (0.5%)
45	G8	1.05	1/804 (0.1%)	1.57	21/1073 (2.0%)
46	H8	0.72	2/1427 (0.1%)	1.28	10/1935 (0.5%)
47	I8	1.03	1/634 (0.2%)	1.40	8/847 (0.9%)
48	J8	1.01	0/769	1.37	11/1022 (1.1%)
49	K8	1.06	1/565 (0.2%)	1.47	8/748 (1.1%)
50	L8	0.91	0/457	1.58	10/613 (1.6%)
51	M8	0.73	0/545	1.26	4/733 (0.5%)
52	N8	0.91	0/467	1.74	11/632 (1.7%)
53	O8	1.07	1/396 (0.3%)	1.51	8/529 (1.5%)
54	P8	1.20	0/399	1.38	2/526 (0.4%)
55	Q8	1.60	5/486 (1.0%)	2.27	28/638 (4.4%)
All	All	0.62	34/280719 (0.0%)	0.90	613/426784 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	12	0	1

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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 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	Q8	25	MET	CA-C	8.17	1.63	1.52
55	Q8	6	THR	CA-CB	8.04	1.66	1.53
28	11	271	ILE	CA-C	7.66	1.62	1.52
37	88	82	ARG	CA-C	7.58	1.63	1.52
37	88	79	LEU	N-CA	7.14	1.55	1.46

The worst 5 of 613 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	Q8	49	VAL	N-CA-C	14.23	125.67	112.29
28	11	271	ILE	N-CA-C	13.56	125.06	112.17
39	A8	110	LEU	N-CA-C	12.66	126.73	108.00
52	N8	41	PRO	CA-C-N	12.59	135.58	119.84
52	N8	41	PRO	C-N-CA	12.59	135.58	119.84

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	836	0
1	1G	32182	0	16243	769	1
2	1L	1627	0	842	40	0
2	3K	1627	0	842	52	0
2	3L	1627	0	842	52	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	9	0
5	14	62647	0	31582	1222	0
5	1H	62707	0	31606	1589	1
6	12	1924	0	1975	120	0
6	1E	1924	0	1975	113	0
7	22	1612	0	1677	88	0
7	2E	1605	0	1668	48	0
8	32	1702	0	1763	90	0
8	3E	1702	0	1763	86	0
9	4E	1155	0	1213	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	5E	842	0	857	32	0
11	6E	1256	0	1296	52	0
12	7E	1115	0	1177	63	0
13	8E	1009	0	1037	59	0
14	1I	801	0	849	59	0
15	2I	884	0	904	40	0
16	3I	975	0	1062	48	0
17	4I	938	0	997	57	0
18	5I	491	0	529	27	0
19	6I	733	0	771	35	0
20	7I	705	0	725	53	0
21	8I	834	0	904	63	0
22	9I	590	0	662	27	0
23	AI	647	0	665	53	0
24	BI	762	0	861	36	0
25	1F	217	0	234	18	0
26	1K	1587	0	822	25	0
27	16	2617	0	1328	73	0
27	1J	2617	0	1328	82	0
28	11	2115	0	2195	107	0
29	21	1568	0	1634	95	0
30	31	1585	0	1632	94	0
31	41	1473	0	1535	100	0
32	51	1336	0	1418	75	0
33	61	1136	0	1223	67	0
34	58	1104	0	1180	63	0
35	68	932	0	996	44	0
36	78	1144	0	1228	97	0
37	88	1086	0	1129	61	0
38	98	967	0	1033	64	0
39	A8	881	0	943	61	0
40	B8	1141	0	1202	72	0
41	C8	963	0	1022	73	0
42	D8	778	0	852	42	0
43	E8	899	0	964	32	0
44	F8	742	0	803	47	0
45	G8	791	0	881	61	0
46	H8	1397	0	1430	79	0
47	I8	626	0	642	40	0
48	J8	762	0	848	40	0
49	K8	563	0	612	31	0
50	L8	452	0	503	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	M8	533	0	526	39	0
52	N8	453	0	475	29	0
53	O8	389	0	404	35	0
54	P8	391	0	432	20	0
55	Q8	480	0	549	112	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

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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	7204	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 7204 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)
30:31:29:ASN:H	30:31:112:MET:HE1	1.13	1.11
5:1H:567:A:OP1	58:1H:3610:HOH:O	1.72	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1H:987:G:OP2	58:1H:4091:HOH:O	1.74	1.03
5:1H:2714:G:OP2	58:1H:3679:HOH:O	1.74	1.03
36:78:19:VAL:HG12	36:78:21:ARG:H	1.24	1.02

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%)	7	25
6	1E	235/256 (92%)	199 (85%)	33 (14%)	3 (1%)	9	31
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%)	12	37
8	3E	206/209 (99%)	186 (90%)	18 (9%)	2 (1%)	12	37
9	4E	149/162 (92%)	138 (93%)	10 (7%)	1 (1%)	18	45
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%)	18	45
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%)	14	39

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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%)	14	39
18	5I	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	13
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%)	3	16
23	AI	79/93 (85%)	66 (84%)	9 (11%)	4 (5%)	1	8
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%)	11	34
29	21	203/206 (98%)	164 (81%)	29 (14%)	10 (5%)	1	8
30	31	200/210 (95%)	182 (91%)	16 (8%)	2 (1%)	12	37
31	41	179/182 (98%)	156 (87%)	20 (11%)	3 (2%)	7	25
32	51	172/180 (96%)	143 (83%)	22 (13%)	7 (4%)	2	10
33	61	144/148 (97%)	117 (81%)	24 (17%)	3 (2%)	5	21
34	58	136/140 (97%)	117 (86%)	15 (11%)	4 (3%)	3	16
35	68	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
36	78	148/150 (99%)	116 (78%)	27 (18%)	5 (3%)	3	13
37	88	134/141 (95%)	110 (82%)	20 (15%)	4 (3%)	3	15
38	98	116/118 (98%)	100 (86%)	15 (13%)	1 (1%)	14	39
39	A8	109/112 (97%)	89 (82%)	19 (17%)	1 (1%)	14	39
40	B8	135/146 (92%)	120 (89%)	14 (10%)	1 (1%)	18	45
41	C8	115/118 (98%)	107 (93%)	5 (4%)	3 (3%)	4	17
42	D8	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	37
43	E8	111/113 (98%)	101 (91%)	10 (9%)	0	100	100
44	F8	92/96 (96%)	83 (90%)	7 (8%)	2 (2%)	5	20
45	G8	102/110 (93%)	80 (78%)	16 (16%)	6 (6%)	1	6
46	H8	173/206 (84%)	141 (82%)	24 (14%)	8 (5%)	2	9
47	I8	78/85 (92%)	66 (85%)	11 (14%)	1 (1%)	9	31
48	J8	95/98 (97%)	85 (90%)	8 (8%)	2 (2%)	5	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	K8	65/72 (90%)	57 (88%)	6 (9%)	2 (3%)	3	14
50	L8	55/60 (92%)	50 (91%)	4 (7%)	1 (2%)	6	24
51	M8	64/71 (90%)	40 (62%)	22 (34%)	2 (3%)	3	14
52	N8	56/60 (93%)	46 (82%)	8 (14%)	2 (4%)	2	12
53	O8	43/54 (80%)	28 (65%)	13 (30%)	2 (5%)	2	9
54	P8	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
55	Q8	58/65 (89%)	33 (57%)	19 (33%)	6 (10%)	0	2
All	All	6312/6731 (94%)	5477 (87%)	730 (12%)	105 (2%)	7	25

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%)	160 (78%)	45 (22%)	1	4
6	1E	205/220 (93%)	158 (77%)	47 (23%)	1	3
7	22	160/188 (85%)	126 (79%)	34 (21%)	1	4
7	2E	159/188 (85%)	126 (79%)	33 (21%)	1	4
8	32	180/181 (99%)	150 (83%)	30 (17%)	2	8
8	3E	180/181 (99%)	143 (79%)	37 (21%)	1	4
9	4E	116/123 (94%)	88 (76%)	28 (24%)	1	2
10	5E	90/90 (100%)	75 (83%)	15 (17%)	2	8
11	6E	126/127 (99%)	97 (77%)	29 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	7E	119/119 (100%)	95 (80%)	24 (20%)	1	4
13	8E	98/99 (99%)	75 (76%)	23 (24%)	1	3
14	1I	89/92 (97%)	70 (79%)	19 (21%)	1	4
15	2I	90/99 (91%)	77 (86%)	13 (14%)	3	12
16	3I	104/109 (95%)	83 (80%)	21 (20%)	1	4
17	4I	94/101 (93%)	68 (72%)	26 (28%)	0	1
18	5I	49/50 (98%)	41 (84%)	8 (16%)	2	9
19	6I	79/80 (99%)	64 (81%)	15 (19%)	1	6
20	7I	72/74 (97%)	54 (75%)	18 (25%)	0	2
21	8I	95/97 (98%)	77 (81%)	18 (19%)	1	6
22	9I	63/77 (82%)	56 (89%)	7 (11%)	6	21
23	AI	70/80 (88%)	46 (66%)	24 (34%)	0	0
24	BI	76/82 (93%)	56 (74%)	20 (26%)	0	2
25	1F	20/22 (91%)	19 (95%)	1 (5%)	22	49
28	11	214/218 (98%)	166 (78%)	48 (22%)	1	3
29	21	165/166 (99%)	121 (73%)	44 (27%)	0	1
30	31	161/166 (97%)	123 (76%)	38 (24%)	1	3
31	41	155/156 (99%)	120 (77%)	35 (23%)	1	3
32	51	145/148 (98%)	106 (73%)	39 (27%)	0	1
33	61	122/124 (98%)	81 (66%)	41 (34%)	0	0
34	58	117/119 (98%)	89 (76%)	28 (24%)	1	3
35	68	100/100 (100%)	80 (80%)	20 (20%)	1	5
36	78	116/116 (100%)	77 (66%)	39 (34%)	0	0
37	88	104/111 (94%)	77 (74%)	27 (26%)	0	2
38	98	101/101 (100%)	71 (70%)	30 (30%)	0	1
39	A8	87/88 (99%)	62 (71%)	25 (29%)	0	1
40	B8	120/127 (94%)	88 (73%)	32 (27%)	0	1
41	C8	93/94 (99%)	74 (80%)	19 (20%)	1	4
42	D8	82/82 (100%)	62 (76%)	20 (24%)	1	2
43	E8	92/92 (100%)	69 (75%)	23 (25%)	0	2
44	F8	76/78 (97%)	59 (78%)	17 (22%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	G8	85/91 (93%)	52 (61%)	33 (39%)	0	0
46	H8	154/179 (86%)	114 (74%)	40 (26%)	0	2
47	I8	61/67 (91%)	47 (77%)	14 (23%)	1	3
48	J8	82/83 (99%)	62 (76%)	20 (24%)	1	2
49	K8	62/67 (92%)	41 (66%)	21 (34%)	0	0
50	L8	49/52 (94%)	40 (82%)	9 (18%)	1	7
51	M8	59/63 (94%)	40 (68%)	19 (32%)	0	0
52	N8	51/52 (98%)	36 (71%)	15 (29%)	0	1
53	O8	44/52 (85%)	30 (68%)	14 (32%)	0	0
54	P8	38/42 (90%)	31 (82%)	7 (18%)	1	7
55	Q8	50/55 (91%)	30 (60%)	20 (40%)	0	0
All	All	5324/5588 (95%)	4052 (76%)	1272 (24%)	1	3

5 of 1272 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	E8	70	TYR
55	Q8	26	LYS
45	G8	7	VAL
43	E8	69	LEU
48	J8	19	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
43	E8	60	ASN
7	22	98	ASN
44	F8	31	HIS
49	K8	56	GLN
7	22	170	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1495/1522 (98%)	355 (23%)	38 (2%)
1	1G	1495/1522 (98%)	376 (25%)	37 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1L	75/76 (98%)	33 (44%)	3 (4%)
2	3K	75/76 (98%)	36 (48%)	5 (6%)
2	3L	75/76 (98%)	33 (44%)	1 (1%)
26	1K	71/76 (93%)	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%)	756 (25%)	46 (1%)
5	1H	2911/2917 (99%)	688 (23%)	62 (2%)
All	All	9520/9640 (98%)	2404 (25%)	207 (2%)

5 of 2404 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
5	1H	685	A
5	1H	1762	A
1	1G	1145	C
5	1H	880	G
5	1H	1312	U

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
2	H2U	3K	20	2	18,21,22	2.25	4 (22%)	19,30,33	1.75	4 (21%)
2	PSU	3L	32	2	18,21,22	1.33	2 (11%)	21,30,33	1.64	3 (14%)
3	OMC	2K	33	3	19,22,23	1.87	3 (15%)	25,31,34	0.92	2 (8%)
3	4SU	2L	8	3	18,21,22	2.11	4 (22%)	25,30,33	2.60	5 (20%)
2	H2U	1L	16	2	18,21,22	2.33	4 (22%)	19,30,33	1.74	4 (21%)
26	MIA	1K	37	26	28,31,32	2.35	4 (14%)	38,44,47	2.63	11 (28%)
3	PSU	2K	56	3	18,21,22	1.21	2 (11%)	21,30,33	2.10	5 (23%)
2	PSU	1L	39	2	18,21,22	1.19	1 (5%)	21,30,33	1.63	4 (19%)
2	MIA	1L	37	2	28,31,32	2.33	5 (17%)	38,44,47	2.67	12 (31%)
2	PSU	3L	55	2	18,21,22	1.19	1 (5%)	21,30,33	1.68	3 (14%)
3	PSU	2L	56	3	18,21,22	1.56	2 (11%)	21,30,33	1.81	3 (14%)
26	4SU	1K	8	26	18,21,22	1.85	4 (22%)	25,30,33	2.38	5 (20%)
3	OMC	2L	33	3	19,22,23	1.74	3 (15%)	25,31,34	1.08	2 (8%)
2	PSU	3K	32	2	18,21,22	1.28	1 (5%)	21,30,33	1.81	4 (19%)
2	H2U	3L	16	2	18,21,22	2.22	4 (22%)	19,30,33	1.62	3 (15%)
2	MIA	3L	37	2	28,31,32	2.75	5 (17%)	38,44,47	3.71	14 (36%)
2	4SU	1L	8	2	18,21,22	1.90	4 (22%)	25,30,33	2.14	5 (20%)
26	PSU	1K	55	26	18,21,22	1.36	2 (11%)	21,30,33	1.63	4 (19%)
2	7MG	1L	46	2	23,26,27	3.16	9 (39%)	27,39,42	2.72	9 (33%)
2	PSU	3K	55	2	18,21,22	1.21	1 (5%)	21,30,33	2.05	6 (28%)
26	7MG	1K	46	26	23,26,27	3.00	7 (30%)	27,39,42	2.87	10 (37%)
2	7MG	3K	46	2	23,26,27	3.04	7 (30%)	27,39,42	2.81	10 (37%)
3	7MG	2K	47	3	23,26,27	2.97	8 (34%)	27,39,42	2.78	9 (33%)
2	4SU	3K	8	2	18,21,22	2.00	3 (16%)	25,30,33	2.53	5 (20%)
26	H2U	1K	16	26	18,21,22	2.59	3 (16%)	19,30,33	1.57	4 (21%)
2	PSU	3L	39	2	18,21,22	1.18	1 (5%)	21,30,33	1.75	4 (19%)
3	4SU	2K	8	3	18,21,22	2.01	3 (16%)	25,30,33	2.74	5 (20%)
3	7MG	2L	47	3	23,26,27	3.13	8 (34%)	27,39,42	2.86	10 (37%)
2	4SU	3L	8	2	18,21,22	2.01	5 (27%)	25,30,33	2.03	5 (20%)
3	H2U	2K	21	3	18,21,22	2.88	4 (22%)	19,30,33	1.61	3 (15%)
3	H2U	2L	21	3	18,21,22	2.17	4 (22%)	19,30,33	1.50	3 (15%)
2	H2U	3K	16	2	18,21,22	2.26	4 (22%)	19,30,33	1.70	4 (21%)
2	H2U	3L	20	2	18,21,22	2.29	4 (22%)	19,30,33	1.66	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	3K	39	2	18,21,22	1.37	1 (5%)	21,30,33	1.59	3 (14%)
2	PSU	1L	32	2	18,21,22	1.33	1 (5%)	21,30,33	1.59	5 (23%)
2	MIA	3K	37	2	28,31,32	2.45	4 (14%)	38,44,47	3.76	14 (36%)
2	7MG	3L	46	2	23,26,27	3.23	7 (30%)	27,39,42	2.77	9 (33%)
26	PSU	1K	39	26	18,21,22	1.14	2 (11%)	21,30,33	1.77	3 (14%)
26	PSU	1K	32	26,56	18,21,22	1.48	3 (16%)	21,30,33	1.69	4 (19%)
2	PSU	1L	55	2	18,21,22	1.43	1 (5%)	21,30,33	1.57	4 (19%)
2	H2U	1L	20	2	18,21,22	2.21	4 (22%)	19,30,33	1.73	4 (21%)

