



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:55 PM BST

PDB ID : 4V9C  
Title : Allosteric control of the ribosome by small-molecule antibiotics  
Authors : Cate, J.H.D.; Pulk, A.; Blanchard, S.C.; Wang, L.; Feldman, M.B.; Wasserman, M.R.; Altman, R.  
Deposited on : 2012-07-25  
Resolution : 3.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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

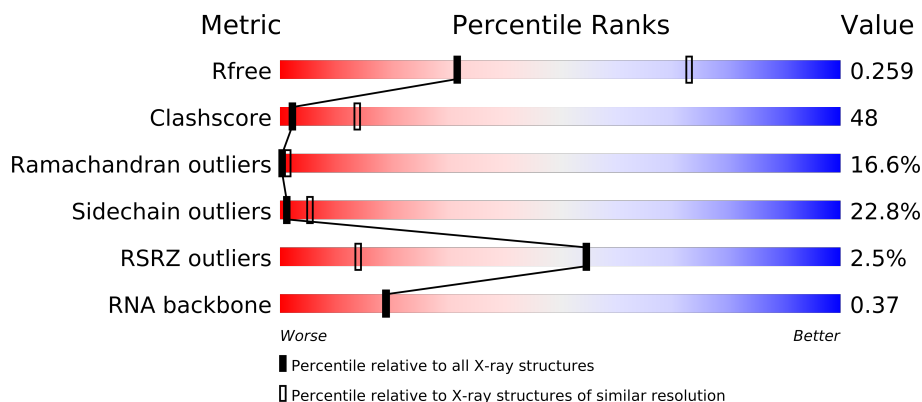
MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23397  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23397



# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 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))
$R_{free}$	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1542	
1	CA	1542	
2	AB	241	
2	CB	241	
3	AC	233	
3	CC	233	
4	AD	206	
4	CD	206	
5	AE	167	
5	CE	167	
6	AF	135	
6	CF	135	

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Mol	Chain	Length	Quality of chain
7	AG	179	
7	CG	179	
8	AH	130	
8	CH	130	
9	AI	130	
9	CI	130	
10	AJ	103	
10	CJ	103	
11	AK	129	
11	CK	129	
12	AL	124	
12	CL	124	
13	AM	118	
13	CM	118	
14	AN	101	
14	CN	101	
15	AO	89	
15	CO	89	
16	AP	82	
16	CP	82	
17	AQ	84	
17	CQ	84	
18	AR	75	
18	CR	75	
19	AS	92	
19	CS	92	
20	AT	87	
20	CT	87	
21	AU	71	
21	CU	71	
22	AV	76	
22	CV	76	
23	AX	24	
23	CX	24	
24	BA	2904	
24	DA	2904	
25	BB	120	
25	DB	120	
26	BC	273	
26	DC	273	
27	BD	209	
27	DD	209	

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Mol	Chain	Length	Quality of chain
28	BE	201	
28	DE	201	
29	BF	179	
29	DF	179	
30	BG	177	
30	DG	177	
31	BH	149	
31	DH	149	
32	BI	142	
32	DI	142	
33	BJ	142	
33	DJ	142	
34	BK	123	
34	DK	123	
35	BL	144	
35	DL	144	
36	BM	136	
36	DM	136	
37	BN	127	
37	DN	127	
38	BO	117	
38	DO	117	
39	BP	115	
39	DP	115	
40	BQ	118	
40	DQ	118	
41	BR	103	
41	DR	103	
42	BS	110	
42	DS	110	
43	BT	100	
43	DT	100	
44	BU	104	
44	DU	104	
45	BV	94	
45	DV	94	
46	BW	85	
46	DW	85	
47	BX	78	
47	DX	78	
48	BY	63	
48	DY	63	