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
2	H2U	3K	20	2	-	0/7/38/39	0/2/2/2
2	PSU	3L	32	2	-	1/7/25/26	0/2/2/2
3	OMC	2K	33	3	-	0/9/27/28	0/2/2/2
3	4SU	2L	8	3	-	0/7/25/26	0/2/2/2
2	H2U	1L	16	2	-	5/7/38/39	0/2/2/2
26	MIA	1K	37	26	-	7/15/33/34	0/3/3/3
3	PSU	2K	56	3	-	0/7/25/26	0/2/2/2
2	PSU	1L	39	2	-	0/7/25/26	0/2/2/2
2	MIA	1L	37	2	-	6/15/33/34	0/3/3/3
2	PSU	3L	55	2	-	2/7/25/26	0/2/2/2
3	PSU	2L	56	3	-	0/7/25/26	0/2/2/2
26	4SU	1K	8	26	-	1/7/25/26	0/2/2/2
3	OMC	2L	33	3	-	1/9/27/28	0/2/2/2
2	PSU	3K	32	2	-	0/7/25/26	0/2/2/2
2	H2U	3L	16	2	-	3/7/38/39	0/2/2/2
2	MIA	3L	37	2	-	8/15/33/34	0/3/3/3
2	4SU	1L	8	2	-	7/7/25/26	0/2/2/2
26	PSU	1K	55	26	-	2/7/25/26	0/2/2/2
2	7MG	1L	46	2	-	4/7/37/38	0/3/3/3
2	PSU	3K	55	2	-	4/7/25/26	0/2/2/2
26	7MG	1K	46	26	-	2/7/37/38	0/3/3/3
2	7MG	3K	46	2	-	2/7/37/38	0/3/3/3
3	7MG	2K	47	3	-	5/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4SU	3K	8	2	-	5/7/25/26	0/2/2/2
26	H2U	1K	16	26	-	3/7/38/39	0/2/2/2
2	PSU	3L	39	2	-	2/7/25/26	0/2/2/2
3	4SU	2K	8	3	-	0/7/25/26	0/2/2/2
3	7MG	2L	47	3	-	4/7/37/38	0/3/3/3
2	4SU	3L	8	2	-	1/7/25/26	0/2/2/2
3	H2U	2K	21	3	-	2/7/38/39	0/2/2/2
3	H2U	2L	21	3	-	4/7/38/39	0/2/2/2
2	H2U	3K	16	2	-	0/7/38/39	0/2/2/2
2	H2U	3L	20	2	-	6/7/38/39	0/2/2/2
2	PSU	3K	39	2	-	0/7/25/26	0/2/2/2
2	PSU	1L	32	2	-	3/7/25/26	0/2/2/2
2	MIA	3K	37	2	-	6/15/33/34	0/3/3/3
2	7MG	3L	46	2	-	2/7/37/38	0/3/3/3
26	PSU	1K	39	26	-	0/7/25/26	0/2/2/2
26	PSU	1K	32	26,56	-	0/7/25/26	0/2/2/2
2	PSU	1L	55	2	-	0/7/25/26	0/2/2/2
2	H2U	1L	20	2	-	4/7/38/39	0/2/2/2

The worst 5 of 149 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3L	46	7MG	C5-N7	9.21	1.47	1.35
3	2K	21	H2U	C2-N1	8.98	1.48	1.35
2	3K	46	7MG	C5-N7	8.81	1.46	1.35
26	1K	37	MIA	C13-C14	8.64	1.58	1.32
2	1L	46	7MG	C5-N7	8.53	1.46	1.35

The worst 5 of 230 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3K	37	MIA	C11-S10-C2	14.86	113.40	102.25
2	3L	37	MIA	C11-S10-C2	14.32	113.00	102.25
26	1K	37	MIA	C12-C13-C14	-10.37	108.41	127.01
2	3K	37	MIA	C12-C13-C14	-9.55	109.87	127.01
3	2K	8	4SU	C4-N3-C2	-9.34	118.36	127.31

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1L	8	4SU	C2'-C1'-N1-C2
2	1L	8	4SU	C2'-C1'-N1-C6
2	3K	8	4SU	C2'-C1'-N1-C2
2	3K	8	4SU	C2'-C1'-N1-C6
2	1L	16	H2U	O4'-C1'-N1-C6

There are no ring outliers.

26 monomers are involved in 55 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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%)	0.26	45 (3%)	52	30	62, 106, 190, 319	0
1	1G	1497/1522 (98%)	0.49	81 (5%)	31	16	78, 126, 199, 313	0
2	1L	68/76 (89%)	1.11	9 (13%)	7	4	144, 237, 271, 321	0
2	3K	68/76 (89%)	1.24	15 (22%)	2	1	76, 227, 273, 285	0
2	3L	68/76 (89%)	1.16	14 (20%)	2	1	95, 217, 254, 268	0
3	2K	72/77 (93%)	-0.04	0	100	100	74, 96, 125, 136	0
3	2L	72/77 (93%)	0.37	4 (5%)	30	15	87, 122, 154, 170	0
4	4K	13/30 (43%)	0.59	1 (7%)	19	10	74, 92, 138, 142	0
4	4L	9/30 (30%)	1.25	1 (11%)	10	5	104, 111, 123, 125	0
5	14	2909/2917 (99%)	0.09	70 (2%)	59	37	59, 96, 254, 399	0
5	1H	2912/2917 (99%)	-0.17	57 (1%)	65	42	45, 78, 243, 371	0
6	12	237/256 (92%)	1.11	42 (17%)	4	2	143, 177, 205, 218	0
6	1E	237/256 (92%)	0.89	31 (13%)	7	4	114, 148, 178, 191	0
7	22	206/239 (86%)	1.05	30 (14%)	6	3	139, 159, 187, 204	0
7	2E	205/239 (85%)	0.48	8 (3%)	43	23	92, 114, 150, 155	0
8	32	208/209 (99%)	1.10	32 (15%)	5	2	103, 127, 150, 155	0
8	3E	208/209 (99%)	0.74	24 (11%)	9	5	87, 115, 142, 155	0
9	4E	151/162 (93%)	0.43	4 (2%)	57	34	82, 104, 128, 177	0
10	5E	101/101 (100%)	0.20	0	100	100	85, 108, 131, 146	0
11	6E	155/156 (99%)	0.72	17 (10%)	10	5	104, 120, 156, 189	0
12	7E	138/138 (100%)	0.61	13 (9%)	14	7	98, 116, 128, 138	0
13	8E	127/128 (99%)	1.11	23 (18%)	3	2	91, 137, 163, 179	0
14	1I	99/105 (94%)	0.98	9 (9%)	15	8	86, 134, 171, 177	0
15	2I	119/129 (92%)	0.90	18 (15%)	5	3	79, 110, 145, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
16	3I	125/132 (94%)	0.47	11 (8%) 15 8	73, 84, 121, 204	0
17	4I	118/126 (93%)	0.97	16 (13%) 7 4	85, 123, 147, 162	0
18	5I	60/61 (98%)	0.69	4 (6%) 24 12	91, 103, 123, 133	0
19	6I	88/89 (98%)	0.62	5 (5%) 29 15	85, 109, 123, 143	0
20	7I	84/88 (95%)	1.45	18 (21%) 2 1	108, 119, 153, 170	0
21	8I	100/105 (95%)	0.77	10 (10%) 12 6	96, 114, 125, 128	0
22	9I	72/88 (81%)	0.34	1 (1%) 73 51	93, 111, 145, 177	0
23	AI	81/93 (87%)	0.91	9 (11%) 10 5	99, 123, 149, 161	0
24	BI	99/106 (93%)	0.99	12 (12%) 8 5	113, 127, 166, 172	0
25	1F	25/27 (92%)	1.38	8 (32%) 1 0	99, 111, 125, 154	0
26	1K	67/76 (88%)	0.80	9 (13%) 7 4	92, 192, 262, 271	0
27	16	122/122 (100%)	-0.22	3 (2%) 58 35	73, 96, 118, 204	0
27	1J	122/122 (100%)	0.58	6 (4%) 35 17	94, 140, 168, 212	0
28	11	272/276 (98%)	0.18	12 (4%) 39 20	46, 70, 87, 96	0
29	21	205/206 (99%)	0.71	24 (11%) 9 5	56, 97, 145, 164	0
30	31	202/210 (96%)	0.16	3 (1%) 72 50	52, 80, 120, 139	0
31	41	181/182 (99%)	0.46	11 (6%) 27 14	84, 107, 142, 155	0
32	51	174/180 (96%)	0.55	10 (5%) 29 15	86, 110, 126, 154	0
33	61	146/148 (98%)	0.67	13 (8%) 15 8	81, 136, 154, 161	0
34	58	138/140 (98%)	0.70	12 (8%) 16 9	71, 96, 137, 154	0
35	68	122/122 (100%)	0.16	1 (0%) 82 63	64, 83, 101, 116	0
36	78	150/150 (100%)	0.51	6 (4%) 42 23	51, 84, 109, 169	0
37	88	138/141 (97%)	0.40	7 (5%) 33 17	58, 84, 104, 139	0
38	98	118/118 (100%)	0.38	4 (3%) 48 27	70, 90, 114, 121	0
39	A8	111/112 (99%)	0.35	4 (3%) 46 25	78, 94, 125, 141	0
40	B8	137/146 (93%)	0.60	9 (6%) 24 12	79, 99, 157, 179	0
41	C8	117/118 (99%)	0.59	9 (7%) 19 10	60, 83, 118, 150	0
42	D8	101/101 (100%)	0.87	11 (10%) 10 5	63, 106, 143, 159	0
43	E8	113/113 (100%)	0.18	2 (1%) 67 45	64, 80, 116, 169	0
44	F8	94/96 (97%)	0.08	2 (2%) 63 40	59, 75, 98, 115	0
45	G8	104/110 (94%)	0.81	15 (14%) 6 3	76, 98, 138, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
46	H8	175/206 (84%)	0.64	8 (4%) 37 19	88, 128, 212, 220	0
47	I8	80/85 (94%)	0.52	9 (11%) 10 5	61, 76, 110, 122	0
48	J8	97/98 (98%)	0.59	9 (9%) 14 7	57, 77, 129, 175	0
49	K8	67/72 (93%)	0.62	11 (16%) 4 2	66, 84, 101, 143	0
50	L8	57/60 (95%)	0.15	1 (1%) 67 45	66, 85, 111, 117	0
51	M8	66/71 (92%)	1.03	12 (18%) 3 2	119, 163, 218, 238	0
52	N8	58/60 (96%)	0.85	6 (10%) 12 6	57, 104, 194, 203	0
53	O8	45/54 (83%)	1.45	12 (26%) 1 1	115, 146, 171, 183	0
54	P8	45/49 (91%)	-0.07	2 (4%) 39 20	46, 55, 70, 82	0
55	Q8	60/65 (92%)	1.41	15 (25%) 2 1	62, 77, 102, 118	0
All	All	15912/16371 (97%)	0.35	900 (5%) 29 15	45, 103, 202, 399	0

The worst 5 of 900 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	1H	2116	G	9.6
5	1H	2113	U	8.8
26	1K	73	A	8.7
5	1H	2477	C	8.5
17	4I	8	GLU	8.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PSU	1L	55	20/21	0.45	0.13	165,197,211,225	0
2	PSU	3L	55	20/21	0.46	0.13	180,202,212,213	0
2	PSU	3K	55	20/21	0.51	0.12	190,210,228,233	0
2	7MG	1L	46	24/25	0.52	0.11	172,200,218,231	0
2	H2U	1L	20	20/21	0.52	0.14	141,165,187,195	0
2	7MG	3K	46	24/25	0.53	0.14	193,206,217,221	0
2	H2U	3L	20	20/21	0.60	0.12	180,188,201,202	0
2	7MG	3L	46	24/25	0.60	0.13	190,197,206,218	0
2	PSU	3L	32	20/21	0.61	0.15	133,144,152,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	H2U	3K	20	20/21	0.62	0.24	140,167,205,206	0
3	H2U	2L	21	20/21	0.63	0.12	135,143,147,157	0
2	H2U	1L	16	20/21	0.65	0.16	157,192,217,227	0
2	H2U	3K	16	20/21	0.66	0.14	165,195,210,211	0
26	7MG	1K	46	24/25	0.66	0.09	149,160,172,176	0
2	H2U	3L	16	20/21	0.67	0.14	181,194,205,211	0
26	4SU	1K	8	20/21	0.68	0.11	164,174,189,190	0
2	4SU	3L	8	20/21	0.68	0.11	191,196,208,218	0
2	PSU	3L	39	20/21	0.70	0.13	134,144,154,160	0
2	4SU	3K	8	20/21	0.70	0.11	200,207,220,233	0
2	MIA	3L	37	29/30	0.71	0.19	148,168,178,187	0
26	H2U	1K	16	20/21	0.72	0.16	122,160,190,196	0
26	PSU	1K	55	20/21	0.72	0.11	133,151,166,168	0
2	4SU	1L	8	20/21	0.75	0.09	185,201,207,213	0
3	7MG	2L	47	24/25	0.76	0.12	126,134,139,140	0
3	H2U	2K	21	20/21	0.77	0.12	114,124,134,134	0
2	PSU	3K	32	20/21	0.79	0.14	127,135,142,151	0
2	PSU	1L	32	20/21	0.81	0.17	149,152,163,169	0
2	MIA	3K	37	29/30	0.85	0.20	123,142,147,157	0
3	PSU	2L	56	20/21	0.85	0.10	123,130,136,139	0
3	4SU	2L	8	20/21	0.86	0.11	115,120,123,126	0
3	7MG	2K	47	24/25	0.87	0.10	97,106,114,116	0
2	PSU	3K	39	20/21	0.88	0.10	117,127,130,138	0
2	PSU	1L	39	20/21	0.88	0.09	140,150,158,160	0
3	4SU	2K	8	20/21	0.88	0.12	89,95,103,105	0
3	PSU	2K	56	20/21	0.89	0.10	101,106,113,119	0
2	MIA	1L	37	29/30	0.92	0.15	131,147,155,157	0
26	PSU	1K	32	20/21	0.92	0.15	107,112,124,131	0
26	PSU	1K	39	20/21	0.94	0.09	86,100,107,110	0
3	OMC	2K	33	21/22	0.95	0.12	75,80,86,87	0
26	MIA	1K	37	29/30	0.96	0.11	84,92,107,113	0
3	OMC	2L	33	21/22	0.96	0.10	104,109,112,118	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	14	3241	1/1	0.09	0.28	139,139,139,139	0
56	MG	13	1699	1/1	0.27	0.23	146,146,146,146	0
56	MG	14	3255	1/1	0.31	0.54	102,102,102,102	0
56	MG	14	3140	1/1	0.36	0.56	113,113,113,113	0
57	ZN	14	3422	1/1	0.38	0.18	181,181,181,181	0
56	MG	1H	3316	1/1	0.39	0.34	102,102,102,102	0
56	MG	1G	1621	1/1	0.42	0.45	122,122,122,122	0
56	MG	13	1708	1/1	0.44	0.38	112,112,112,112	0
56	MG	13	1681	1/1	0.46	0.48	116,116,116,116	0
56	MG	13	1702	1/1	0.46	0.34	109,109,109,109	0
56	MG	13	1690	1/1	0.46	0.62	109,109,109,109	0
56	MG	1H	3248	1/1	0.47	0.33	82,82,82,82	0
56	MG	1H	3255	1/1	0.48	0.26	110,110,110,110	0
56	MG	1H	3271	1/1	0.50	0.40	100,100,100,100	0
56	MG	13	1679	1/1	0.51	0.35	94,94,94,94	0
56	MG	13	1688	1/1	0.52	0.55	106,106,106,106	0
56	MG	1G	1663	1/1	0.52	0.32	120,120,120,120	0
56	MG	1H	3323	1/1	0.52	0.31	100,100,100,100	0
56	MG	13	1607	1/1	0.55	0.41	88,88,88,88	0
56	MG	13	1643	1/1	0.55	0.33	96,96,96,96	0
56	MG	13	1700	1/1	0.56	0.33	103,103,103,103	0
56	MG	14	3266	1/1	0.56	0.24	107,107,107,107	0
56	MG	14	3228	1/1	0.57	0.33	109,109,109,109	0
56	MG	1G	1661	1/1	0.57	0.22	104,104,104,104	0
56	MG	14	3118	1/1	0.58	0.34	110,110,110,110	0
56	MG	1G	1634	1/1	0.59	0.38	114,114,114,114	0
56	MG	14	3217	1/1	0.59	0.18	159,159,159,159	0
56	MG	3E	302	1/1	0.60	0.32	121,121,121,121	0
56	MG	1H	3222	1/1	0.60	0.42	97,97,97,97	0
56	MG	14	3119	1/1	0.60	0.32	97,97,97,97	0
56	MG	1H	3283	1/1	0.61	0.21	103,103,103,103	0
56	MG	14	3243	1/1	0.61	0.35	93,93,93,93	0
56	MG	13	1684	1/1	0.61	0.37	108,108,108,108	0
56	MG	1J	204	1/1	0.61	0.34	108,108,108,108	0
56	MG	1G	1616	1/1	0.61	0.47	97,97,97,97	0
56	MG	13	1675	1/1	0.62	0.18	131,131,131,131	0
56	MG	13	1654	1/1	0.62	0.49	125,125,125,125	0
56	MG	3L	101	1/1	0.62	0.24	116,116,116,116	0
56	MG	14	3225	1/1	0.63	0.33	103,103,103,103	0
56	MG	1H	3205	1/1	0.63	0.38	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	13	1685	1/1	0.63	0.37	91,91,91,91	0
56	MG	1G	1623	1/1	0.63	0.35	108,108,108,108	0
56	MG	14	3227	1/1	0.64	0.34	106,106,106,106	0
56	MG	1H	3109	1/1	0.64	0.32	79,79,79,79	0
56	MG	14	3101	1/1	0.64	0.25	99,99,99,99	0
56	MG	1H	3217	1/1	0.64	0.32	96,96,96,96	0
56	MG	14	3259	1/1	0.64	0.20	104,104,104,104	0
56	MG	14	3059	1/1	0.64	0.34	83,83,83,83	0
56	MG	1G	1607	1/1	0.64	0.26	96,96,96,96	0
56	MG	1G	1649	1/1	0.65	0.36	84,84,84,84	0
56	MG	1H	3301	1/1	0.65	0.48	110,110,110,110	0
56	MG	14	3221	1/1	0.65	0.29	99,99,99,99	0
56	MG	14	3198	1/1	0.65	0.30	90,90,90,90	0
56	MG	1G	1602	1/1	0.66	0.28	76,76,76,76	0
56	MG	14	3219	1/1	0.66	0.57	100,100,100,100	0
56	MG	14	3244	1/1	0.66	0.29	82,82,82,82	0
56	MG	14	3050	1/1	0.66	0.32	74,74,74,74	0
56	MG	2K	103	1/1	0.66	0.33	88,88,88,88	0
56	MG	1H	3286	1/1	0.67	0.32	88,88,88,88	0
56	MG	13	1698	1/1	0.67	0.30	91,91,91,91	0
56	MG	1H	3266	1/1	0.67	0.29	94,94,94,94	0
56	MG	14	3216	1/1	0.67	0.33	106,106,106,106	0
56	MG	14	3016	1/1	0.67	0.27	65,65,65,65	0
56	MG	1H	3227	1/1	0.68	0.29	77,77,77,77	0
56	MG	1G	1645	1/1	0.68	0.24	102,102,102,102	0
56	MG	14	3183	1/1	0.68	0.28	74,74,74,74	0
56	MG	2K	105	1/1	0.68	0.39	102,102,102,102	0
56	MG	14	3070	1/1	0.68	0.37	92,92,92,92	0
56	MG	1G	1625	1/1	0.68	0.33	108,108,108,108	0
56	MG	13	1703	1/1	0.69	0.32	105,105,105,105	0
56	MG	1H	3273	1/1	0.69	0.39	101,101,101,101	0
56	MG	1H	3277	1/1	0.69	0.43	98,98,98,98	0
56	MG	13	1667	1/1	0.69	0.29	91,91,91,91	0
56	MG	1G	1657	1/1	0.69	0.19	112,112,112,112	0
56	MG	1H	3125	1/1	0.69	0.22	97,97,97,97	0
56	MG	13	1648	1/1	0.69	0.33	91,91,91,91	0
56	MG	13	1642	1/1	0.69	0.39	76,76,76,76	0
56	MG	1G	1635	1/1	0.70	0.32	82,82,82,82	0
56	MG	1H	3315	1/1	0.70	0.40	93,93,93,93	0
56	MG	1H	3263	1/1	0.70	0.46	87,87,87,87	0
56	MG	13	1706	1/1	0.70	0.28	93,93,93,93	0
56	MG	1H	3117	1/1	0.70	0.11	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	16	207	1/1	0.70	0.24	96,96,96,96	0
56	MG	1G	1678	1/1	0.70	0.32	98,98,98,98	0
56	MG	14	3162	1/1	0.70	0.26	107,107,107,107	0
56	MG	14	3121	1/1	0.71	0.20	91,91,91,91	0
56	MG	14	3185	1/1	0.71	0.40	80,80,80,80	0
56	MG	14	3197	1/1	0.71	0.23	83,83,83,83	0
56	MG	13	1617	1/1	0.71	0.31	85,85,85,85	0
56	MG	1G	1612	1/1	0.71	0.28	109,109,109,109	0
56	MG	1H	3260	1/1	0.71	0.37	93,93,93,93	0
56	MG	14	3209	1/1	0.71	0.36	71,71,71,71	0
56	MG	14	3045	1/1	0.71	0.43	82,82,82,82	0
56	MG	14	3238	1/1	0.71	0.21	94,94,94,94	0
56	MG	14	3263	1/1	0.72	0.24	97,97,97,97	0
56	MG	14	3230	1/1	0.72	0.32	86,86,86,86	0
56	MG	14	3376	1/1	0.72	0.18	122,122,122,122	0
56	MG	1G	1632	1/1	0.72	0.37	92,92,92,92	0
56	MG	13	1704	1/1	0.72	0.31	113,113,113,113	0
56	MG	14	3074	1/1	0.72	0.21	89,89,89,89	0
56	MG	13	1693	1/1	0.72	0.16	86,86,86,86	0
56	MG	1H	3261	1/1	0.72	0.32	98,98,98,98	0
56	MG	1H	3105	1/1	0.72	0.45	89,89,89,89	0
56	MG	13	1653	1/1	0.72	0.31	91,91,91,91	0
56	MG	14	3248	1/1	0.72	0.32	91,91,91,91	0
56	MG	1G	1669	1/1	0.72	0.35	105,105,105,105	0
56	MG	1G	1676	1/1	0.72	0.19	113,113,113,113	0
56	MG	1G	1677	1/1	0.72	0.31	96,96,96,96	0
56	MG	13	1683	1/1	0.72	0.45	101,101,101,101	0
56	MG	14	3229	1/1	0.72	0.40	107,107,107,107	0
56	MG	16	210	1/1	0.73	0.14	105,105,105,105	0
56	MG	1G	1641	1/1	0.73	0.39	92,92,92,92	0
56	MG	21	302	1/1	0.73	0.44	84,84,84,84	0
56	MG	14	3038	1/1	0.73	0.26	96,96,96,96	0
56	MG	1H	3311	1/1	0.73	0.42	93,93,93,93	0
56	MG	13	1626	1/1	0.73	0.28	56,56,56,56	0
56	MG	1H	3181	1/1	0.73	0.27	84,84,84,84	0
56	MG	1G	1665	1/1	0.73	0.32	99,99,99,99	0
56	MG	1H	3318	1/1	0.73	0.23	101,101,101,101	0
56	MG	14	3192	1/1	0.73	0.28	102,102,102,102	0
56	MG	1J	202	1/1	0.73	0.29	93,93,93,93	0
56	MG	14	3143	1/1	0.73	0.38	88,88,88,88	0
56	MG	13	1610	1/1	0.73	0.29	86,86,86,86	0
56	MG	1H	3186	1/1	0.74	0.17	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3191	1/1	0.74	0.23	83,83,83,83	0
56	MG	1G	1639	1/1	0.74	0.25	104,104,104,104	0
56	MG	1G	1640	1/1	0.74	0.26	107,107,107,107	0
56	MG	1H	3203	1/1	0.74	0.49	101,101,101,101	0
56	MG	14	3246	1/1	0.74	0.23	97,97,97,97	0
56	MG	1H	3216	1/1	0.74	0.40	87,87,87,87	0
56	MG	14	3261	1/1	0.74	0.28	91,91,91,91	0
56	MG	14	3133	1/1	0.74	0.37	82,82,82,82	0
56	MG	1H	3122	1/1	0.74	0.20	77,77,77,77	0
56	MG	1H	3294	1/1	0.74	0.38	88,88,88,88	0
56	MG	1H	3234	1/1	0.74	0.29	96,96,96,96	0
56	MG	14	3148	1/1	0.74	0.20	96,96,96,96	0
56	MG	1H	3254	1/1	0.74	0.27	90,90,90,90	0
56	MG	1H	3137	1/1	0.74	0.29	87,87,87,87	0
56	MG	1H	3030	1/1	0.74	0.22	87,87,87,87	0
57	ZN	1G	1697	1/1	0.74	0.27	149,149,149,149	0
56	MG	1G	1618	1/1	0.75	0.17	102,102,102,102	0
56	MG	1H	3293	1/1	0.75	0.27	95,95,95,95	0
56	MG	13	1692	1/1	0.75	0.20	85,85,85,85	0
56	MG	1H	3239	1/1	0.75	0.24	88,88,88,88	0
56	MG	1H	3009	1/1	0.75	0.27	58,58,58,58	0
56	MG	14	3030	1/1	0.75	0.32	84,84,84,84	0
56	MG	1G	1674	1/1	0.75	0.39	92,92,92,92	0
56	MG	1G	1601	1/1	0.75	0.27	90,90,90,90	0
56	MG	14	3396	1/1	0.75	0.19	101,101,101,101	0
56	MG	14	3170	1/1	0.75	0.19	77,77,77,77	0
56	MG	14	3130	1/1	0.75	0.32	98,98,98,98	0
56	MG	1J	201	1/1	0.75	0.15	123,123,123,123	0
56	MG	1G	1646	1/1	0.76	0.48	108,108,108,108	0
56	MG	14	3153	1/1	0.76	0.27	82,82,82,82	0
56	MG	14	3135	1/1	0.76	0.23	84,84,84,84	0
56	MG	14	3203	1/1	0.76	0.26	103,103,103,103	0
56	MG	14	3164	1/1	0.76	0.19	76,76,76,76	0
56	MG	16	201	1/1	0.76	0.28	91,91,91,91	0
56	MG	14	3139	1/1	0.76	0.35	97,97,97,97	0
56	MG	1H	3262	1/1	0.76	0.19	86,86,86,86	0
56	MG	14	3069	1/1	0.76	0.32	73,73,73,73	0
56	MG	13	1651	1/1	0.76	0.25	76,76,76,76	0
56	MG	13	1663	1/1	0.76	0.18	107,107,107,107	0
56	MG	1H	3247	1/1	0.76	0.39	105,105,105,105	0
56	MG	1H	3319	1/1	0.76	0.32	87,87,87,87	0
56	MG	14	3097	1/1	0.77	0.25	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3236	1/1	0.77	0.19	92,92,92,92	0