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Mol	Chain	Length	Quality of chain
49	BZ	59	
49	DZ	59	
50	B0	57	
50	D0	57	
51	B1	55	
51	D1	55	
52	B2	46	
52	D2	46	
53	B3	65	
53	D3	65	
54	B4	38	
54	D4	38	
55	CY	185	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
56	MG	AA	1601	-	X
56	MG	AA	1602	-	X
56	MG	AA	1603	-	X
56	MG	AA	1605	-	X
56	MG	AA	1606	-	X
56	MG	AA	1608	-	X
56	MG	AA	1609	-	X
56	MG	AA	1610	-	X
56	MG	AA	1613	-	X
56	MG	AA	1614	-	X
56	MG	AA	1616	-	X
56	MG	AA	1617	-	X
56	MG	AA	1618	-	X
56	MG	AA	1620	-	X
56	MG	AA	1621	-	X
56	MG	AA	1622	-	X
56	MG	AA	1623	-	X
56	MG	AA	1624	-	X
56	MG	AA	1625	-	X
56	MG	AA	1626	-	X
56	MG	AA	1627	-	X
56	MG	AA	1628	-	X
56	MG	AA	1629	-	X
56	MG	AA	1630	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
56	MG	AA	1631	-	X
56	MG	AA	1633	-	X
56	MG	AA	1634	-	X
56	MG	AA	1635	-	X
56	MG	AA	1636	-	X
56	MG	AA	1638	-	X
56	MG	AA	1639	-	X
56	MG	AA	1640	-	X
56	MG	AA	1642	-	X
56	MG	AA	1643	-	X
56	MG	AA	1644	-	X
56	MG	AA	1645	-	X
56	MG	AA	1646	-	X
56	MG	AA	1647	-	X
56	MG	AA	1648	-	X
56	MG	AA	1649	-	X
56	MG	AA	1650	-	X
56	MG	AA	1651	-	X
56	MG	AA	1652	-	X
56	MG	AA	1653	-	X
56	MG	AA	1654	-	X
56	MG	AD	301	-	X
56	MG	AN	201	-	X
56	MG	BA	3003	-	X
56	MG	BA	3004	-	X
56	MG	BA	3005	-	X
56	MG	BA	3007	-	X
56	MG	BA	3008	-	X
56	MG	BA	3009	-	X
56	MG	BA	3011	-	X
56	MG	BA	3012	-	X
56	MG	BA	3013	-	X
56	MG	BA	3014	-	X
56	MG	BA	3015	-	X
56	MG	BA	3018	-	X
56	MG	BA	3019	-	X
56	MG	BA	3020	-	X
56	MG	BA	3021	-	X
56	MG	BA	3022	-	X
56	MG	BA	3023	-	X
56	MG	BA	3024	-	X
56	MG	BA	3025	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
56	MG	BA	3026	-	X
56	MG	BA	3027	-	X
56	MG	BA	3028	-	X
56	MG	BA	3030	-	X
56	MG	BA	3031	-	X
56	MG	BA	3032	-	X
56	MG	BA	3033	-	X
56	MG	BA	3037	-	X
56	MG	BA	3038	-	X
56	MG	BA	3044	-	X
56	MG	BA	3047	-	X
56	MG	BA	3049	-	X
56	MG	BA	3050	-	X
56	MG	BA	3051	-	X
56	MG	BA	3053	-	X
56	MG	BA	3054	-	X
56	MG	BA	3055	-	X
56	MG	BA	3056	-	X
56	MG	BA	3058	-	X
56	MG	BA	3059	-	X
56	MG	BA	3060	-	X
56	MG	BA	3061	-	X
56	MG	BA	3062	-	X
56	MG	BA	3063	-	X
56	MG	BA	3065	-	X
56	MG	BA	3066	-	X
56	MG	BA	3068	-	X
56	MG	BA	3069	-	X
56	MG	BA	3070	-	X
56	MG	BA	3071	-	X
56	MG	BA	3072	-	X
56	MG	BA	3074	-	X
56	MG	BA	3075	-	X
56	MG	BA	3077	-	X
56	MG	BA	3078	-	X
56	MG	BA	3079	-	X
56	MG	BA	3081	-	X
56	MG	BA	3082	-	X
56	MG	BA	3083	-	X
56	MG	BA	3087	-	X
56	MG	BA	3088	-	X
56	MG	BA	3089	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
56	MG	BA	3090	-	X
56	MG	BA	3091	-	X
56	MG	BA	3092	-	X
56	MG	BA	3093	-	X
56	MG	BA	3094	-	X
56	MG	BA	3095	-	X
56	MG	BA	3096	-	X
56	MG	BA	3097	-	X
56	MG	BA	3098	-	X
56	MG	BA	3099	-	X
56	MG	BA	3100	-	X
56	MG	BA	3101	-	X
56	MG	BA	3102	-	X
56	MG	BA	3103	-	X
56	MG	BA	3104	-	X
56	MG	BA	3105	-	X
56	MG	BA	3106	-	X
56	MG	BA	3107	-	X
56	MG	BA	3108	-	X
56	MG	BA	3109	-	X
56	MG	BA	3110	-	X
56	MG	BA	3111	-	X
56	MG	BA	3112	-	X
56	MG	BA	3113	-	X
56	MG	BA	3115	-	X
56	MG	BA	3116	-	X
56	MG	BA	3118	-	X
56	MG	BA	3119	-	X
56	MG	BA	3120	-	X
56	MG	BA	3121	-	X
56	MG	BA	3122	-	X
56	MG	BA	3123	-	X
56	MG	BA	3124	-	X
56	MG	BA	3125	-	X
56	MG	BA	3126	-	X
56	MG	BA	3127	-	X
56	MG	BA	3129	-	X
56	MG	BA	3130	-	X
56	MG	BA	3131	-	X
56	MG	BA	3133	-	X
56	MG	BA	3134	-	X
56	MG	BA	3135	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
56	MG	BA	3136	-	X
56	MG	BA	3137	-	X
56	MG	BA	3138	-	X
56	MG	BA	3139	-	X
56	MG	BA	3142	-	X
56	MG	BA	3143	-	X
56	MG	BA	3144	-	X
56	MG	BA	3145	-	X
56	MG	BA	3146	-	X
56	MG	BA	3147	-	X
56	MG	BA	3148	-	X
56	MG	BA	3149	-	X
56	MG	BA	3150	-	X
56	MG	BA	3151	-	X
56	MG	BA	3152	-	X
56	MG	BA	3153	-	X
56	MG	BA	3154	-	X
56	MG	BA	3155	-	X
56	MG	BA	3156	-	X
56	MG	BA	3157	-	X
56	MG	BA	3158	-	X
56	MG	BA	3159	-	X
56	MG	BA	3160	-	X
56	MG	BA	3168	-	X
56	MG	BA	3169	-	X
56	MG	BA	3170	-	X
56	MG	BB	201	-	X
56	MG	BB	202	-	X
56	MG	BC	301	-	X
56	MG	BQ	201	-	X
56	MG	CA	1601	-	X
56	MG	CA	1602	-	X
56	MG	CA	1603	-	X
56	MG	CA	1605	-	X
56	MG	CA	1607	-	X
56	MG	CA	1608	-	X
56	MG	CA	1609	-	X
56	MG	CA	1611	-	X
56	MG	CA	1612	-	X
56	MG	CA	1613	-	X
56	MG	CA	1614	-	X
56	MG	CA	1615	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
56	MG	CA	1617	-	X
56	MG	CA	1618	-	X
56	MG	CA	1620	-	X
56	MG	CA	1622	-	X
56	MG	CA	1623	-	X
56	MG	CA	1624	-	X
56	MG	CA	1625	-	X
56	MG	CA	1626	-	X
56	MG	CA	1627	-	X
56	MG	CA	1628	-	X
56	MG	CA	1629	-	X
56	MG	CA	1631	-	X
56	MG	CA	1632	-	X
56	MG	CA	1633	-	X
56	MG	CA	1634	-	X
56	MG	CA	1636	-	X
56	MG	CA	1637	-	X
56	MG	CA	1638	-	X
56	MG	CA	1640	-	X
56	MG	CA	1641	-	X
56	MG	CA	1642	-	X
56	MG	CA	1643	-	X
56	MG	CA	1644	-	X
56	MG	CA	1645	-	X
56	MG	CA	1646	-	X
56	MG	CA	1647	-	X
56	MG	CA	1648	-	X
56	MG	CA	1650	-	X
56	MG	CA	1651	-	X
56	MG	CA	1652	-	X
56	MG	CA	1653	-	X
56	MG	CA	1654	-	X
56	MG	CA	1655	-	X
56	MG	CA	1656	-	X
56	MG	CA	1658	-	X
56	MG	CA	1659	-	X
56	MG	CA	1660	-	X
56	MG	CA	1661	-	X
56	MG	CA	1663	-	X
56	MG	CA	1664	-	X
56	MG	CA	1665	-	X
56	MG	CA	1666	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
56	MG	CA	1667	-	X
56	MG	CA	1668	-	X
56	MG	CA	1669	-	X
56	MG	CA	1670	-	X
56	MG	CA	1671	-	X
56	MG	CX	101	-	X
56	MG	DA	3004	-	X
56	MG	DA	3006	-	X
56	MG	DA	3007	-	X
56	MG	DA	3008	-	X
56	MG	DA	3009	-	X
56	MG	DA	3010	-	X
56	MG	DA	3011	-	X
56	MG	DA	3012	-	X
56	MG	DA	3013	-	X
56	MG	DA	3014	-	X
56	MG	DA	3015	-	X
56	MG	DA	3016	-	X
56	MG	DA	3017	-	X
56	MG	DA	3018	-	X
56	MG	DA	3019	-	X
56	MG	DA	3020	-	X
56	MG	DA	3021	-	X
56	MG	DA	3022	-	X
56	MG	DA	3023	-	X
56	MG	DA	3024	-	X
56	MG	DA	3025	-	X
56	MG	DA	3026	-	X
56	MG	DA	3028	-	X
56	MG	DA	3029	-	X
56	MG	DA	3031	-	X
56	MG	DA	3032	-	X
56	MG	DA	3035	-	X
56	MG	DA	3036	-	X
56	MG	DA	3037	-	X
56	MG	DA	3038	-	X
56	MG	DA	3042	-	X
56	MG	DA	3044	-	X
56	MG	DA	3048	-	X
56	MG	DA	3049	-	X
56	MG	DA	3050	-	X
56	MG	DA	3051	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
56	MG	DA	3052	-	X
56	MG	DA	3054	-	X
56	MG	DA	3055	-	X
56	MG	DA	3057	-	X
56	MG	DA	3058	-	X
56	MG	DA	3059	-	X
56	MG	DA	3060	-	X
56	MG	DA	3061	-	X
56	MG	DA	3064	-	X
56	MG	DA	3065	-	X
56	MG	DA	3066	-	X
56	MG	DA	3067	-	X
56	MG	DA	3068	-	X
56	MG	DA	3069	-	X
56	MG	DA	3070	-	X
56	MG	DA	3071	-	X
56	MG	DA	3072	-	X
56	MG	DA	3073	-	X
56	MG	DA	3075	-	X
56	MG	DA	3076	-	X
56	MG	DA	3077	-	X
56	MG	DA	3078	-	X
56	MG	DA	3079	-	X
56	MG	DA	3080	-	X
56	MG	DA	3081	-	X
56	MG	DA	3082	-	X
56	MG	DA	3083	-	X
56	MG	DA	3084	-	X
56	MG	DA	3085	-	X
56	MG	DA	3087	-	X
56	MG	DA	3088	-	X
56	MG	DA	3090	-	X
56	MG	DA	3091	-	X
56	MG	DA	3092	-	X
56	MG	DA	3093	-	X
56	MG	DA	3094	-	X
56	MG	DA	3095	-	X
56	MG	DA	3096	-	X
56	MG	DA	3097	-	X
56	MG	DA	3098	-	X
56	MG	DA	3100	-	X
56	MG	DA	3101	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
56	MG	DA	3102	-	X
56	MG	DA	3103	-	X
56	MG	DA	3104	-	X
56	MG	DA	3105	-	X
56	MG	DA	3106	-	X
56	MG	DA	3107	-	X
56	MG	DA	3108	-	X
56	MG	DA	3109	-	X
56	MG	DA	3110	-	X
56	MG	DA	3111	-	X
56	MG	DA	3113	-	X
56	MG	DA	3114	-	X
56	MG	DA	3116	-	X
56	MG	DA	3118	-	X
56	MG	DA	3119	-	X
56	MG	DA	3120	-	X
56	MG	DA	3121	-	X
56	MG	DA	3122	-	X
56	MG	DA	3123	-	X
56	MG	DA	3124	-	X
56	MG	DA	3125	-	X
56	MG	DA	3127	-	X
56	MG	DA	3129	-	X
56	MG	DA	3130	-	X
56	MG	DA	3131	-	X
56	MG	DA	3134	-	X
56	MG	DA	3135	-	X
56	MG	DA	3136	-	X
56	MG	DA	3137	-	X
56	MG	DA	3138	-	X
56	MG	DA	3139	-	X
56	MG	DA	3140	-	X
56	MG	DA	3141	-	X
56	MG	DA	3142	-	X
56	MG	DA	3143	-	X
56	MG	DA	3144	-	X
56	MG	DA	3145	-	X
56	MG	DA	3146	-	X
56	MG	DA	3147	-	X
56	MG	DA	3148	-	X
56	MG	DA	3149	-	X
56	MG	DA	3150	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
56	MG	DA	3151	-	X
56	MG	DA	3152	-	X
56	MG	DA	3154	-	X
56	MG	DA	3155	-	X
56	MG	DA	3156	-	X
56	MG	DA	3157	-	X
56	MG	DA	3158	-	X
56	MG	DA	3159	-	X
56	MG	DA	3160	-	X
56	MG	DA	3161	-	X
56	MG	DA	3162	-	X
56	MG	DA	3163	-	X
56	MG	DA	3164	-	X
56	MG	DA	3165	-	X
56	MG	DA	3166	-	X
56	MG	DA	3167	-	X
56	MG	DA	3168	-	X
56	MG	DA	3169	-	X
56	MG	DA	3170	-	X
56	MG	DA	3171	-	X
56	MG	DA	3172	-	X
56	MG	DA	3173	-	X
56	MG	DA	3174	-	X
56	MG	DA	3175	-	X
56	MG	DA	3176	-	X
56	MG	DA	3177	-	X
56	MG	DA	3178	-	X
56	MG	DA	3179	-	X
56	MG	DA	3180	-	X
56	MG	DA	3181	-	X
56	MG	DA	3182	-	X
56	MG	DA	3183	-	X
56	MG	DA	3192	-	X
56	MG	DA	3193	-	X
56	MG	DA	3194	-	X
56	MG	DB	201	-	X
56	MG	DB	202	-	X
56	MG	DB	203	-	X
56	MG	DB	204	-	X
56	MG	DL	201	-	X
56	MG	DO	201	-	X
57	NMY	AA	1656	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
57	NMY	AA	1657	-	X
57	NMY	BA	3161	-	X
57	NMY	BA	3162	-	X
57	NMY	BA	3163	-	X
57	NMY	BA	3164	-	X
57	NMY	BA	3165	-	X
57	NMY	BA	3167	-	X
57	NMY	CA	1672	-	X
57	NMY	DA	3184	-	X
57	NMY	DA	3185	-	X
57	NMY	DA	3186	-	X
57	NMY	DA	3187	-	X
57	NMY	DA	3189	-	X
57	NMY	DA	3190	-	X



## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 293103 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			
1	CA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
2	CB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
3	CC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
4	CD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
5	CE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
6	CF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
7	CG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	CH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
9	CI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
11	CK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
12	CL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
13	CM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
14	CN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			



- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	CP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
17	CQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			
18	CR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
19	CS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
20	CT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
21	CU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a RNA chain called Phenylalanine specific transfer RNA, tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
22	CV	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 23 is a RNA chain called Messenger RNA, mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	16	Total	C	N	O	P	0	0	0
			346	155	66	109	16			
23	CX	15	Total	C	N	O	P	0	0	0
			324	145	61	103	15			

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
24	DA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
25	DB	119	Total	C	N	O	P	0	0	0
			2549	1135	466	829	119			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	12	C	A	SEE REMARK 999	GB AP012306
DB	12	C	A	SEE REMARK 999	GB AP012306



- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
26	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
27	DD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
28	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
29	DF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
30	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 31 is a protein called 50S ribosomal protein L9.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
31	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
32	DI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
33	DJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
34	DK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
35	DL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
37	DN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BO	116	Total	C	N	O		0	0	0
			892	552	178	162				
38	DO	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
39	DP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
40	DQ	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
41	DR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			



- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
42	DS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
43	DT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BU	102	Total	C	N	O		0	0	0
			779	492	146	141				
44	DU	102	Total	C	N	O		0	0	0
			779	492	146	141				

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
45	DV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BW	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			
46	DW	76	Total	C	N	O	S	0	0	0
			580	359	117	103	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
47	DX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
48	DY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
49	DZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
50	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	B1	50	Total	C	N	O	0	0	0
			409	263	75	71			
51	D1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
53	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
54	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 55 is a protein called Ribosome recycling factor, RRF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	CY	183	Total	C	N	O	S	0	0	0
			1423	874	260	283	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BB	3	Total	Mg	0	0
			3	3		
56	DE	1	Total	Mg	0	0
			1	1		
56	BA	163	Total	Mg	0	0
			163	163		
56	CA	71	Total	Mg	0	0
			71	71		
56	DO	1	Total	Mg	0	0
			1	1		
56	DL	1	Total	Mg	0	0
			1	1		
56	DA	187	Total	Mg	0	0
			187	187		

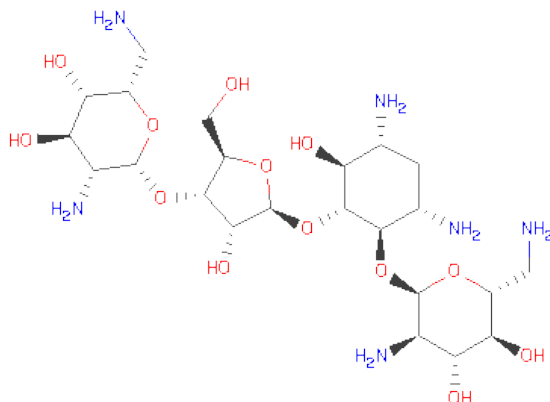
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	54	Total	Mg	0	0
			54	54		
56	BQ	1	Total	Mg	0	0
			1	1		
56	AN	1	Total	Mg	0	0
			1	1		
56	AD	1	Total	Mg	0	0
			1	1		
56	CX	1	Total	Mg	0	0
			1	1		
56	BC	1	Total	Mg	0	0
			1	1		
56	DB	4	Total	Mg	0	0
			4	4		

- Molecule 57 is NEOMYCIN (three-letter code: NMY) (formula:  $C_{23}H_{46}N_6O_{13}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	AA	1	Total	C	N	O	0	0
			42	23	6	13		
57	AA	1	Total	C	N	O	0	0
			42	23	6	13		
57	AA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	BA	1	Total	C	N	O	0	0
			42	23	6	13		
57	CA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		
57	DA	1	Total	C	N	O	0	0
			42	23	6	13		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	B4	1	Total	Zn	0	0
			1	1		
58	D4	1	Total	Zn	0	0
			1	1		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	188	Total	O	0	0
			188	188		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	2	Total 2	O 2	0	0
59	AK	1	Total 1	O 1	0	0
59	AN	4	Total 4	O 4	0	0
59	AT	2	Total 2	O 2	0	0
59	AU	1	Total 1	O 1	0	0
59	BA	616	Total 616	O 616	0	0
59	BB	13	Total 13	O 13	0	0
59	BC	10	Total 10	O 10	0	0
59	BD	4	Total 4	O 4	0	0
59	BL	4	Total 4	O 4	0	0
59	BN	1	Total 1	O 1	0	0
59	BT	3	Total 3	O 3	0	0
59	BU	3	Total 3	O 3	0	0
59	BV	1	Total 1	O 1	0	0
59	B0	1	Total 1	O 1	0	0
59	B3	1	Total 1	O 1	0	0
59	B4	1	Total 1	O 1	0	0
59	CA	192	Total 192	O 192	0	0
59	CC	1	Total 1	O 1	0	0
59	CE	1	Total 1	O 1	0	0
59	CL	1	Total 1	O 1	0	0