56	MG	1H	3149	1/1	0.77	0.28	60,60,60,60	0
56	MG	13	1615	1/1	0.77	0.35	100,100,100,100	0
56	MG	1H	3324	1/1	0.77	0.24	81,81,81,81	0
56	MG	14	3112	1/1	0.77	0.37	85,85,85,85	0
56	MG	1H	3042	1/1	0.77	0.34	62,62,62,62	0
56	MG	1H	3291	1/1	0.77	0.25	93,93,93,93	0
56	MG	1J	205	1/1	0.77	0.28	113,113,113,113	0
56	MG	1H	3062	1/1	0.77	0.21	61,61,61,61	0
56	MG	14	3132	1/1	0.77	0.20	84,84,84,84	0
56	MG	14	3204	1/1	0.77	0.38	87,87,87,87	0
56	MG	14	3147	1/1	0.77	0.23	93,93,93,93	0
56	MG	13	1687	1/1	0.77	0.40	94,94,94,94	0
56	MG	13	1652	1/1	0.78	0.28	83,83,83,83	0
56	MG	14	3021	1/1	0.78	0.31	81,81,81,81	0
56	MG	1H	3139	1/1	0.78	0.21	70,70,70,70	0
56	MG	13	1623	1/1	0.78	0.35	98,98,98,98	0
56	MG	1H	3320	1/1	0.78	0.13	95,95,95,95	0
56	MG	1H	3174	1/1	0.78	0.23	63,63,63,63	0
56	MG	14	3190	1/1	0.78	0.23	90,90,90,90	0
56	MG	13	1695	1/1	0.78	0.47	100,100,100,100	0
56	MG	14	3233	1/1	0.78	0.18	77,77,77,77	0
56	MG	1H	3197	1/1	0.78	0.36	101,101,101,101	0
56	MG	1H	3199	1/1	0.78	0.59	101,101,101,101	0
56	MG	1H	3032	1/1	0.78	0.27	79,79,79,79	0
56	MG	1G	1651	1/1	0.78	0.58	95,95,95,95	0
56	MG	16	206	1/1	0.78	0.16	88,88,88,88	0
56	MG	14	3260	1/1	0.78	0.18	112,112,112,112	0
56	MG	14	3015	1/1	0.78	0.25	83,83,83,83	0
56	MG	14	3220	1/1	0.78	0.34	108,108,108,108	0
56	MG	14	3240	1/1	0.78	0.40	90,90,90,90	0
56	MG	1H	3115	1/1	0.78	0.22	78,78,78,78	0
56	MG	14	3272	1/1	0.78	0.13	100,100,100,100	0
56	MG	14	3094	1/1	0.78	0.26	89,89,89,89	0
56	MG	1H	3308	1/1	0.78	0.26	85,85,85,85	0
56	MG	1G	1617	1/1	0.78	0.37	90,90,90,90	0
57	ZN	G8	201	1/1	0.78	0.21	176,176,176,176	0
56	MG	1H	3242	1/1	0.78	0.32	82,82,82,82	0
56	MG	1H	3304	1/1	0.79	0.38	94,94,94,94	0
56	MG	14	3029	1/1	0.79	0.28	86,86,86,86	0
56	MG	13	1676	1/1	0.79	0.27	89,89,89,89	0
56	MG	3L	103	1/1	0.79	0.18	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	13	1665	1/1	0.79	0.20	90,90,90,90	0
56	MG	14	3157	1/1	0.79	0.23	68,68,68,68	0
56	MG	1H	3171	1/1	0.79	0.32	65,65,65,65	0
56	MG	1H	3054	1/1	0.79	0.32	67,67,67,67	0
56	MG	1H	3178	1/1	0.79	0.17	61,61,61,61	0
56	MG	1H	3278	1/1	0.79	0.20	74,74,74,74	0
56	MG	1G	1667	1/1	0.79	0.31	124,124,124,124	0
56	MG	1G	1620	1/1	0.79	0.28	93,93,93,93	0
56	MG	1H	3325	1/1	0.79	0.19	96,96,96,96	0
56	MG	1H	3240	1/1	0.79	0.29	82,82,82,82	0
56	MG	14	3226	1/1	0.79	0.24	83,83,83,83	0
56	MG	13	1659	1/1	0.79	0.37	94,94,94,94	0
56	MG	14	3106	1/1	0.79	0.17	93,93,93,93	0
56	MG	13	1616	1/1	0.79	0.21	95,95,95,95	0
56	MG	14	3028	1/1	0.79	0.29	101,101,101,101	0
56	MG	13	1646	1/1	0.80	0.33	80,80,80,80	0
56	MG	1H	3213	1/1	0.80	0.42	78,78,78,78	0
56	MG	1H	3267	1/1	0.80	0.25	96,96,96,96	0
56	MG	14	3120	1/1	0.80	0.12	82,82,82,82	0
56	MG	1H	3134	1/1	0.80	0.32	90,90,90,90	0
56	MG	1H	3025	1/1	0.80	0.13	67,67,67,67	0
56	MG	13	1611	1/1	0.80	0.23	79,79,79,79	0
56	MG	14	3201	1/1	0.80	0.29	86,86,86,86	0
56	MG	13	1696	1/1	0.80	0.18	91,91,91,91	0
56	MG	1H	3288	1/1	0.80	0.24	73,73,73,73	0
56	MG	14	3372	1/1	0.80	0.20	114,114,114,114	0
56	MG	1H	3176	1/1	0.80	0.41	76,76,76,76	0
56	MG	1H	3055	1/1	0.80	0.23	77,77,77,77	0
56	MG	11	301	1/1	0.80	0.33	78,78,78,78	0
56	MG	1H	3298	1/1	0.80	0.10	71,71,71,71	0
56	MG	1H	3060	1/1	0.80	0.18	56,56,56,56	0
56	MG	1H	3253	1/1	0.80	0.39	87,87,87,87	0
56	MG	1H	3306	1/1	0.80	0.29	81,81,81,81	0
56	MG	14	3189	1/1	0.80	0.20	72,72,72,72	0
56	MG	1G	1615	1/1	0.80	0.14	86,86,86,86	0
56	MG	1H	3310	1/1	0.80	0.23	84,84,84,84	0
56	MG	13	1633	1/1	0.80	0.15	84,84,84,84	0
56	MG	14	3258	1/1	0.80	0.22	80,80,80,80	0
56	MG	2K	102	1/1	0.80	0.16	92,92,92,92	0
56	MG	14	3239	1/1	0.80	0.26	92,92,92,92	0
56	MG	14	3262	1/1	0.81	0.21	101,101,101,101	0
56	MG	13	1670	1/1	0.81	0.27	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3186	1/1	0.81	0.33	84,84,84,84	0
56	MG	14	3027	1/1	0.81	0.40	89,89,89,89	0
56	MG	14	3080	1/1	0.81	0.28	96,96,96,96	0
56	MG	1H	3130	1/1	0.81	0.19	83,83,83,83	0
56	MG	1G	1622	1/1	0.81	0.20	128,128,128,128	0
56	MG	13	1662	1/1	0.81	0.25	94,94,94,94	0
56	MG	2L	102	1/1	0.81	0.36	85,85,85,85	0
56	MG	14	3237	1/1	0.81	0.34	85,85,85,85	0
56	MG	13	1650	1/1	0.81	0.18	105,105,105,105	0
56	MG	1H	3151	1/1	0.81	0.20	60,60,60,60	0
56	MG	14	3103	1/1	0.81	0.30	84,84,84,84	0
56	MG	14	3144	1/1	0.81	0.41	83,83,83,83	0
56	MG	3L	102	1/1	0.81	0.10	146,146,146,146	0
56	MG	1H	3422	1/1	0.81	0.17	99,99,99,99	0
56	MG	1H	3022	1/1	0.81	0.26	89,89,89,89	0
56	MG	14	3040	1/1	0.81	0.39	86,86,86,86	0
56	MG	1G	1650	1/1	0.81	0.20	91,91,91,91	0
56	MG	14	3210	1/1	0.81	0.22	100,100,100,100	0
56	MG	14	3152	1/1	0.81	0.16	67,67,67,67	0
56	MG	13	1694	1/1	0.81	0.27	94,94,94,94	0
56	MG	14	3008	1/1	0.81	0.35	61,61,61,61	0
56	MG	1H	3282	1/1	0.81	0.25	60,60,60,60	0
56	MG	13	1608	1/1	0.81	0.30	79,79,79,79	0
56	MG	13	1649	1/1	0.81	0.27	102,102,102,102	0
56	MG	1G	1670	1/1	0.81	0.31	96,96,96,96	0
56	MG	1G	1672	1/1	0.81	0.34	98,98,98,98	0
56	MG	14	3128	1/1	0.81	0.36	91,91,91,91	0
56	MG	4I	202	1/1	0.81	0.20	85,85,85,85	0
56	MG	1H	3214	1/1	0.81	0.15	101,101,101,101	0
56	MG	14	3129	1/1	0.81	0.21	89,89,89,89	0
56	MG	1H	3107	1/1	0.81	0.23	84,84,84,84	0
56	MG	1G	1611	1/1	0.81	0.18	89,89,89,89	0
56	MG	1H	3108	1/1	0.81	0.36	44,44,44,44	0
56	MG	13	1622	1/1	0.82	0.24	99,99,99,99	0
56	MG	1H	3158	1/1	0.82	0.26	64,64,64,64	0
56	MG	13	1707	1/1	0.82	0.28	98,98,98,98	0
56	MG	14	3169	1/1	0.82	0.23	65,65,65,65	0
56	MG	13	1664	1/1	0.82	0.29	88,88,88,88	0
56	MG	14	3176	1/1	0.82	0.33	88,88,88,88	0
56	MG	1G	1633	1/1	0.82	0.36	101,101,101,101	0
56	MG	1H	3180	1/1	0.82	0.21	63,63,63,63	0
56	MG	1H	3095	1/1	0.82	0.28	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3180	1/1	0.82	0.29	104,104,104,104	0
56	MG	1H	3190	1/1	0.82	0.41	85,85,85,85	0
56	MG	1H	3444	1/1	0.82	0.16	119,119,119,119	0
56	MG	14	3382	1/1	0.82	0.26	94,94,94,94	0
56	MG	14	3087	1/1	0.82	0.38	89,89,89,89	0
56	MG	1G	1647	1/1	0.82	0.35	102,102,102,102	0
56	MG	14	3088	1/1	0.82	0.29	88,88,88,88	0
56	MG	1H	3113	1/1	0.82	0.32	84,84,84,84	0
56	MG	13	1614	1/1	0.82	0.33	98,98,98,98	0
56	MG	13	1638	1/1	0.82	0.29	68,68,68,68	0
56	MG	1G	1658	1/1	0.82	0.48	91,91,91,91	0
56	MG	1G	1660	1/1	0.82	0.34	105,105,105,105	0
56	MG	13	1641	1/1	0.82	0.35	80,80,80,80	0
56	MG	13	1697	1/1	0.82	0.20	92,92,92,92	0
56	MG	1H	3289	1/1	0.82	0.14	79,79,79,79	0
56	MG	1G	1666	1/1	0.82	0.51	101,101,101,101	0
56	MG	1H	3126	1/1	0.82	0.36	96,96,96,96	0
56	MG	1H	3129	1/1	0.82	0.13	57,57,57,57	0
56	MG	1H	3014	1/1	0.82	0.37	62,62,62,62	0
56	MG	14	3131	1/1	0.82	0.46	89,89,89,89	0
56	MG	1G	1673	1/1	0.82	0.30	93,93,93,93	0
56	MG	1H	3299	1/1	0.82	0.25	83,83,83,83	0
56	MG	1G	1675	1/1	0.82	0.38	93,93,93,93	0
56	MG	14	3105	1/1	0.82	0.26	60,60,60,60	0
56	MG	1H	3303	1/1	0.82	0.27	84,84,84,84	0
56	MG	14	3160	1/1	0.82	0.31	81,81,81,81	0
56	MG	1H	3143	1/1	0.82	0.24	81,81,81,81	0
56	MG	1H	3243	1/1	0.82	0.45	85,85,85,85	0
56	MG	14	3231	1/1	0.82	0.17	79,79,79,79	0
56	MG	1H	3295	1/1	0.83	0.22	72,72,72,72	0
56	MG	1H	3296	1/1	0.83	0.15	71,71,71,71	0
56	MG	1G	1619	1/1	0.83	0.48	87,87,87,87	0
56	MG	1H	3215	1/1	0.83	0.37	88,88,88,88	0
56	MG	1H	3124	1/1	0.83	0.28	72,72,72,72	0
56	MG	14	3188	1/1	0.83	0.25	83,83,83,83	0
56	MG	1H	3218	1/1	0.83	0.31	91,91,91,91	0
56	MG	14	3251	1/1	0.83	0.14	83,83,83,83	0
56	MG	1H	3128	1/1	0.83	0.24	69,69,69,69	0
56	MG	14	3253	1/1	0.83	0.12	73,73,73,73	0
56	MG	14	3254	1/1	0.83	0.33	91,91,91,91	0
56	MG	1H	3132	1/1	0.83	0.18	71,71,71,71	0
56	MG	1H	3023	1/1	0.83	0.27	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3058	1/1	0.83	0.23	89,89,89,89	0
56	MG	13	1629	1/1	0.83	0.40	84,84,84,84	0
56	MG	1G	1644	1/1	0.83	0.36	102,102,102,102	0
56	MG	1H	3140	1/1	0.83	0.25	87,87,87,87	0
56	MG	14	3060	1/1	0.83	0.25	84,84,84,84	0
56	MG	1H	3147	1/1	0.83	0.13	69,69,69,69	0
56	MG	1H	3038	1/1	0.83	0.26	78,78,78,78	0
56	MG	1H	3041	1/1	0.83	0.30	75,75,75,75	0
56	MG	14	3036	1/1	0.83	0.32	80,80,80,80	0
56	MG	1H	3163	1/1	0.83	0.27	82,82,82,82	0
56	MG	14	3037	1/1	0.83	0.22	62,62,62,62	0
56	MG	1H	3264	1/1	0.83	0.22	68,68,68,68	0
56	MG	14	3071	1/1	0.83	0.17	63,63,63,63	0
56	MG	14	3165	1/1	0.83	0.20	69,69,69,69	0
56	MG	14	3107	1/1	0.83	0.26	74,74,74,74	0
56	MG	1H	3272	1/1	0.83	0.25	92,92,92,92	0
56	MG	1H	3092	1/1	0.83	0.17	66,66,66,66	0
56	MG	14	3270	1/1	0.83	0.45	98,98,98,98	0
56	MG	13	1655	1/1	0.83	0.23	68,68,68,68	0
56	MG	1H	3280	1/1	0.83	0.29	101,101,101,101	0
56	MG	14	3175	1/1	0.83	0.13	83,83,83,83	0
56	MG	13	1689	1/1	0.83	0.34	92,92,92,92	0
56	MG	13	1644	1/1	0.83	0.29	87,87,87,87	0
56	MG	13	1631	1/1	0.83	0.24	62,62,62,62	0
56	MG	14	3090	1/1	0.83	0.20	87,87,87,87	0
56	MG	14	3125	1/1	0.83	0.23	77,77,77,77	0
56	MG	1G	1613	1/1	0.83	0.22	98,98,98,98	0
56	MG	1H	3119	1/1	0.83	0.35	70,70,70,70	0
56	MG	14	3223	1/1	0.83	0.33	60,60,60,60	0
56	MG	1H	3204	1/1	0.84	0.35	70,70,70,70	0
56	MG	1H	3269	1/1	0.84	0.30	78,78,78,78	0
56	MG	1G	1626	1/1	0.84	0.20	99,99,99,99	0
56	MG	1G	1628	1/1	0.84	0.39	83,83,83,83	0
56	MG	1H	3322	1/1	0.84	0.37	77,77,77,77	0
56	MG	1H	3058	1/1	0.84	0.34	80,80,80,80	0
56	MG	14	3116	1/1	0.84	0.32	75,75,75,75	0
56	MG	1H	3136	1/1	0.84	0.31	69,69,69,69	0
56	MG	13	1674	1/1	0.84	0.30	83,83,83,83	0
56	MG	1H	3091	1/1	0.84	0.27	65,65,65,65	0
56	MG	1H	3488	1/1	0.84	0.09	134,134,134,134	0
56	MG	14	3154	1/1	0.84	0.22	59,59,59,59	0
56	MG	14	3051	1/1	0.84	0.36	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1J	203	1/1	0.84	0.20	96,96,96,96	0
56	MG	1H	3221	1/1	0.84	0.57	88,88,88,88	0
56	MG	1H	3099	1/1	0.84	0.24	74,74,74,74	0
56	MG	14	3056	1/1	0.84	0.32	69,69,69,69	0
56	MG	1H	3229	1/1	0.84	0.31	82,82,82,82	0
56	MG	2L	103	1/1	0.84	0.20	85,85,85,85	0
56	MG	1H	3292	1/1	0.84	0.30	80,80,80,80	0
56	MG	1H	3237	1/1	0.84	0.36	82,82,82,82	0
56	MG	14	3081	1/1	0.84	0.47	90,90,90,90	0
56	MG	1G	1662	1/1	0.84	0.16	81,81,81,81	0
56	MG	14	3191	1/1	0.84	0.22	90,90,90,90	0
56	MG	14	3127	1/1	0.84	0.21	88,88,88,88	0
56	MG	1H	3026	1/1	0.84	0.20	61,61,61,61	0
56	MG	1H	3029	1/1	0.84	0.26	91,91,91,91	0
56	MG	1G	1608	1/1	0.84	0.25	86,86,86,86	0
56	MG	1H	3300	1/1	0.84	0.23	102,102,102,102	0
56	MG	1H	3118	1/1	0.84	0.33	87,87,87,87	0
56	MG	13	1624	1/1	0.84	0.32	89,89,89,89	0
56	MG	14	3146	1/1	0.84	0.33	91,91,91,91	0
56	MG	14	3336	1/1	0.84	0.32	114,114,114,114	0
56	MG	14	3247	1/1	0.84	0.30	89,89,89,89	0
56	MG	14	3174	1/1	0.84	0.31	82,82,82,82	0
56	MG	1H	3193	1/1	0.84	0.31	89,89,89,89	0
56	MG	1G	1696	1/1	0.84	0.12	113,113,113,113	0
56	MG	1H	3044	1/1	0.84	0.28	76,76,76,76	0
56	MG	13	1620	1/1	0.84	0.20	81,81,81,81	0
56	MG	14	3017	1/1	0.84	0.25	70,70,70,70	0
56	MG	1G	1631	1/1	0.85	0.29	88,88,88,88	0
56	MG	1H	3078	1/1	0.85	0.39	80,80,80,80	0
56	MG	14	3199	1/1	0.85	0.30	83,83,83,83	0
56	MG	1H	3475	1/1	0.85	0.19	114,114,114,114	0
56	MG	1H	3279	1/1	0.85	0.13	80,80,80,80	0
56	MG	14	3034	1/1	0.85	0.24	78,78,78,78	0
56	MG	14	3014	1/1	0.85	0.14	73,73,73,73	0
56	MG	1H	3144	1/1	0.85	0.17	63,63,63,63	0
56	MG	1H	3097	1/1	0.85	0.12	76,76,76,76	0
56	MG	1H	3223	1/1	0.85	0.18	88,88,88,88	0
56	MG	1H	3225	1/1	0.85	0.41	87,87,87,87	0
56	MG	13	1731	1/1	0.85	0.12	115,115,115,115	0
56	MG	1H	3103	1/1	0.85	0.28	60,60,60,60	0
56	MG	14	3177	1/1	0.85	0.12	81,81,81,81	0
56	MG	13	1637	1/1	0.85	0.17	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1G	1656	1/1	0.85	0.24	112,112,112,112	0
56	MG	1H	3165	1/1	0.85	0.22	45,45,45,45	0
56	MG	14	3214	1/1	0.85	0.37	88,88,88,88	0
56	MG	14	3073	1/1	0.85	0.24	64,64,64,64	0
56	MG	13	1672	1/1	0.85	0.16	103,103,103,103	0
56	MG	1H	3177	1/1	0.85	0.41	72,72,72,72	0
56	MG	14	3268	1/1	0.85	0.20	96,96,96,96	0
56	MG	1G	1610	1/1	0.85	0.16	103,103,103,103	0
56	MG	13	1705	1/1	0.85	0.17	82,82,82,82	0
56	MG	14	3158	1/1	0.85	0.57	83,83,83,83	0
56	MG	1H	3185	1/1	0.85	0.25	70,70,70,70	0
56	MG	1H	3039	1/1	0.85	0.18	87,87,87,87	0
56	MG	14	3114	1/1	0.85	0.24	69,69,69,69	0
56	MG	13	1677	1/1	0.85	0.44	96,96,96,96	0
56	MG	14	3374	1/1	0.85	0.10	131,131,131,131	0
56	MG	13	1668	1/1	0.85	0.10	98,98,98,98	0
56	MG	13	1691	1/1	0.85	0.29	87,87,87,87	0
56	MG	1H	3056	1/1	0.85	0.23	74,74,74,74	0
56	MG	14	3250	1/1	0.85	0.14	98,98,98,98	0
56	MG	14	3009	1/1	0.85	0.21	73,73,73,73	0
56	MG	14	3032	1/1	0.85	0.27	87,87,87,87	0
56	MG	1H	3063	1/1	0.85	0.21	54,54,54,54	0
56	MG	1H	3276	1/1	0.85	0.15	87,87,87,87	0
56	MG	1H	3007	1/1	0.86	0.25	58,58,58,58	0
56	MG	1H	3188	1/1	0.86	0.26	67,67,67,67	0
56	MG	1H	3244	1/1	0.86	0.49	85,85,85,85	0
56	MG	14	3053	1/1	0.86	0.51	78,78,78,78	0
56	MG	14	3104	1/1	0.86	0.27	78,78,78,78	0
56	MG	14	3242	1/1	0.86	0.33	89,89,89,89	0
56	MG	14	3265	1/1	0.86	0.36	96,96,96,96	0
56	MG	13	1680	1/1	0.86	0.23	107,107,107,107	0
56	MG	14	3057	1/1	0.86	0.25	74,74,74,74	0
56	MG	14	3013	1/1	0.86	0.21	65,65,65,65	0
56	MG	14	3200	1/1	0.86	0.30	94,94,94,94	0
56	MG	1H	3208	1/1	0.86	0.16	53,53,53,53	0
56	MG	14	3109	1/1	0.86	0.23	67,67,67,67	0
56	MG	1H	3265	1/1	0.86	0.28	94,94,94,94	0
56	MG	14	3178	1/1	0.86	0.22	86,86,86,86	0
56	MG	14	3111	1/1	0.86	0.37	98,98,98,98	0
56	MG	1H	3152	1/1	0.86	0.39	75,75,75,75	0
56	MG	1G	1614	1/1	0.86	0.28	92,92,92,92	0
56	MG	1H	3040	1/1	0.86	0.32	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3019	1/1	0.86	0.26	73,73,73,73	0
56	MG	14	3041	1/1	0.86	0.19	59,59,59,59	0
56	MG	14	3063	1/1	0.86	0.29	70,70,70,70	0
56	MG	1H	3051	1/1	0.86	0.12	71,71,71,71	0
56	MG	1H	3175	1/1	0.86	0.32	69,69,69,69	0
56	MG	14	3410	1/1	0.86	0.19	112,112,112,112	0
56	MG	14	3257	1/1	0.86	0.17	93,93,93,93	0
56	MG	1H	3231	1/1	0.86	0.32	92,92,92,92	0
56	MG	1H	3468	1/1	0.86	0.11	115,115,115,115	0
56	MG	1K	101	1/1	0.86	0.15	91,91,91,91	0
56	MG	13	1673	1/1	0.86	0.26	84,84,84,84	0
56	MG	1H	3529	1/1	0.86	0.11	113,113,113,113	0
56	MG	1H	3238	1/1	0.86	0.20	98,98,98,98	0
56	MG	14	3025	1/1	0.86	0.20	87,87,87,87	0
56	MG	13	1656	1/1	0.86	0.25	84,84,84,84	0
56	MG	14	3123	1/1	0.87	0.42	93,93,93,93	0
56	MG	14	3124	1/1	0.87	0.33	80,80,80,80	0
56	MG	1H	3246	1/1	0.87	0.26	81,81,81,81	0
56	MG	16	203	1/1	0.87	0.33	82,82,82,82	0
56	MG	1H	3021	1/1	0.87	0.41	84,84,84,84	0
56	MG	14	3166	1/1	0.87	0.21	85,85,85,85	0
56	MG	1G	1642	1/1	0.87	0.16	130,130,130,130	0
56	MG	1G	1643	1/1	0.87	0.24	147,147,147,147	0
56	MG	16	208	1/1	0.87	0.26	88,88,88,88	0
56	MG	13	1701	1/1	0.87	0.11	71,71,71,71	0
56	MG	13	1630	1/1	0.87	0.15	80,80,80,80	0
56	MG	1H	3138	1/1	0.87	0.26	72,72,72,72	0
56	MG	14	3033	1/1	0.87	0.14	63,63,63,63	0
56	MG	78	201	1/1	0.87	0.32	79,79,79,79	0
56	MG	14	3076	1/1	0.87	0.24	60,60,60,60	0
56	MG	1G	1653	1/1	0.87	0.18	99,99,99,99	0
56	MG	14	3115	1/1	0.87	0.23	82,82,82,82	0
56	MG	14	3007	1/1	0.87	0.16	69,69,69,69	0
56	MG	14	3202	1/1	0.87	0.13	106,106,106,106	0
56	MG	13	1634	1/1	0.87	0.15	76,76,76,76	0
56	MG	1H	3150	1/1	0.87	0.46	86,86,86,86	0
56	MG	14	3155	1/1	0.87	0.13	68,68,68,68	0
56	MG	1H	3111	1/1	0.87	0.17	67,67,67,67	0
56	MG	14	3256	1/1	0.87	0.33	86,86,86,86	0
56	MG	1H	3220	1/1	0.87	0.50	82,82,82,82	0
56	MG	1H	3161	1/1	0.87	0.32	101,101,101,101	0
56	MG	1H	3114	1/1	0.87	0.40	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3416	1/1	0.87	0.16	116,116,116,116	0
56	MG	1G	1671	1/1	0.87	0.10	92,92,92,92	0
56	MG	14	3083	1/1	0.87	0.32	86,86,86,86	0
56	MG	1H	3172	1/1	0.87	0.19	60,60,60,60	0
56	MG	1H	3047	1/1	0.87	0.25	62,62,62,62	0
56	MG	13	1640	1/1	0.87	0.22	81,81,81,81	0
56	MG	1H	3120	1/1	0.87	0.24	89,89,89,89	0
56	MG	14	3211	1/1	0.87	0.12	94,94,94,94	0
56	MG	14	3212	1/1	0.87	0.36	85,85,85,85	0
56	MG	14	3137	1/1	0.87	0.14	96,96,96,96	0
56	MG	1G	1629	1/1	0.87	0.25	75,75,75,75	0
56	MG	1H	3003	1/1	0.87	0.29	60,60,60,60	0
56	MG	14	3018	1/1	0.87	0.23	96,96,96,96	0
56	MG	1G	1630	1/1	0.88	0.52	92,92,92,92	0
56	MG	1H	3212	1/1	0.88	0.27	79,79,79,79	0
56	MG	14	3378	1/1	0.88	0.09	126,126,126,126	0
56	MG	14	3234	1/1	0.88	0.41	81,81,81,81	0
56	MG	16	202	1/1	0.88	0.23	68,68,68,68	0
56	MG	1H	3259	1/1	0.88	0.29	79,79,79,79	0
56	MG	1G	1636	1/1	0.88	0.23	89,89,89,89	0
56	MG	1H	3052	1/1	0.88	0.26	77,77,77,77	0
56	MG	14	3039	1/1	0.88	0.17	81,81,81,81	0
56	MG	13	1602	1/1	0.88	0.19	70,70,70,70	0
56	MG	14	3052	1/1	0.88	0.24	75,75,75,75	0
56	MG	14	3215	1/1	0.88	0.41	91,91,91,91	0
56	MG	21	301	1/1	0.88	0.28	56,56,56,56	0
56	MG	14	3089	1/1	0.88	0.12	54,54,54,54	0
56	MG	41	201	1/1	0.88	0.20	85,85,85,85	0
56	MG	1H	3307	1/1	0.88	0.35	86,86,86,86	0
56	MG	14	3179	1/1	0.88	0.09	71,71,71,71	0
56	MG	L8	101	1/1	0.88	0.20	81,81,81,81	0
56	MG	1H	3035	1/1	0.88	0.23	76,76,76,76	0
56	MG	1H	3268	1/1	0.88	0.33	84,84,84,84	0
56	MG	1G	1654	1/1	0.88	0.14	115,115,115,115	0
56	MG	1G	1603	1/1	0.88	0.17	77,77,77,77	0
56	MG	1G	1605	1/1	0.88	0.24	95,95,95,95	0
56	MG	1G	1606	1/1	0.88	0.14	102,102,102,102	0
56	MG	1G	1659	1/1	0.88	0.17	150,150,150,150	0
56	MG	14	3271	1/1	0.88	0.18	99,99,99,99	0
56	MG	1H	3080	1/1	0.88	0.23	76,76,76,76	0
56	MG	1G	1609	1/1	0.88	0.22	96,96,96,96	0
56	MG	1H	3317	1/1	0.88	0.21	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3001	1/1	0.88	0.27	62,62,62,62	0
56	MG	1H	3230	1/1	0.88	0.24	73,73,73,73	0
56	MG	13	1604	1/1	0.88	0.20	80,80,80,80	0
56	MG	1H	3194	1/1	0.88	0.20	83,83,83,83	0
56	MG	1H	3236	1/1	0.88	0.31	72,72,72,72	0
56	MG	1H	3093	1/1	0.88	0.18	56,56,56,56	0
56	MG	14	3232	1/1	0.88	0.28	100,100,100,100	0
56	MG	1H	3420	1/1	0.88	0.09	114,114,114,114	0
56	MG	1H	3281	1/1	0.88	0.37	85,85,85,85	0
56	MG	1H	3200	1/1	0.88	0.15	77,77,77,77	0
56	MG	1H	3202	1/1	0.88	0.30	87,87,87,87	0
56	MG	14	3245	1/1	0.88	0.14	83,83,83,83	0
56	MG	14	3047	1/1	0.88	0.25	68,68,68,68	0
56	MG	1H	3167	1/1	0.88	0.27	59,59,59,59	0
56	MG	1H	3207	1/1	0.88	0.35	76,76,76,76	0
56	MG	1H	3045	1/1	0.88	0.33	66,66,66,66	0
56	MG	1H	3210	1/1	0.88	0.25	71,71,71,71	0
56	MG	16	205	1/1	0.89	0.16	87,87,87,87	0
56	MG	13	1657	1/1	0.89	0.61	84,84,84,84	0
56	MG	1H	3004	1/1	0.89	0.21	63,63,63,63	0
56	MG	14	3046	1/1	0.89	0.26	70,70,70,70	0
56	MG	13	1636	1/1	0.89	0.27	74,74,74,74	0
56	MG	1H	3166	1/1	0.89	0.31	53,53,53,53	0
56	MG	14	3273	1/1	0.89	0.16	106,106,106,106	0
56	MG	1H	3015	1/1	0.89	0.27	54,54,54,54	0
56	MG	1H	3016	1/1	0.89	0.17	61,61,61,61	0
56	MG	1H	3173	1/1	0.89	0.20	73,73,73,73	0
56	MG	1H	3313	1/1	0.89	0.18	86,86,86,86	0
56	MG	14	3134	1/1	0.89	0.19	82,82,82,82	0
56	MG	14	3235	1/1	0.89	0.37	92,92,92,92	0
56	MG	14	3096	1/1	0.89	0.18	64,64,64,64	0
56	MG	1H	3073	1/1	0.89	0.30	55,55,55,55	0
56	MG	14	3218	1/1	0.89	0.33	95,95,95,95	0
56	MG	14	3136	1/1	0.89	0.20	92,92,92,92	0
56	MG	1H	3321	1/1	0.89	0.43	93,93,93,93	0
56	MG	1H	3089	1/1	0.89	0.22	56,56,56,56	0
56	MG	1H	3183	1/1	0.89	0.10	61,61,61,61	0
56	MG	14	3156	1/1	0.89	0.32	92,92,92,92	0
56	MG	13	1669	1/1	0.89	0.20	78,78,78,78	0
56	MG	1H	3403	1/1	0.89	0.13	78,78,78,78	0
56	MG	14	3113	1/1	0.89	0.13	57,57,57,57	0
56	MG	1H	3189	1/1	0.89	0.40	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3033	1/1	0.89	0.24	72,72,72,72	0
56	MG	1H	3458	1/1	0.89	0.13	126,126,126,126	0
56	MG	13	1618	1/1	0.89	0.23	67,67,67,67	0
56	MG	1H	3287	1/1	0.89	0.21	88,88,88,88	0
56	MG	1H	3484	1/1	0.89	0.10	105,105,105,105	0
56	MG	1H	3037	1/1	0.89	0.26	51,51,51,51	0
56	MG	14	3141	1/1	0.89	0.32	72,72,72,72	0
56	MG	1H	3531	1/1	0.89	0.09	109,109,109,109	0
56	MG	1H	3535	1/1	0.89	0.09	115,115,115,115	0
56	MG	3I	201	1/1	0.89	0.26	68,68,68,68	0
56	MG	14	3206	1/1	0.89	0.22	86,86,86,86	0
56	MG	2K	101	1/1	0.89	0.21	74,74,74,74	0
56	MG	13	1625	1/1	0.89	0.20	74,74,74,74	0
56	MG	13	1635	1/1	0.89	0.30	85,85,85,85	0
56	MG	13	1645	1/1	0.89	0.25	94,94,94,94	0
56	MG	1H	3153	1/1	0.89	0.21	77,77,77,77	0
56	MG	1H	3156	1/1	0.89	0.40	85,85,85,85	0
56	MG	1G	1627	1/1	0.90	0.34	83,83,83,83	0
56	MG	1H	3123	1/1	0.90	0.26	90,90,90,90	0
56	MG	14	3282	1/1	0.90	0.11	76,76,76,76	0
56	MG	1H	3232	1/1	0.90	0.22	46,46,46,46	0