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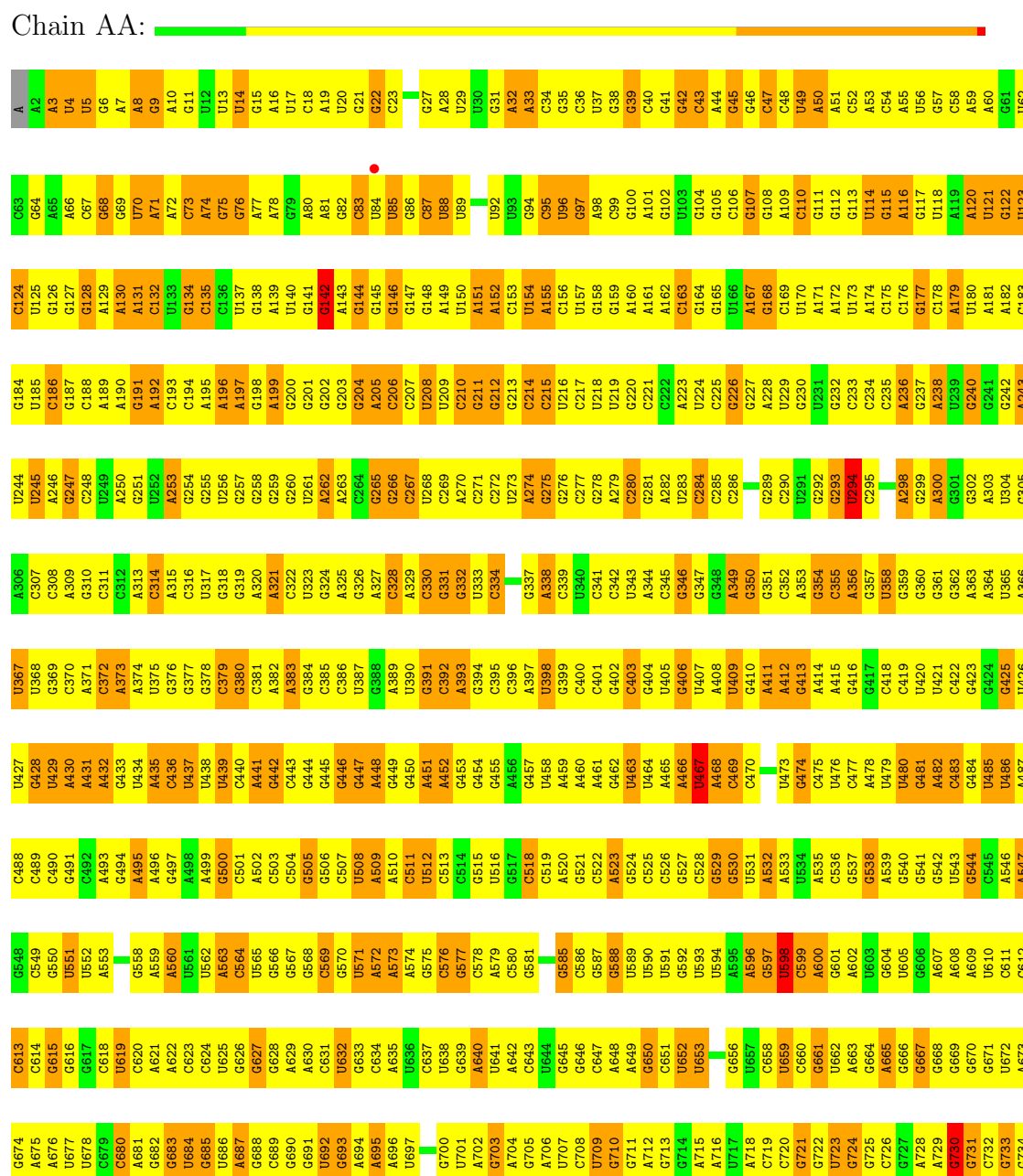
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CN	6	Total 6	O 6	0	0
59	CT	2	Total 2	O 2	0	0
59	DA	627	Total 627	O 627	0	0
59	DB	13	Total 13	O 13	0	0
59	DC	4	Total 4	O 4	0	0
59	DD	2	Total 2	O 2	0	0
59	DE	4	Total 4	O 4	0	0
59	DF	1	Total 1	O 1	0	0
59	DL	7	Total 7	O 7	0	0
59	DN	2	Total 2	O 2	0	0
59	DQ	1	Total 1	O 1	0	0
59	DS	1	Total 1	O 1	0	0
59	DT	1	Total 1	O 1	0	0
59	DU	1	Total 1	O 1	0	0
59	DV	1	Total 1	O 1	0	0
59	D3	2	Total 2	O 2	0	0
59	D4	1	Total 1	O 1	0	0



### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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





U1537	G1475	A1350	C1228	G1166	A1102	A1042	U981	U920	G859	G799	C735
C1538	A1476	U1351	A1229	A1167	C1103	G1043	U982	U921	A860	G800	C736
C1539	U1477	C1352	C1230	U1168	A1104	A1044	A983	G922	G861	U801	C737
U1540	G1478	G1353	G1292	A1169	G1105	C1045	C984	A922	C862	A802	C738
U	C1479	U1354	U1233	A1170	G1106	A1046	C985	C924	U863	G803	
A	A1480	G1415	G1294	C1171	C1107	G1047	U986	G925	A864	U804	G741
	U1481	G1416	U1295	C1172	G1108	G1048	G987	G926	A865	C805	G742
	G1482	A1357	C1296	U1173	C1109	U1049	G988	G927	C866	C806	A743
	A1483	U1358	C1297	G1174	A1110	G1050	U989	G928	A867	A807	G744
	C1484	C1359	U1298	U1175	C1111	U1051	C990	G929	C868	G808	G745
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	G1486	G1361	A1239	G1178	C1113	G1053	U992	C931	U870	C810	A747
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	G1488	C1302	G1241	A1180	U1115	A1055	A994	G933	A872	C812	A749
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	A1500	C1314	G1253	C1192	C1129	A1067	G945	G945	U884	G824	C764
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		C1400	G1279	G1218	A1155	A1092	G971	G971	A909	G849	U789
		G1401	A1280	A1219	G1156	A1093	C972	C972	C910	U850	A790
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		G1403	G1282	G1221	C1158	U1095	A974	A974	C912	G852	A792
		C1404	U1283	G1222	U1159	C1096	A975	A975	A913	C853	U793
		U1345	C1284	C1223	G1160	C1097	G976	G976	A914	U854	A794
		A1346	A1285	U1224	C1161	C1098	A977	A977	U855	C795	C795
		U1286	U1286	A1225	G1162	G1099	A978	A978	C856	C796	C796
		C1347	U1287	C1226	A1163	C1100	C979	C979	C857	A918	
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• Molecule 1: 16S ribosomal RNA