56	MG	14	3159	1/1	0.90	0.19	64,64,64,64	0
56	MG	1H	3019	1/1	0.90	0.13	48,48,48,48	0
56	MG	1H	3020	1/1	0.90	0.31	67,67,67,67	0
56	MG	13	1619	1/1	0.90	0.27	71,71,71,71	0
56	MG	1H	3184	1/1	0.90	0.41	73,73,73,73	0
56	MG	1H	3064	1/1	0.90	0.11	52,52,52,52	0
56	MG	14	3161	1/1	0.90	0.13	100,100,100,100	0
56	MG	1H	3075	1/1	0.90	0.27	52,52,52,52	0
56	MG	1H	3076	1/1	0.90	0.14	64,64,64,64	0
56	MG	1H	3302	1/1	0.90	0.28	88,88,88,88	0
56	MG	16	209	1/1	0.90	0.14	74,74,74,74	0
56	MG	14	3213	1/1	0.90	0.31	76,76,76,76	0
56	MG	13	1632	1/1	0.90	0.22	74,74,74,74	0
56	MG	11	302	1/1	0.90	0.12	42,42,42,42	0
56	MG	1H	3084	1/1	0.90	0.27	64,64,64,64	0
56	MG	13	1671	1/1	0.90	0.14	92,92,92,92	0
56	MG	14	3145	1/1	0.90	0.16	57,57,57,57	0
56	MG	14	3402	1/1	0.90	0.10	105,105,105,105	0
56	MG	14	3072	1/1	0.90	0.24	82,82,82,82	0
56	MG	1H	3148	1/1	0.90	0.22	65,65,65,65	0
56	MG	14	3195	1/1	0.90	0.11	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3419	1/1	0.90	0.07	135,135,135,135	0
56	MG	14	3048	1/1	0.90	0.17	63,63,63,63	0
56	MG	5E	201	1/1	0.90	0.19	93,93,93,93	0
56	MG	14	3010	1/1	0.90	0.14	65,65,65,65	0
56	MG	1H	3209	1/1	0.90	0.17	68,68,68,68	0
56	MG	14	3150	1/1	0.90	0.21	57,57,57,57	0
56	MG	14	3264	1/1	0.90	0.10	78,78,78,78	0
56	MG	1G	1664	1/1	0.90	0.35	90,90,90,90	0
56	MG	1H	3160	1/1	0.90	0.20	81,81,81,81	0
56	MG	13	1682	1/1	0.90	0.23	135,135,135,135	0
56	MG	1H	3162	1/1	0.90	0.19	69,69,69,69	0
56	MG	1H	3358	1/1	0.90	0.34	65,65,65,65	0
56	MG	1H	3043	1/1	0.90	0.34	62,62,62,62	0
56	MG	1H	3164	1/1	0.90	0.18	56,56,56,56	0
56	MG	14	3061	1/1	0.90	0.19	49,49,49,49	0
56	MG	14	3062	1/1	0.90	0.11	70,70,70,70	0
56	MG	14	3269	1/1	0.90	0.12	84,84,84,84	0
56	MG	14	3035	1/1	0.90	0.27	68,68,68,68	0
56	MG	14	3084	1/1	0.90	0.25	70,70,70,70	0
56	MG	1H	3053	1/1	0.90	0.20	56,56,56,56	0
56	MG	14	3086	1/1	0.90	0.22	72,72,72,72	0
56	MG	1H	3525	1/1	0.90	0.11	113,113,113,113	0
56	MG	1G	1624	1/1	0.90	0.18	88,88,88,88	0
56	MG	1H	3228	1/1	0.90	0.19	67,67,67,67	0
56	MG	14	3067	1/1	0.90	0.26	76,76,76,76	0
56	MG	14	3361	1/1	0.91	0.10	119,119,119,119	0
56	MG	14	3252	1/1	0.91	0.08	74,74,74,74	0
56	MG	14	3011	1/1	0.91	0.26	65,65,65,65	0
56	MG	14	3208	1/1	0.91	0.12	69,69,69,69	0
56	MG	13	1730	1/1	0.91	0.10	111,111,111,111	0
56	MG	13	1647	1/1	0.91	0.11	83,83,83,83	0
56	MG	1H	3305	1/1	0.91	0.33	76,76,76,76	0
56	MG	14	3393	1/1	0.91	0.08	111,111,111,111	0
56	MG	1H	3067	1/1	0.91	0.34	75,75,75,75	0
56	MG	14	3142	1/1	0.91	0.18	89,89,89,89	0
56	MG	1H	3309	1/1	0.91	0.32	94,94,94,94	0
56	MG	14	3126	1/1	0.91	0.26	80,80,80,80	0
56	MG	14	3020	1/1	0.91	0.28	62,62,62,62	0
56	MG	1H	3077	1/1	0.91	0.34	81,81,81,81	0
56	MG	1H	3314	1/1	0.91	0.17	81,81,81,81	0
56	MG	14	3163	1/1	0.91	0.14	109,109,109,109	0
56	MG	14	3079	1/1	0.91	0.23	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3133	1/1	0.91	0.46	69,69,69,69	0
56	MG	1G	1648	1/1	0.91	0.44	85,85,85,85	0
56	MG	14	3095	1/1	0.91	0.20	87,87,87,87	0
56	MG	1H	3135	1/1	0.91	0.18	74,74,74,74	0
56	MG	88	201	1/1	0.91	0.20	73,73,73,73	0
56	MG	1H	3274	1/1	0.91	0.33	87,87,87,87	0
56	MG	P8	101	1/1	0.91	0.24	76,76,76,76	0
56	MG	1H	3275	1/1	0.91	0.32	83,83,83,83	0
56	MG	13	1621	1/1	0.91	0.46	64,64,64,64	0
56	MG	14	3167	1/1	0.91	0.23	67,67,67,67	0
56	MG	14	3196	1/1	0.91	0.18	69,69,69,69	0
56	MG	14	3022	1/1	0.91	0.18	83,83,83,83	0
56	MG	14	3098	1/1	0.91	0.20	53,53,53,53	0
56	MG	1H	3363	1/1	0.91	0.08	83,83,83,83	0
56	MG	1H	3141	1/1	0.91	0.22	78,78,78,78	0
56	MG	1H	3187	1/1	0.91	0.27	72,72,72,72	0
56	MG	14	3172	1/1	0.91	0.36	87,87,87,87	0
56	MG	1H	3433	1/1	0.91	0.11	92,92,92,92	0
56	MG	14	3100	1/1	0.91	0.31	69,69,69,69	0
56	MG	14	3043	1/1	0.91	0.16	52,52,52,52	0
56	MG	1H	3466	1/1	0.91	0.10	105,105,105,105	0
56	MG	14	3102	1/1	0.91	0.32	73,73,73,73	0
56	MG	1H	3006	1/1	0.91	0.33	48,48,48,48	0
56	MG	1H	3483	1/1	0.91	0.09	116,116,116,116	0
56	MG	14	3249	1/1	0.91	0.18	89,89,89,89	0
56	MG	14	3024	1/1	0.91	0.24	64,64,64,64	0
56	MG	1H	3515	1/1	0.91	0.12	107,107,107,107	0
56	MG	1H	3517	1/1	0.91	0.09	105,105,105,105	0
56	MG	1H	3198	1/1	0.91	0.32	82,82,82,82	0
56	MG	1G	1684	1/1	0.91	0.08	121,121,121,121	0
56	MG	1G	1690	1/1	0.91	0.08	120,120,120,120	0
56	MG	1G	1694	1/1	0.91	0.13	105,105,105,105	0
56	MG	1H	3010	1/1	0.91	0.24	46,46,46,46	0
56	MG	1H	3012	1/1	0.91	0.18	52,52,52,52	0
56	MG	1H	3155	1/1	0.91	0.14	65,65,65,65	0
56	MG	13	1725	1/1	0.91	0.14	114,114,114,114	0
56	MG	1H	3069	1/1	0.92	0.28	53,53,53,53	0
56	MG	1H	3520	1/1	0.92	0.24	91,91,91,91	0
56	MG	1H	3524	1/1	0.92	0.12	104,104,104,104	0
56	MG	1H	3024	1/1	0.92	0.08	61,61,61,61	0
56	MG	1H	3182	1/1	0.92	0.33	69,69,69,69	0
56	MG	1H	3530	1/1	0.92	0.08	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3091	1/1	0.92	0.13	64,64,64,64	0
56	MG	1H	3534	1/1	0.92	0.13	101,101,101,101	0
56	MG	13	1747	1/1	0.92	0.10	107,107,107,107	0
56	MG	1L	101	1/1	0.92	0.16	94,94,94,94	0
56	MG	14	3077	1/1	0.92	0.28	68,68,68,68	0
56	MG	14	3078	1/1	0.92	0.22	67,67,67,67	0
56	MG	13	1612	1/1	0.92	0.23	68,68,68,68	0
56	MG	1H	3085	1/1	0.92	0.24	64,64,64,64	0
56	MG	14	3193	1/1	0.92	0.30	78,78,78,78	0
56	MG	14	3099	1/1	0.92	0.29	82,82,82,82	0
56	MG	14	3292	1/1	0.92	0.08	73,73,73,73	0
56	MG	14	3319	1/1	0.92	0.09	86,86,86,86	0
56	MG	1H	3195	1/1	0.92	0.17	91,91,91,91	0
56	MG	2K	108	1/1	0.92	0.11	92,92,92,92	0
56	MG	1H	3257	1/1	0.92	0.24	85,85,85,85	0
56	MG	1H	3096	1/1	0.92	0.27	66,66,66,66	0
56	MG	13	1660	1/1	0.92	0.31	76,76,76,76	0
56	MG	1H	3312	1/1	0.92	0.42	83,83,83,83	0
56	MG	14	3349	1/1	0.92	0.20	82,82,82,82	0
56	MG	1H	3102	1/1	0.92	0.12	45,45,45,45	0
56	MG	1H	3005	1/1	0.92	0.20	51,51,51,51	0
56	MG	14	3358	1/1	0.92	0.18	98,98,98,98	0
56	MG	13	1639	1/1	0.92	0.17	87,87,87,87	0
56	MG	14	3364	1/1	0.92	0.08	132,132,132,132	0
56	MG	1H	3050	1/1	0.92	0.32	62,62,62,62	0
56	MG	1H	3157	1/1	0.92	0.22	57,57,57,57	0
56	MG	14	3366	1/1	0.92	0.08	90,90,90,90	0
56	MG	1H	3270	1/1	0.92	0.28	75,75,75,75	0
56	MG	13	1613	1/1	0.92	0.30	79,79,79,79	0
56	MG	1H	3013	1/1	0.92	0.24	59,59,59,59	0
56	MG	13	1601	1/1	0.92	0.17	71,71,71,71	0
56	MG	1H	3328	1/1	0.92	0.11	75,75,75,75	0
56	MG	1H	3116	1/1	0.92	0.10	66,66,66,66	0
56	MG	13	1606	1/1	0.92	0.20	83,83,83,83	0
56	MG	1H	3375	1/1	0.92	0.08	103,103,103,103	0
56	MG	14	3006	1/1	0.92	0.26	68,68,68,68	0
56	MG	1H	3018	1/1	0.92	0.16	67,67,67,67	0
56	MG	14	3054	1/1	0.92	0.35	70,70,70,70	0
56	MG	1H	3168	1/1	0.92	0.30	77,77,77,77	0
56	MG	1H	3121	1/1	0.92	0.17	59,59,59,59	0
56	MG	14	3224	1/1	0.92	0.12	66,66,66,66	0
56	MG	1H	3459	1/1	0.92	0.08	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3224	1/1	0.92	0.23	67,67,67,67	0
56	MG	14	3181	1/1	0.92	0.08	84,84,84,84	0
56	MG	13	1658	1/1	0.92	0.23	79,79,79,79	0
56	MG	1H	3066	1/1	0.92	0.11	48,48,48,48	0
56	MG	14	3042	1/1	0.92	0.36	69,69,69,69	0
56	MG	1H	3127	1/1	0.92	0.24	64,64,64,64	0
56	MG	1H	3504	1/1	0.92	0.07	117,117,117,117	0
56	MG	1H	3068	1/1	0.92	0.36	68,68,68,68	0
56	MG	1H	3284	1/1	0.93	0.14	81,81,81,81	0
56	MG	1H	3354	1/1	0.93	0.07	106,106,106,106	0
56	MG	1G	1637	1/1	0.93	0.18	89,89,89,89	0
56	MG	13	1749	1/1	0.93	0.11	107,107,107,107	0
56	MG	14	3412	1/1	0.93	0.13	93,93,93,93	0
56	MG	14	3138	1/1	0.93	0.09	71,71,71,71	0
56	MG	1H	3389	1/1	0.93	0.21	98,98,98,98	0
56	MG	1H	3392	1/1	0.93	0.10	67,67,67,67	0
56	MG	1H	3396	1/1	0.93	0.14	61,61,61,61	0
56	MG	1H	3087	1/1	0.93	0.18	69,69,69,69	0
56	MG	1H	3411	1/1	0.93	0.08	80,80,80,80	0
56	MG	14	3005	1/1	0.93	0.18	59,59,59,59	0
56	MG	13	1723	1/1	0.93	0.08	85,85,85,85	0
56	MG	1H	3249	1/1	0.93	0.16	75,75,75,75	0
56	MG	1H	3252	1/1	0.93	0.16	82,82,82,82	0
56	MG	14	3351	1/1	0.93	0.16	70,70,70,70	0
56	MG	1H	3131	1/1	0.93	0.09	71,71,71,71	0
56	MG	2L	101	1/1	0.93	0.18	86,86,86,86	0
56	MG	1H	3256	1/1	0.93	0.17	83,83,83,83	0
56	MG	1H	3474	1/1	0.93	0.10	103,103,103,103	0
56	MG	5I	101	1/1	0.93	0.08	82,82,82,82	0
56	MG	14	3049	1/1	0.93	0.13	60,60,60,60	0
56	MG	13	1628	1/1	0.93	0.10	51,51,51,51	0
56	MG	13	1686	1/1	0.93	0.15	84,84,84,84	0
56	MG	13	1609	1/1	0.93	0.11	83,83,83,83	0
56	MG	14	3117	1/1	0.93	0.33	69,69,69,69	0
56	MG	13	1733	1/1	0.93	0.07	102,102,102,102	0
56	MG	1H	3061	1/1	0.93	0.14	52,52,52,52	0
56	MG	1H	3521	1/1	0.93	0.14	89,89,89,89	0
56	MG	1H	3001	1/1	0.93	0.22	49,49,49,49	0
56	MG	1G	1668	1/1	0.93	0.28	90,90,90,90	0
56	MG	1H	3002	1/1	0.93	0.16	43,43,43,43	0
56	MG	14	3092	1/1	0.93	0.07	61,61,61,61	0
56	MG	1H	3146	1/1	0.93	0.30	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3112	1/1	0.93	0.20	72,72,72,72	0
56	MG	1H	3226	1/1	0.93	0.22	87,87,87,87	0
56	MG	1H	3065	1/1	0.93	0.18	51,51,51,51	0
56	MG	14	3093	1/1	0.93	0.19	58,58,58,58	0
56	MG	1H	3034	1/1	0.93	0.19	46,46,46,46	0
56	MG	14	3187	1/1	0.93	0.25	63,63,63,63	0
56	MG	1H	3036	1/1	0.93	0.15	59,59,59,59	0
56	MG	1H	3072	1/1	0.93	0.28	52,52,52,52	0
56	MG	14	3394	1/1	0.93	0.13	102,102,102,102	0
56	MG	1G	1693	1/1	0.93	0.07	109,109,109,109	0
56	MG	13	1678	1/1	0.93	0.11	85,85,85,85	0
56	MG	14	3122	1/1	0.93	0.21	77,77,77,77	0
56	MG	14	3405	1/1	0.93	0.10	93,93,93,93	0
56	MG	1H	3159	1/1	0.93	0.19	53,53,53,53	0
56	MG	1H	3011	1/1	0.93	0.23	51,51,51,51	0
56	MG	14	3399	1/1	0.94	0.10	116,116,116,116	0
56	MG	1H	3235	1/1	0.94	0.09	61,61,61,61	0
56	MG	14	3400	1/1	0.94	0.09	112,112,112,112	0
56	MG	1H	3074	1/1	0.94	0.20	46,46,46,46	0
56	MG	1H	3196	1/1	0.94	0.09	56,56,56,56	0
56	MG	1H	3008	1/1	0.94	0.17	41,41,41,41	0
56	MG	14	3325	1/1	0.94	0.06	110,110,110,110	0
56	MG	1H	3241	1/1	0.94	0.14	87,87,87,87	0
56	MG	16	204	1/1	0.94	0.09	68,68,68,68	0
56	MG	13	1726	1/1	0.94	0.09	96,96,96,96	0
56	MG	1H	3285	1/1	0.94	0.10	82,82,82,82	0
56	MG	14	3342	1/1	0.94	0.09	79,79,79,79	0
56	MG	14	3068	1/1	0.94	0.58	64,64,64,64	0
56	MG	1H	3376	1/1	0.94	0.13	88,88,88,88	0
56	MG	1H	3381	1/1	0.94	0.12	78,78,78,78	0
56	MG	1H	3245	1/1	0.94	0.19	73,73,73,73	0
56	MG	14	3415	1/1	0.94	0.06	121,121,121,121	0
56	MG	14	3026	1/1	0.94	0.16	55,55,55,55	0
56	MG	1H	3086	1/1	0.94	0.19	75,75,75,75	0
56	MG	1H	3046	1/1	0.94	0.14	46,46,46,46	0
56	MG	1H	3419	1/1	0.94	0.11	86,86,86,86	0
56	MG	1H	3250	1/1	0.94	0.18	78,78,78,78	0
56	MG	14	3267	1/1	0.94	0.27	79,79,79,79	0
56	MG	88	202	1/1	0.94	0.14	60,60,60,60	0
56	MG	1H	3429	1/1	0.94	0.09	64,64,64,64	0
56	MG	1H	3090	1/1	0.94	0.22	65,65,65,65	0
56	MG	1H	3437	1/1	0.94	0.10	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3297	1/1	0.94	0.25	79,79,79,79	0
56	MG	1H	3453	1/1	0.94	0.09	83,83,83,83	0
56	MG	1H	3048	1/1	0.94	0.27	52,52,52,52	0
56	MG	14	3420	1/1	0.94	0.10	91,91,91,91	0
56	MG	1H	3463	1/1	0.94	0.09	81,81,81,81	0
56	MG	14	3359	1/1	0.94	0.07	117,117,117,117	0
56	MG	13	1603	1/1	0.94	0.23	67,67,67,67	0
56	MG	14	3363	1/1	0.94	0.06	120,120,120,120	0
56	MG	13	1741	1/1	0.94	0.11	99,99,99,99	0
56	MG	14	3194	1/1	0.94	0.12	73,73,73,73	0
56	MG	14	3368	1/1	0.94	0.07	105,105,105,105	0
56	MG	1H	3179	1/1	0.94	0.28	75,75,75,75	0
56	MG	1H	3501	1/1	0.94	0.09	81,81,81,81	0
56	MG	1H	3057	1/1	0.94	0.23	64,64,64,64	0
56	MG	1H	3508	1/1	0.94	0.06	117,117,117,117	0
56	MG	14	3023	1/1	0.94	0.29	67,67,67,67	0
56	MG	14	3184	1/1	0.94	0.11	79,79,79,79	0
56	MG	14	3044	1/1	0.94	0.18	52,52,52,52	0
56	MG	1H	3028	1/1	0.94	0.23	59,59,59,59	0
56	MG	1G	1680	1/1	0.94	0.06	126,126,126,126	0
56	MG	2K	106	1/1	0.94	0.13	94,94,94,94	0
56	MG	13	1744	1/1	0.94	0.12	112,112,112,112	0
56	MG	14	3031	1/1	0.94	0.16	83,83,83,83	0
56	MG	14	3301	1/1	0.94	0.11	87,87,87,87	0
56	MG	14	3314	1/1	0.94	0.07	59,59,59,59	0
56	MG	1H	3532	1/1	0.94	0.12	116,116,116,116	0
57	ZN	3E	303	1/1	0.94	0.31	127,127,127,127	0
56	MG	14	3066	1/1	0.94	0.15	62,62,62,62	0
56	MG	14	3397	1/1	0.94	0.12	94,94,94,94	0
56	MG	1H	3502	1/1	0.95	0.06	109,109,109,109	0
56	MG	14	3417	1/1	0.95	0.05	118,118,118,118	0
56	MG	1H	3219	1/1	0.95	0.09	73,73,73,73	0
56	MG	1H	3513	1/1	0.95	0.10	104,104,104,104	0
56	MG	1H	3049	1/1	0.95	0.13	59,59,59,59	0
56	MG	1H	3516	1/1	0.95	0.07	114,114,114,114	0
56	MG	14	3075	1/1	0.95	0.09	83,83,83,83	0
56	MG	1H	3518	1/1	0.95	0.11	89,89,89,89	0
56	MG	1H	3519	1/1	0.95	0.10	93,93,93,93	0
56	MG	14	3182	1/1	0.95	0.10	66,66,66,66	0
56	MG	14	3421	1/1	0.95	0.08	136,136,136,136	0
56	MG	14	3064	1/1	0.95	0.26	60,60,60,60	0
56	MG	1H	3094	1/1	0.95	0.15	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3149	1/1	0.95	0.16	58,58,58,58	0
56	MG	14	3065	1/1	0.95	0.05	71,71,71,71	0
56	MG	14	3370	1/1	0.95	0.07	90,90,90,90	0
56	MG	1H	3098	1/1	0.95	0.24	63,63,63,63	0
56	MG	1G	1638	1/1	0.95	0.14	89,89,89,89	0
56	MG	14	3371	1/1	0.95	0.06	102,102,102,102	0
56	MG	1H	3101	1/1	0.95	0.24	57,57,57,57	0
56	MG	1K	102	1/1	0.95	0.19	107,107,107,107	0
56	MG	1H	3059	1/1	0.95	0.28	70,70,70,70	0
56	MG	1H	3330	1/1	0.95	0.08	53,53,53,53	0
56	MG	1H	3333	1/1	0.95	0.07	64,64,64,64	0
56	MG	1H	3345	1/1	0.95	0.07	66,66,66,66	0
56	MG	1J	206	1/1	0.95	0.06	106,106,106,106	0
56	MG	1H	3347	1/1	0.95	0.07	54,54,54,54	0
56	MG	13	1742	1/1	0.95	0.05	124,124,124,124	0
56	MG	1H	3027	1/1	0.95	0.28	58,58,58,58	0
56	MG	1H	3360	1/1	0.95	0.12	94,94,94,94	0
56	MG	1H	3361	1/1	0.95	0.08	103,103,103,103	0
56	MG	14	3373	1/1	0.95	0.05	138,138,138,138	0
56	MG	1H	3366	1/1	0.95	0.09	74,74,74,74	0
56	MG	1H	3192	1/1	0.95	0.12	81,81,81,81	0
56	MG	13	1711	1/1	0.95	0.07	106,106,106,106	0
56	MG	1H	3110	1/1	0.95	0.31	75,75,75,75	0
56	MG	14	3298	1/1	0.95	0.11	79,79,79,79	0
56	MG	14	3002	1/1	0.95	0.12	62,62,62,62	0
56	MG	14	3379	1/1	0.95	0.06	126,126,126,126	0
56	MG	1H	3290	1/1	0.95	0.32	82,82,82,82	0
56	MG	1H	3405	1/1	0.95	0.07	78,78,78,78	0
56	MG	14	3012	1/1	0.95	0.26	54,54,54,54	0
56	MG	1H	3412	1/1	0.95	0.07	70,70,70,70	0
56	MG	1H	3415	1/1	0.95	0.11	94,94,94,94	0
56	MG	14	3383	1/1	0.95	0.08	114,114,114,114	0
56	MG	14	3173	1/1	0.95	0.17	66,66,66,66	0
56	MG	1H	3201	1/1	0.95	0.25	68,68,68,68	0
56	MG	1H	3071	1/1	0.95	0.14	38,38,38,38	0
56	MG	14	3324	1/1	0.95	0.07	63,63,63,63	0
56	MG	14	3082	1/1	0.95	0.17	75,75,75,75	0
56	MG	14	3328	1/1	0.95	0.12	73,73,73,73	0
56	MG	14	3004	1/1	0.95	0.18	61,61,61,61	0
56	MG	14	3340	1/1	0.95	0.11	104,104,104,104	0
56	MG	13	1732	1/1	0.95	0.08	99,99,99,99	0
56	MG	14	3085	1/1	0.95	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3211	1/1	0.95	0.44	69,69,69,69	0
56	MG	1H	3258	1/1	0.95	0.42	63,63,63,63	0
56	MG	1G	1683	1/1	0.95	0.08	97,97,97,97	0
56	MG	2L	104	1/1	0.95	0.14	95,95,95,95	0
56	MG	1G	1688	1/1	0.95	0.07	122,122,122,122	0
56	MG	1H	3082	1/1	0.95	0.15	40,40,40,40	0
56	MG	1G	1691	1/1	0.95	0.06	98,98,98,98	0
56	MG	1H	3479	1/1	0.95	0.09	72,72,72,72	0
56	MG	1H	3170	1/1	0.95	0.10	71,71,71,71	0
56	MG	1G	1695	1/1	0.95	0.07	94,94,94,94	0
56	MG	14	3355	1/1	0.95	0.10	78,78,78,78	0
56	MG	1H	3485	1/1	0.95	0.12	105,105,105,105	0
56	MG	1H	3486	1/1	0.95	0.06	97,97,97,97	0
56	MG	13	1718	1/1	0.95	0.07	108,108,108,108	0
56	MG	13	1661	1/1	0.95	0.08	75,75,75,75	0
56	MG	14	3388	1/1	0.96	0.06	90,90,90,90	0
56	MG	14	3392	1/1	0.96	0.13	77,77,77,77	0
56	MG	14	3207	1/1	0.96	0.21	72,72,72,72	0
56	MG	1H	3494	1/1	0.96	0.05	107,107,107,107	0
56	MG	1H	3498	1/1	0.96	0.07	74,74,74,74	0
56	MG	1H	3500	1/1	0.96	0.11	82,82,82,82	0
56	MG	14	3341	1/1	0.96	0.09	65,65,65,65	0
56	MG	1H	3088	1/1	0.96	0.15	71,71,71,71	0
56	MG	13	1627	1/1	0.96	0.13	64,64,64,64	0
56	MG	14	3348	1/1	0.96	0.05	111,111,111,111	0
56	MG	1H	3326	1/1	0.96	0.08	54,54,54,54	0
56	MG	14	3151	1/1	0.96	0.14	56,56,56,56	0
56	MG	1H	3329	1/1	0.96	0.10	52,52,52,52	0
56	MG	14	3222	1/1	0.96	0.10	62,62,62,62	0
56	MG	14	3353	1/1	0.96	0.14	94,94,94,94	0
56	MG	14	3285	1/1	0.96	0.06	68,68,68,68	0
56	MG	14	3408	1/1	0.96	0.06	96,96,96,96	0
56	MG	1H	3352	1/1	0.96	0.08	106,106,106,106	0
56	MG	1H	3522	1/1	0.96	0.21	74,74,74,74	0
56	MG	1H	3523	1/1	0.96	0.07	115,115,115,115	0
56	MG	1H	3353	1/1	0.96	0.06	100,100,100,100	0
56	MG	14	3409	1/1	0.96	0.05	109,109,109,109	0
56	MG	1H	3527	1/1	0.96	0.11	103,103,103,103	0
56	MG	14	3286	1/1	0.96	0.09	62,62,62,62	0
56	MG	1H	3359	1/1	0.96	0.07	93,93,93,93	0
56	MG	1H	3142	1/1	0.96	0.22	82,82,82,82	0
56	MG	14	3168	1/1	0.96	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3413	1/1	0.96	0.13	100,100,100,100	0
56	MG	1H	3145	1/1	0.96	0.13	70,70,70,70	0
56	MG	1H	3368	1/1	0.96	0.07	58,58,58,58	0
56	MG	1H	3369	1/1	0.96	0.07	58,58,58,58	0
56	MG	1H	3373	1/1	0.96	0.09	75,75,75,75	0
56	MG	1H	3100	1/1	0.96	0.10	48,48,48,48	0
56	MG	14	3414	1/1	0.96	0.06	99,99,99,99	0
56	MG	1G	1652	1/1	0.96	0.15	81,81,81,81	0
56	MG	1H	3378	1/1	0.96	0.18	77,77,77,77	0
56	MG	14	3296	1/1	0.96	0.10	97,97,97,97	0
56	MG	1G	1655	1/1	0.96	0.09	127,127,127,127	0
56	MG	1H	3388	1/1	0.96	0.08	90,90,90,90	0
56	MG	13	1743	1/1	0.96	0.06	125,125,125,125	0
56	MG	1H	3104	1/1	0.96	0.21	57,57,57,57	0
56	MG	14	3110	1/1	0.96	0.07	61,61,61,61	0
56	MG	1H	3400	1/1	0.96	0.12	72,72,72,72	0
56	MG	1H	3401	1/1	0.96	0.06	87,87,87,87	0
56	MG	14	3365	1/1	0.96	0.05	89,89,89,89	0
56	MG	14	3305	1/1	0.96	0.08	89,89,89,89	0
56	MG	1H	3154	1/1	0.96	0.33	77,77,77,77	0
56	MG	14	3306	1/1	0.96	0.10	66,66,66,66	0
56	MG	3E	301	1/1	0.96	0.08	116,116,116,116	0
56	MG	14	3309	1/1	0.96	0.08	53,53,53,53	0
56	MG	14	3311	1/1	0.96	0.06	62,62,62,62	0
56	MG	14	3171	1/1	0.96	0.07	84,84,84,84	0
56	MG	1H	3423	1/1	0.96	0.07	77,77,77,77	0
56	MG	14	3055	1/1	0.96	0.13	59,59,59,59	0
56	MG	14	3322	1/1	0.96	0.07	80,80,80,80	0
56	MG	14	3375	1/1	0.96	0.12	92,92,92,92	0
56	MG	J8	101	1/1	0.96	0.32	67,67,67,67	0
56	MG	1H	3439	1/1	0.96	0.06	77,77,77,77	0
56	MG	1H	3442	1/1	0.96	0.12	74,74,74,74	0
56	MG	13	1605	1/1	0.96	0.09	82,82,82,82	0
56	MG	13	1713	1/1	0.96	0.06	99,99,99,99	0
56	MG	1H	3455	1/1	0.96	0.05	101,101,101,101	0
56	MG	14	3205	1/1	0.96	0.14	99,99,99,99	0
56	MG	2K	104	1/1	0.96	0.26	88,88,88,88	0
56	MG	13	1748	1/1	0.96	0.08	96,96,96,96	0
56	MG	14	3337	1/1	0.96	0.05	90,90,90,90	0
56	MG	1H	3169	1/1	0.96	0.06	49,49,49,49	0
56	MG	1G	1692	1/1	0.96	0.06	106,106,106,106	0
56	MG	1H	3473	1/1	0.96	0.09	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2K	107	1/1	0.96	0.22	86,86,86,86	0
56	MG	14	3384	1/1	0.96	0.08	98,98,98,98	0
56	MG	1H	3081	1/1	0.96	0.15	54,54,54,54	0
56	MG	1H	3480	1/1	0.96	0.05	100,100,100,100	0
56	MG	1H	3482	1/1	0.96	0.14	81,81,81,81	0
56	MG	14	3386	1/1	0.96	0.07	96,96,96,96	0
56	MG	1H	3083	1/1	0.96	0.12	51,51,51,51	0
56	MG	14	3003	1/1	0.97	0.12	49,49,49,49	0
56	MG	14	3279	1/1	0.97	0.04	115,115,115,115	0
56	MG	1H	3335	1/1	0.97	0.05	45,45,45,45	0
56	MG	1H	3430	1/1	0.97	0.11	50,50,50,50	0
56	MG	1H	3431	1/1	0.97	0.05	71,71,71,71	0
56	MG	1H	3337	1/1	0.97	0.07	65,65,65,65	0
56	MG	1H	3436	1/1	0.97	0.06	73,73,73,73	0
56	MG	1H	3533	1/1	0.97	0.06	106,106,106,106	0
56	MG	1H	3342	1/1	0.97	0.11	60,60,60,60	0
56	MG	1H	3438	1/1	0.97	0.08	63,63,63,63	0
56	MG	13	1739	1/1	0.97	0.06	103,103,103,103	0
56	MG	14	3343	1/1	0.97	0.10	81,81,81,81	0
56	MG	1H	3348	1/1	0.97	0.09	60,60,60,60	0
56	MG	1H	3451	1/1	0.97	0.10	88,88,88,88	0
56	MG	1H	3233	1/1	0.97	0.11	65,65,65,65	0
56	MG	1H	3454	1/1	0.97	0.08	87,87,87,87	0
56	MG	14	3307	1/1	0.97	0.07	81,81,81,81	0
56	MG	1H	3457	1/1	0.97	0.13	81,81,81,81	0
56	MG	14	3284	1/1	0.97	0.06	104,104,104,104	0
56	MG	1H	3106	1/1	0.97	0.28	70,70,70,70	0
56	MG	13	1745	1/1	0.97	0.07	104,104,104,104	0
56	MG	14	3352	1/1	0.97	0.07	91,91,91,91	0
56	MG	14	3312	1/1	0.97	0.07	93,93,93,93	0
56	MG	1H	3471	1/1	0.97	0.10	91,91,91,91	0
56	MG	1H	3472	1/1	0.97	0.07	95,95,95,95	0
56	MG	1H	3017	1/1	0.97	0.07	63,63,63,63	0
56	MG	16	211	1/1	0.97	0.06	80,80,80,80	0
56	MG	16	213	1/1	0.97	0.07	102,102,102,102	0
56	MG	1H	3079	1/1	0.97	0.16	46,46,46,46	0
56	MG	14	3390	1/1	0.97	0.05	111,111,111,111	0
56	MG	1H	3476	1/1	0.97	0.07	95,95,95,95	0
56	MG	1H	3477	1/1	0.97	0.05	114,114,114,114	0
56	MG	14	3391	1/1	0.97	0.04	96,96,96,96	0
56	MG	1H	3371	1/1	0.97	0.06	73,73,73,73	0
56	MG	14	3108	1/1	0.97	0.07	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3315	1/1	0.97	0.06	76,76,76,76	0
56	MG	14	3318	1/1	0.97	0.06	69,69,69,69	0
56	MG	I8	101	1/1	0.97	0.09	89,89,89,89	0
56	MG	1H	3377	1/1	0.97	0.06	90,90,90,90	0
56	MG	14	3287	1/1	0.97	0.11	70,70,70,70	0
56	MG	1H	3487	1/1	0.97	0.05	101,101,101,101	0
56	MG	1H	3380	1/1	0.97	0.05	44,44,44,44	0
56	MG	1H	3489	1/1	0.97	0.12	89,89,89,89	0
56	MG	1H	3490	1/1	0.97	0.11	147,147,147,147	0
56	MG	1G	1604	1/1	0.97	0.08	90,90,90,90	0
56	MG	1H	3492	1/1	0.97	0.08	90,90,90,90	0
56	MG	14	3289	1/1	0.97	0.06	77,77,77,77	0
56	MG	1H	3385	1/1	0.97	0.07	62,62,62,62	0
56	MG	1H	3499	1/1	0.97	0.09	66,66,66,66	0
56	MG	14	3290	1/1	0.97	0.07	68,68,68,68	0
56	MG	13	1720	1/1	0.97	0.05	105,105,105,105	0
56	MG	14	3326	1/1	0.97	0.06	58,58,58,58	0
56	MG	1G	1679	1/1	0.97	0.06	109,109,109,109	0
56	MG	14	3403	1/1	0.97	0.18	70,70,70,70	0
56	MG	1G	1681	1/1	0.97	0.06	93,93,93,93	0
56	MG	1H	3507	1/1	0.97	0.05	101,101,101,101	0
56	MG	14	3367	1/1	0.97	0.05	115,115,115,115	0
56	MG	1G	1685	1/1	0.97	0.05	91,91,91,91	0
56	MG	1H	3509	1/1	0.97	0.06	91,91,91,91	0
56	MG	1G	1689	1/1	0.97	0.06	114,114,114,114	0
56	MG	1H	3510	1/1	0.97	0.07	99,99,99,99	0
56	MG	14	3327	1/1	0.97	0.05	70,70,70,70	0
56	MG	1H	3031	1/1	0.97	0.24	58,58,58,58	0
56	MG	14	3293	1/1	0.97	0.05	73,73,73,73	0
56	MG	1H	3408	1/1	0.97	0.07	60,60,60,60	0
56	MG	14	3331	1/1	0.97	0.06	73,73,73,73	0
56	MG	14	3411	1/1	0.97	0.06	106,106,106,106	0
56	MG	13	1724	1/1	0.97	0.11	116,116,116,116	0
56	MG	1H	3417	1/1	0.97	0.07	65,65,65,65	0
56	MG	13	1738	1/1	0.97	0.04	109,109,109,109	0
56	MG	14	3338	1/1	0.97	0.05	62,62,62,62	0
56	MG	1H	3070	1/1	0.98	0.31	61,61,61,61	0
56	MG	1H	3491	1/1	0.98	0.06	99,99,99,99	0
56	MG	14	3389	1/1	0.98	0.05	72,72,72,72	0
56	MG	13	1709	1/1	0.98	0.06	72,72,72,72	0
56	MG	1H	3495	1/1	0.98	0.20	75,75,75,75	0
56	MG	1H	3497	1/1	0.98	0.04	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3393	1/1	0.98	0.04	51,51,51,51	0
56	MG	1H	3394	1/1	0.98	0.06	58,58,58,58	0
56	MG	1H	3395	1/1	0.98	0.04	59,59,59,59	0
56	MG	14	3313	1/1	0.98	0.05	65,65,65,65	0
56	MG	13	1666	1/1	0.98	0.03	86,86,86,86	0
56	MG	1H	3503	1/1	0.98	0.17	64,64,64,64	0
56	MG	14	3288	1/1	0.98	0.07	78,78,78,78	0
56	MG	1H	3402	1/1	0.98	0.04	102,102,102,102	0
56	MG	13	1719	1/1	0.98	0.07	100,100,100,100	0
56	MG	14	3395	1/1	0.98	0.04	105,105,105,105	0
56	MG	1H	3407	1/1	0.98	0.12	59,59,59,59	0
56	MG	1H	3511	1/1	0.98	0.06	84,84,84,84	0
56	MG	13	1735	1/1	0.98	0.05	78,78,78,78	0
56	MG	1H	3409	1/1	0.98	0.04	50,50,50,50	0
56	MG	14	3321	1/1	0.98	0.15	62,62,62,62	0
56	MG	14	3398	1/1	0.98	0.05	76,76,76,76	0
56	MG	14	3291	1/1	0.98	0.04	52,52,52,52	0
56	MG	1H	3416	1/1	0.98	0.10	48,48,48,48	0
56	MG	14	3362	1/1	0.98	0.12	101,101,101,101	0
56	MG	1H	3418	1/1	0.98	0.04	77,77,77,77	0
56	MG	14	3401	1/1	0.98	0.04	90,90,90,90	0
56	MG	13	1737	1/1	0.98	0.06	116,116,116,116	0
56	MG	1H	3332	1/1	0.98	0.05	64,64,64,64	0
56	MG	13	1712	1/1	0.98	0.04	84,84,84,84	0
56	MG	1H	3426	1/1	0.98	0.05	59,59,59,59	0
56	MG	1H	3528	1/1	0.98	0.06	61,61,61,61	0
56	MG	1H	3206	1/1	0.98	0.31	76,76,76,76	0
56	MG	1H	3336	1/1	0.98	0.06	53,53,53,53	0
56	MG	14	3404	1/1	0.98	0.05	97,97,97,97	0
56	MG	1H	3432	1/1	0.98	0.06	69,69,69,69	0
56	MG	1H	3338	1/1	0.98	0.07	64,64,64,64	0
56	MG	1H	3434	1/1	0.98	0.03	107,107,107,107	0
56	MG	1H	3340	1/1	0.98	0.04	76,76,76,76	0
56	MG	1H	3537	1/1	0.98	0.06	55,55,55,55	0
56	MG	14	3294	1/1	0.98	0.05	59,59,59,59	0
56	MG	14	3406	1/1	0.98	0.18	84,84,84,84	0
56	MG	1H	3346	1/1	0.98	0.08	58,58,58,58	0
56	MG	1H	3440	1/1	0.98	0.10	98,98,98,98	0
56	MG	1H	3441	1/1	0.98	0.08	73,73,73,73	0
56	MG	1H	3251	1/1	0.98	0.10	115,115,115,115	0
56	MG	1J	207	1/1	0.98	0.05	100,100,100,100	0
56	MG	1H	3443	1/1	0.98	0.09	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3407	1/1	0.98	0.06	110,110,110,110	0
56	MG	1H	3446	1/1	0.98	0.10	87,87,87,87	0
56	MG	1H	3449	1/1	0.98	0.06	91,91,91,91	0
56	MG	1H	3450	1/1	0.98	0.04	88,88,88,88	0
56	MG	14	3295	1/1	0.98	0.08	90,90,90,90	0
56	MG	14	3276	1/1	0.98	0.05	85,85,85,85	0
56	MG	14	3329	1/1	0.98	0.06	88,88,88,88	0
56	MG	1H	3355	1/1	0.98	0.07	72,72,72,72	0
56	MG	1H	3356	1/1	0.98	0.04	81,81,81,81	0
56	MG	13	1727	1/1	0.98	0.06	111,111,111,111	0
56	MG	16	212	1/1	0.98	0.07	84,84,84,84	0
56	MG	14	3332	1/1	0.98	0.06	94,94,94,94	0
56	MG	1H	3462	1/1	0.98	0.07	106,106,106,106	0
56	MG	14	3334	1/1	0.98	0.05	111,111,111,111	0
56	MG	1H	3464	1/1	0.98	0.04	90,90,90,90	0
56	MG	14	3299	1/1	0.98	0.05	68,68,68,68	0
56	MG	14	3280	1/1	0.98	0.06	64,64,64,64	0
56	MG	1H	3469	1/1	0.98	0.07	95,95,95,95	0
56	MG	1H	3470	1/1	0.98	0.06	81,81,81,81	0
56	MG	1H	3364	1/1	0.98	0.11	71,71,71,71	0
56	MG	14	3281	1/1	0.98	0.05	74,74,74,74	0
56	MG	1G	1682	1/1	0.98	0.04	86,86,86,86	0
56	MG	1H	3367	1/1	0.98	0.05	50,50,50,50	0
56	MG	13	1728	1/1	0.98	0.05	80,80,80,80	0
56	MG	14	3418	1/1	0.98	0.07	128,128,128,128	0
56	MG	1G	1686	1/1	0.98	0.06	117,117,117,117	0
56	MG	1G	1687	1/1	0.98	0.09	134,134,134,134	0
56	MG	14	3283	1/1	0.98	0.04	78,78,78,78	0
56	MG	1H	3372	1/1	0.98	0.05	65,65,65,65	0
56	MG	14	3308	1/1	0.98	0.06	69,69,69,69	0
56	MG	14	3381	1/1	0.98	0.05	110,110,110,110	0
56	MG	1H	3481	1/1	0.98	0.04	76,76,76,76	0
56	MG	13	1729	1/1	0.98	0.04	73,73,73,73	0
56	MG	14	3344	1/1	0.98	0.10	100,100,100,100	0
56	MG	14	3346	1/1	0.98	0.07	88,88,88,88	0
56	MG	1H	3379	1/1	0.98	0.11	90,90,90,90	0
56	MG	14	3385	1/1	0.98	0.04	83,83,83,83	0
56	MG	14	3347	1/1	0.98	0.06	88,88,88,88	0
56	MG	1H	3382	1/1	0.98	0.09	55,55,55,55	0
56	MG	13	1721	1/1	0.98	0.05	99,99,99,99	0
57	ZN	32	301	1/1	0.98	0.22	119,119,119,119	0
56	MG	1H	3370	1/1	0.99	0.06	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	14	3297	1/1	0.99	0.04	80,80,80,80	0
56	MG	14	3316	1/1	0.99	0.04	57,57,57,57	0
56	MG	14	3317	1/1	0.99	0.08	98,98,98,98	0
56	MG	1H	3374	1/1	0.99	0.04	70,70,70,70	0
56	MG	13	1710	1/1	0.99	0.03	61,61,61,61	0
56	MG	14	3377	1/1	0.99	0.04	88,88,88,88	0
56	MG	1H	3327	1/1	0.99	0.04	61,61,61,61	0
56	MG	14	3345	1/1	0.99	0.03	82,82,82,82	0
56	MG	1H	3445	1/1	0.99	0.04	81,81,81,81	0
56	MG	1H	3526	1/1	0.99	0.14	78,78,78,78	0
56	MG	13	1714	1/1	0.99	0.04	79,79,79,79	0
56	MG	1H	3447	1/1	0.99	0.04	74,74,74,74	0
56	MG	1H	3448	1/1	0.99	0.03	75,75,75,75	0
56	MG	14	3380	1/1	0.99	0.03	87,87,87,87	0
56	MG	1H	3331	1/1	0.99	0.04	49,49,49,49	0
56	MG	14	3320	1/1	0.99	0.10	84,84,84,84	0
56	MG	1H	3452	1/1	0.99	0.04	50,50,50,50	0
56	MG	1H	3383	1/1	0.99	0.05	59,59,59,59	0
56	MG	1H	3384	1/1	0.99	0.05	50,50,50,50	0
56	MG	1H	3536	1/1	0.99	0.10	43,43,43,43	0
56	MG	14	3300	1/1	0.99	0.04	69,69,69,69	0
56	MG	1H	3386	1/1	0.99	0.04	58,58,58,58	0
56	MG	1H	3387	1/1	0.99	0.04	63,63,63,63	0
56	MG	13	1740	1/1	0.99	0.02	83,83,83,83	0
56	MG	1H	3460	1/1	0.99	0.04	81,81,81,81	0
56	MG	1H	3461	1/1	0.99	0.03	89,89,89,89	0
56	MG	14	3350	1/1	0.99	0.04	64,64,64,64	0
56	MG	1H	3390	1/1	0.99	0.03	61,61,61,61	0
56	MG	1H	3391	1/1	0.99	0.03	58,58,58,58	0
56	MG	1H	3465	1/1	0.99	0.04	85,85,85,85	0
56	MG	14	3323	1/1	0.99	0.06	59,59,59,59	0
56	MG	14	3302	1/1	0.99	0.07	76,76,76,76	0
56	MG	1H	3339	1/1	0.99	0.06	60,60,60,60	0
56	MG	14	3387	1/1	0.99	0.08	90,90,90,90	0
56	MG	14	3303	1/1	0.99	0.03	92,92,92,92	0
56	MG	1H	3397	1/1	0.99	0.04	52,52,52,52	0
56	MG	1H	3398	1/1	0.99	0.06	58,58,58,58	0
56	MG	1H	3399	1/1	0.99	0.07	50,50,50,50	0
56	MG	1H	3343	1/1	0.99	0.07	52,52,52,52	0
56	MG	1H	3344	1/1	0.99	0.06	69,69,69,69	0
56	MG	14	3354	1/1	0.99	0.07	90,90,90,90	0
56	MG	14	3304	1/1	0.99	0.05	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3404	1/1	0.99	0.03	74,74,74,74	0
56	MG	14	3356	1/1	0.99	0.05	85,85,85,85	0
56	MG	1H	3406	1/1	0.99	0.03	76,76,76,76	0
56	MG	14	3357	1/1	0.99	0.05	82,82,82,82	0
56	MG	1H	3350	1/1	0.99	0.04	52,52,52,52	0
56	MG	1H	3351	1/1	0.99	0.07	65,65,65,65	0
56	MG	1H	3410	1/1	0.99	0.10	66,66,66,66	0
56	MG	13	1715	1/1	0.99	0.06	85,85,85,85	0
56	MG	14	3277	1/1	0.99	0.07	54,54,54,54	0
56	MG	1H	3413	1/1	0.99	0.04	82,82,82,82	0
56	MG	1H	3414	1/1	0.99	0.06	67,67,67,67	0
56	MG	14	3360	1/1	0.99	0.04	104,104,104,104	0
56	MG	14	3278	1/1	0.99	0.05	62,62,62,62	0
56	MG	13	1716	1/1	0.99	0.04	58,58,58,58	0
56	MG	1H	3357	1/1	0.99	0.07	72,72,72,72	0
56	MG	1H	3496	1/1	0.99	0.04	103,103,103,103	0
56	MG	13	1734	1/1	0.99	0.04	79,79,79,79	0
56	MG	14	3333	1/1	0.99	0.02	74,74,74,74	0
56	MG	1H	3421	1/1	0.99	0.02	74,74,74,74	0
56	MG	14	3310	1/1	0.99	0.04	65,65,65,65	0
56	MG	14	3335	1/1	0.99	0.08	89,89,89,89	0
56	MG	1H	3425	1/1	0.99	0.04	77,77,77,77	0
56	MG	1H	3362	1/1	0.99	0.07	68,68,68,68	0
56	MG	1H	3428	1/1	0.99	0.04	56,56,56,56	0
56	MG	1H	3505	1/1	0.99	0.05	78,78,78,78	0
56	MG	1H	3506	1/1	0.99	0.04	57,57,57,57	0
56	MG	13	1722	1/1	0.99	0.11	87,87,87,87	0
56	MG	13	1736	1/1	0.99	0.05	95,95,95,95	0
56	MG	14	3369	1/1	0.99	0.06	73,73,73,73	0
56	MG	13	1746	1/1	0.99	0.04	102,102,102,102	0
56	MG	14	3339	1/1	0.99	0.05	56,56,56,56	0
56	MG	1H	3512	1/1	0.99	0.03	80,80,80,80	0
57	ZN	5I	102	1/1	0.99	0.03	96,96,96,96	0
56	MG	13	1717	1/1	0.99	0.08	64,64,64,64	0
56	MG	1H	3514	1/1	0.99	0.03	96,96,96,96	0
56	MG	1H	3435	1/1	0.99	0.03	52,52,52,52	0
56	MG	1H	3467	1/1	1.00	0.04	57,57,57,57	0
56	MG	1H	3341	1/1	1.00	0.03	43,43,43,43	0
56	MG	1H	3493	1/1	1.00	0.02	68,68,68,68	0
56	MG	1H	3365	1/1	1.00	0.06	71,71,71,71	0
56	MG	14	3274	1/1	1.00	0.04	69,69,69,69	0
56	MG	1H	3334	1/1	1.00	0.07	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1H	3424	1/1	1.00	0.03	92,92,92,92	0
56	MG	1H	3349	1/1	1.00	0.03	68,68,68,68	0
56	MG	14	3275	1/1	1.00	0.02	58,58,58,58	0
56	MG	1H	3427	1/1	1.00	0.03	56,56,56,56	0
56	MG	14	3330	1/1	1.00	0.01	50,50,50,50	0
56	MG	1H	3456	1/1	1.00	0.02	69,69,69,69	0
56	MG	1H	3478	1/1	1.00	0.02	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.