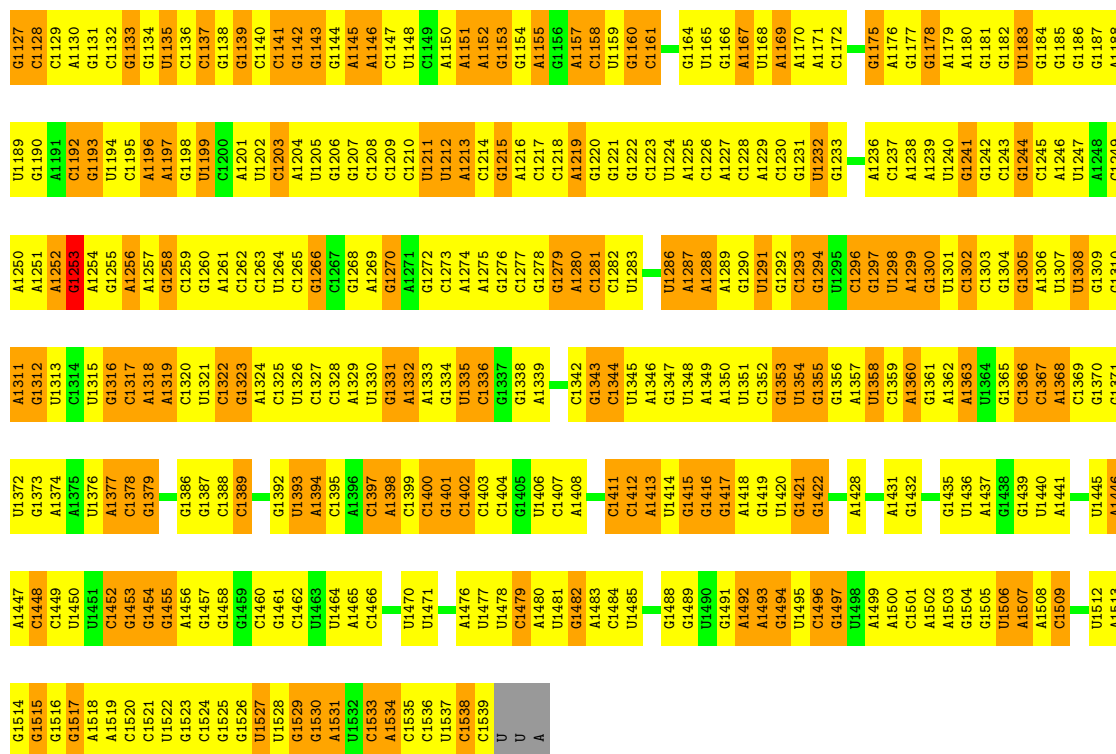
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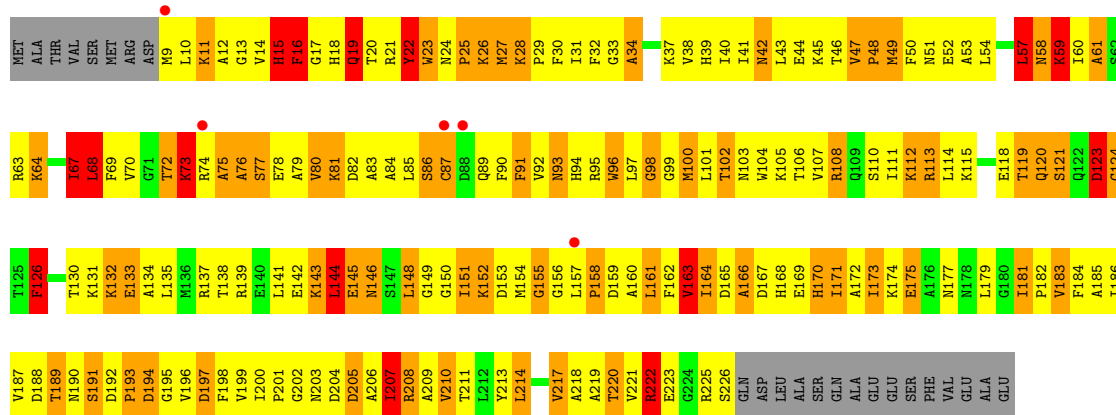
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C1066	A1004	A938	A873	A814	G749	G888	U625	C565	G501	C440	G379	A315	G251	C188	G126	A66
A1067	A1005	G939	A874	A815	C750	G889	U626	G566	A502	C316	C381	C316	U251	A189	G127	A66
G1068	G1006	C940	U875	A816	U751	G890	U627	G567	C503	G443	C382	U317	A253	A190	C67	C67
	U1007	G941	C876	A817	G752	G891	U628	C568	C504	G444	A382	G318	G254	G191	A130	G68
G1072	U1008	G942	G877	C817	A753	U892	A629	C569	G505	G445	A383	G319	G255	A192	A131	G69
U1073	U1009	U943	A878	G818	C754	G893	A630	G570	G506	G446	G384	A320	U256	C193	A132	U70
G1074	G944	C879	A879	A819	G755	A894	C631	U571		G447	C385	G321	G257	C194	G132	A71
U1075	A1012	C945	C880	U820	C756	A895	U632	A572	A510	A448	U387	C322	G258	A196	C135	A72
U1076	G1013	A946	C881	G921	U757	A896	U633	A573	A511	A449	U387	C323	G259	A196	C135	C73
G1077	U1076	G947	C882	U822	C758	U697	C634	A574	C511	A450	A388	G324	G260	A197	C136	A74
	A1014	G948	C883	C823	A759		A635	A575	U512	A451	A389	G325	U261	G198	U137	G75
A1080	A1016	A949	U884	G824	G760	G700	U636	C576	C513	A452	U390	G326	A282	A199	G138	G76
A1081	U1017	U950	G885	A825	G761	U701		G577	C514	A453	G391	A327	A283	G200	A139	A77
A1082	G1018	G951	C886	C826	U762	A702	U639	C578	C515	A454	C392	A328	C284	G201	U140	A78
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G1087	G1024	U956	U891	A831	A767	U707	U644	C583	C520	A459	U398		C289	G206	G145	C83
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U1095	G1032	G966	A900	C839	G775	A715	U653	U591	U530	U467	C406	C345	C277	C214	C153	U91
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G1098	A1035	A969		U842	C778	A718	C656	U594		C470	U409	G348	C281	C217	C156	G94
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G1100	C1037	C972	A907	G844	C780	U720	C658	A596	C537	U472	A411	G350	A283	U219	G158	U96
A1101	C1038	G973	A908	A845	A781	G721	U659	G597	G537	G473	A412	G351	C284	G220	G159	U97
A1102	G1039	A974	A909	G846	A782	G722	C660	U598	C538	G474	C413	C352	C285	C321	A160	A98
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A1111	G1048	A983	U920	U855	A792	G731	C669	A607	A547	C483	C422	G361	U294	G230	G169	G107
G1112	U1049		U921	C856	C793	G732	G670	A608	G548	C484	G423	G362	C295	U231	U170	G108
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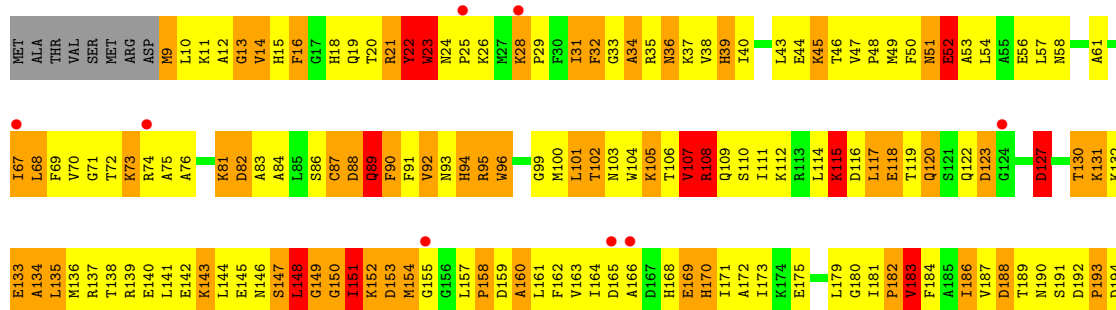
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Chain AB:



### • Molecule 2: 30S ribosomal protein S2

Chain CB:

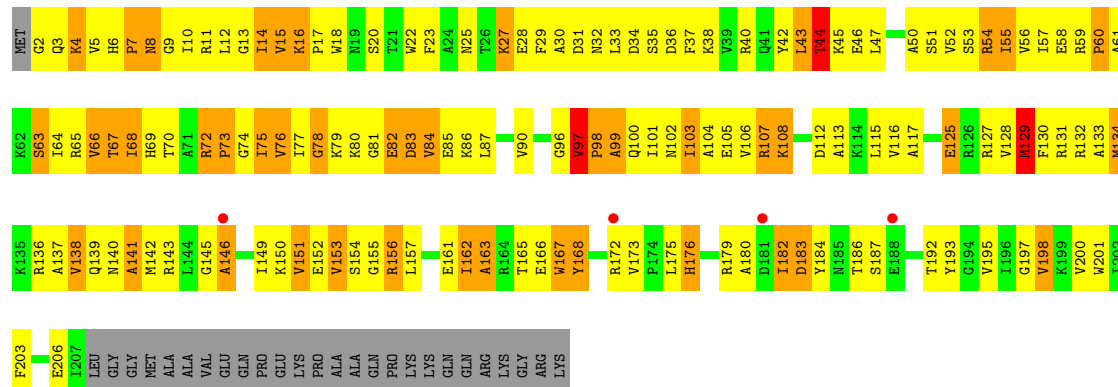






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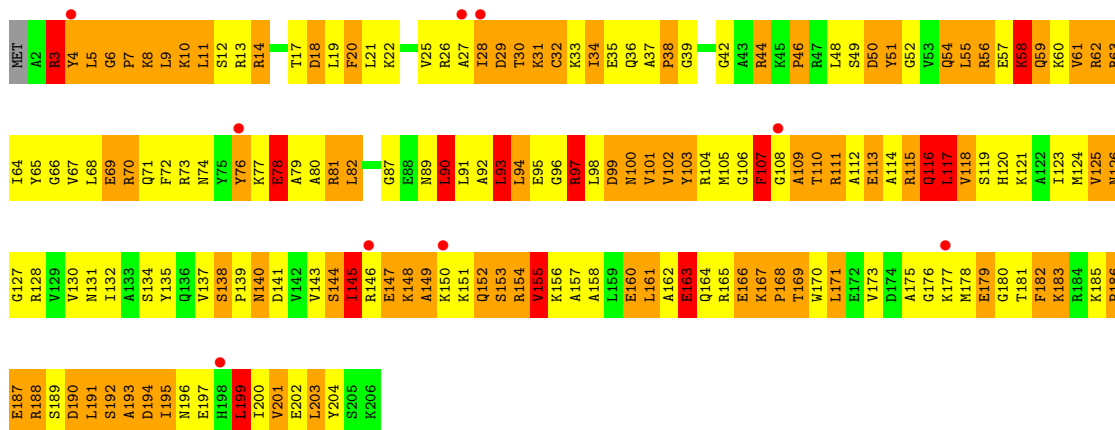
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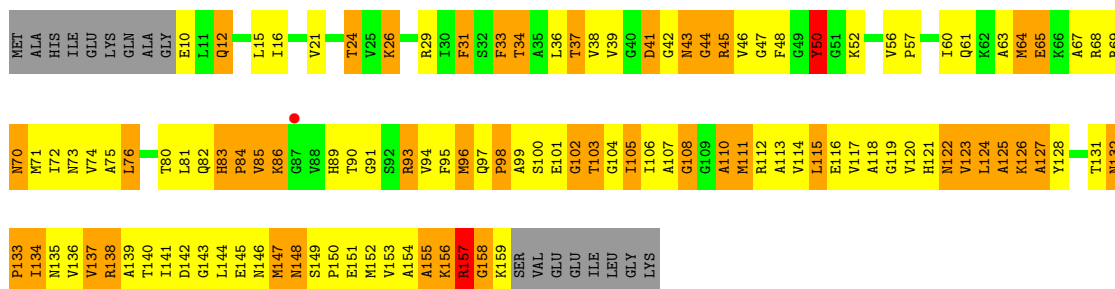
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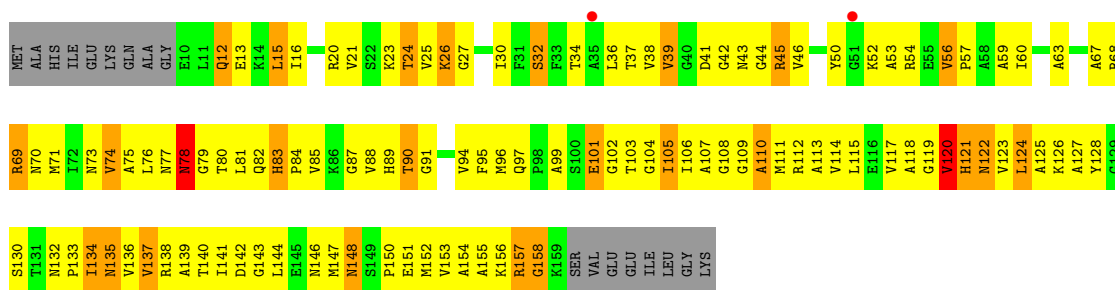
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Chain AE:



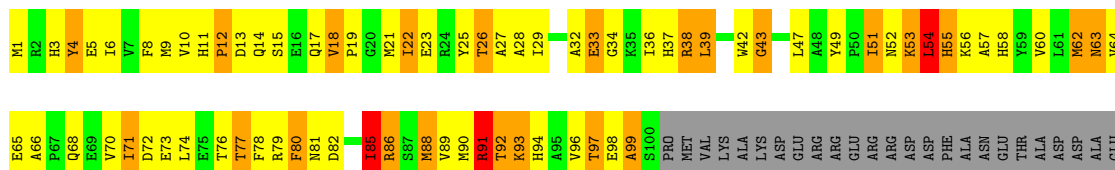
- Molecule 5: 30S ribosomal protein S5

Chain CE:



- Molecule 6: 30S ribosomal protein S6

Chain AF:

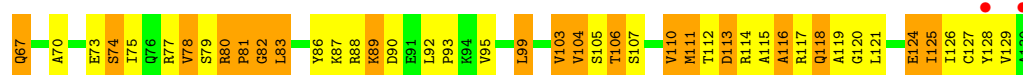






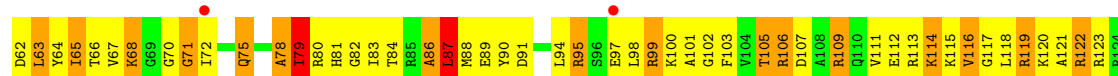


Chain CH: 



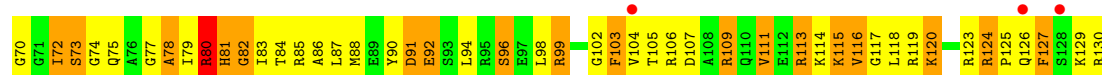
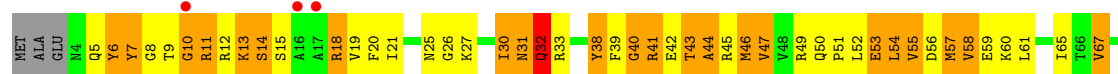
- Molecule 9: 30S ribosomal protein S9

Chain AI: 



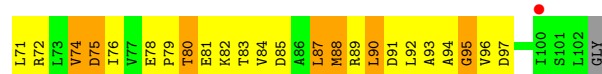
- Molecule 9: 30S ribosomal protein S9

Chain CI: 



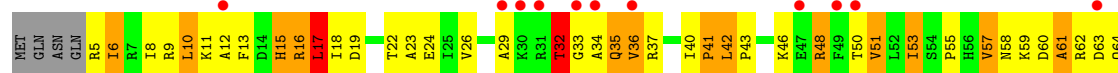
- Molecule 10: 30S ribosomal protein S10

Chain AJ: 



- Molecule 10: 30S ribosomal protein S10

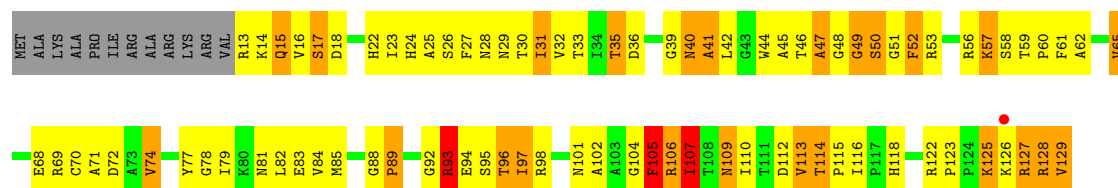
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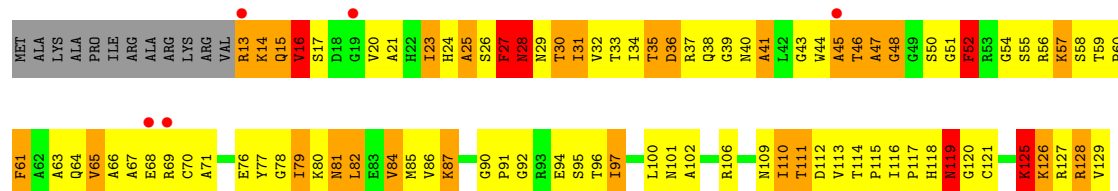
- Molecule 11: 30S ribosomal protein S11

Chain AK:



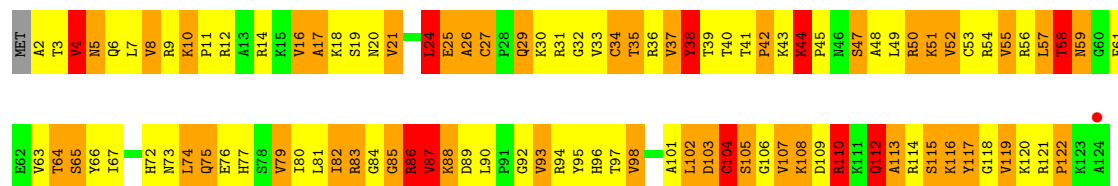
- Molecule 11: 30S ribosomal protein S11

Chain CK:



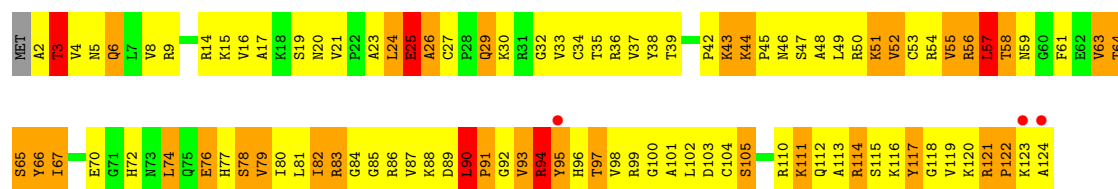
- Molecule 12: 30S ribosomal protein S12

Chain AL:



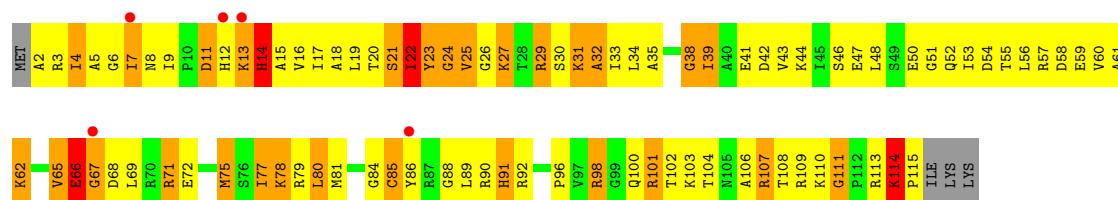
- Molecule 12: 30S ribosomal protein S12

Chain CL:



- Molecule 13: 30S ribosomal protein S13

Chain AM:

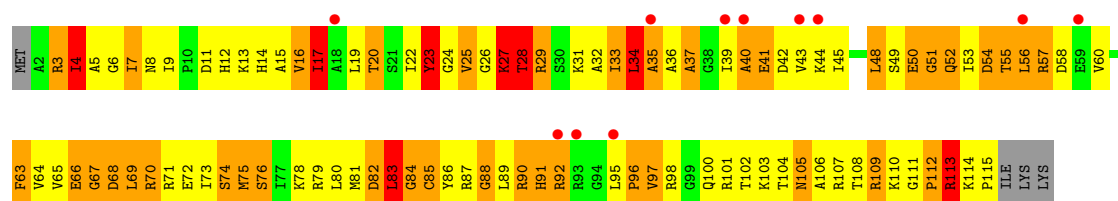


- Molecule 13: 30S ribosomal protein S13

Chain CM:

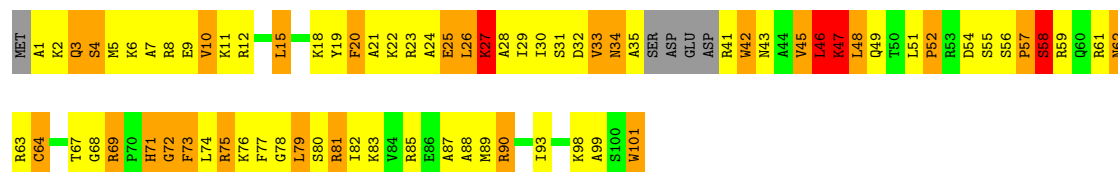






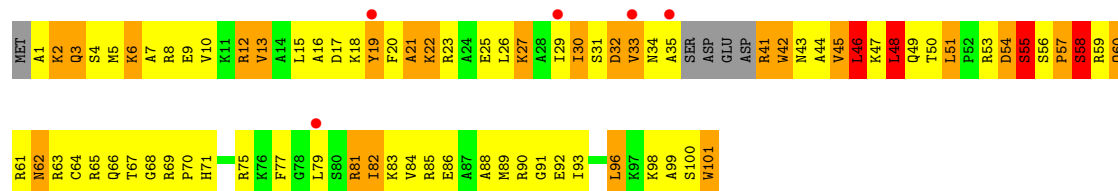
• Molecule 14: 30S ribosomal protein S14

Chain AN:



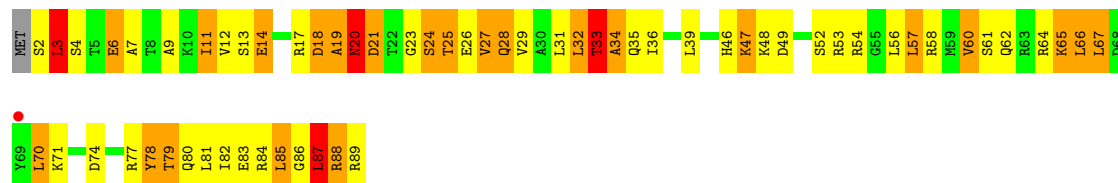
• Molecule 14: 30S ribosomal protein S14

Chain CN:



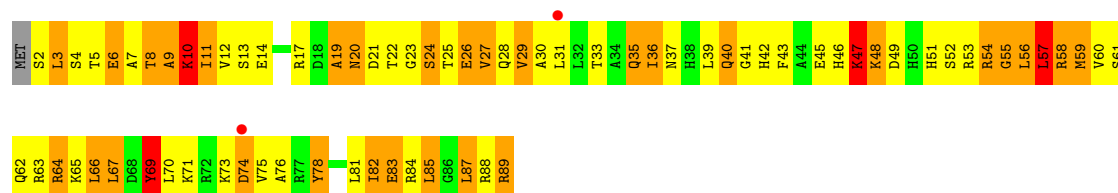
• Molecule 15: 30S ribosomal protein S15

Chain AO:



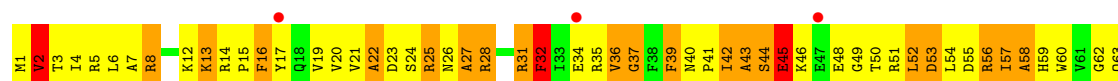
• Molecule 15: 30S ribosomal protein S15

Chain CO:

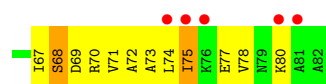


• Molecule 16: 30S ribosomal protein S16

Chain AP:

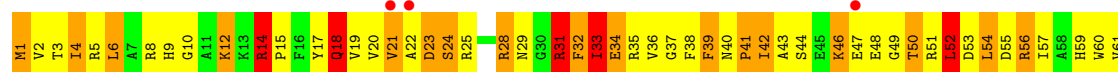






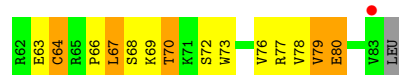
- Molecule 16: 30S ribosomal protein S16

Chain CP:



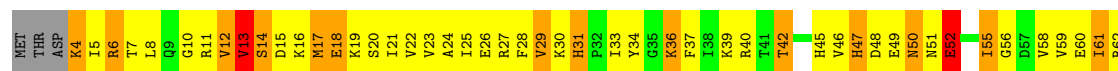
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



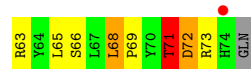
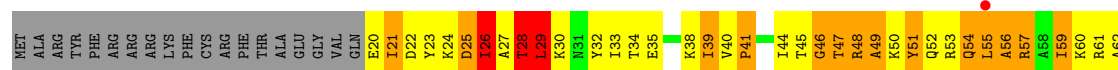
- Molecule 17: 30S ribosomal protein S17

Chain CQ:



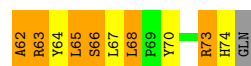
- Molecule 18: 30S ribosomal protein S18

Chain AR:



- Molecule 18: 30S ribosomal protein S18

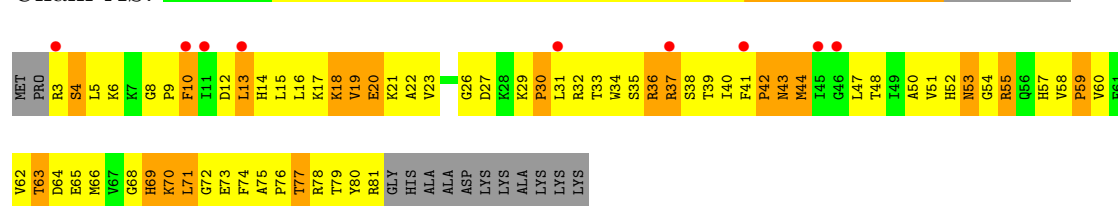
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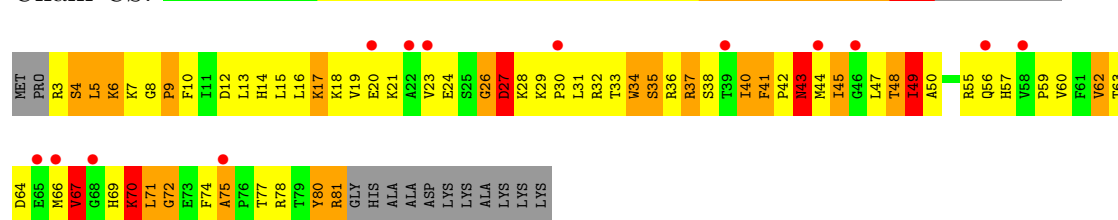
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Chain AS:



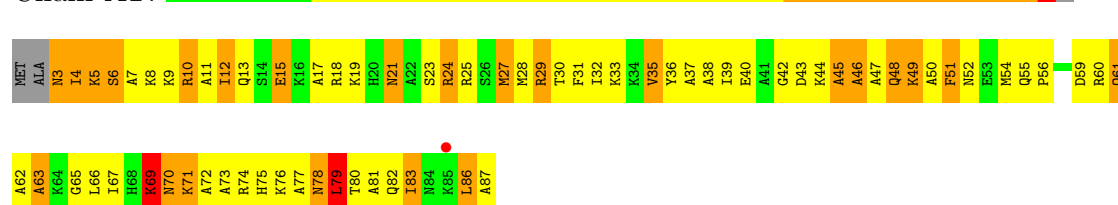
- Molecule 19: 30S ribosomal protein S19

Chain CS:



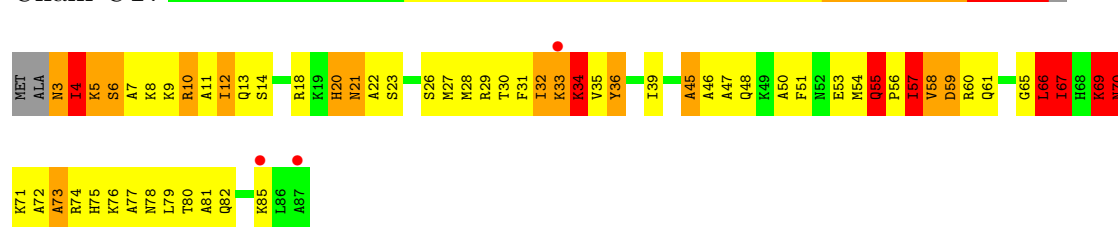
- Molecule 20: 30S ribosomal protein S20

Chain AT:



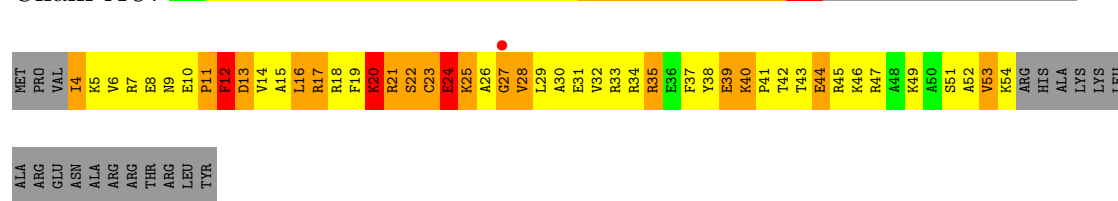
- Molecule 20: 30S ribosomal protein S20

Chain CT:



- Molecule 21: 30S ribosomal protein S21

Chain AU:



- Molecule 21: 30S ribosomal protein S21

Chain CU:









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WORLDWIDE  
**PDB**  
PROTEIN DATA BANK





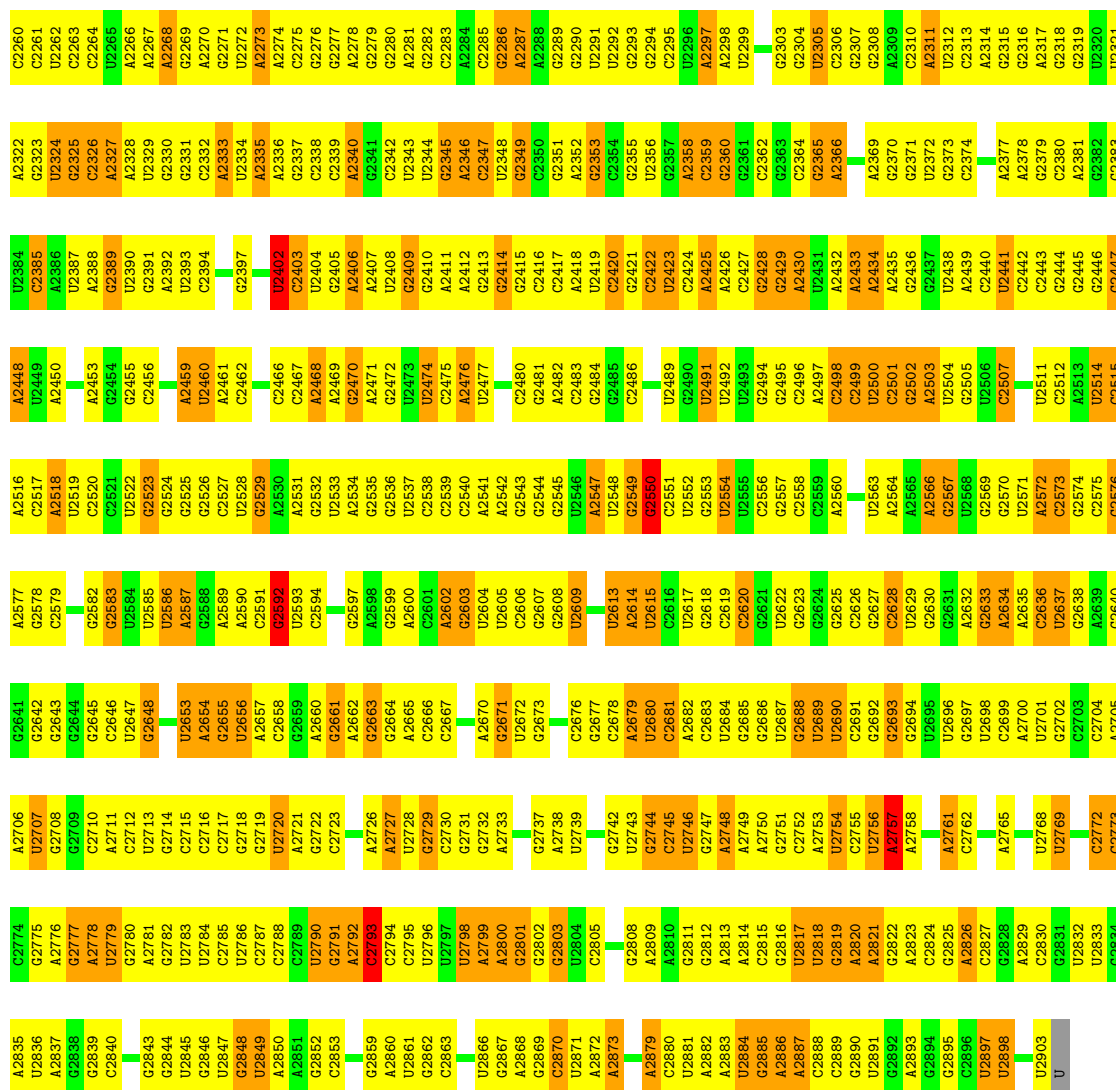


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G1182	G1114	G1047	A980	C915	U850	G784	G718	U653	A592	U529	G463	G401	C331	G263	U201
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U1188	G1120	G1056		C921	G856	U790	G723	U659	U598	U535	G469	G407	C338	A270	U206
A1189	C1121	A1057	A988	C922	G857	C791	U724	C660	A599	G536	A470	G408	U339	G271	A207
G1190	G1122	U1058	G989	G923	G858	A792	G725	A661	G600	G537		G409	U339	A272	C208
G1191	C1123	G1059	A990		G859	A793	G726	G662	C601	A538	G473	G410	C340	G273	C209
G1192	G1124	U1060	C991	G926	U860	A794	G727	G663	A602	G539	G474	C341	C340	C274	C210
G1193	G1125	U1061	C992	A927	A861		G728	U664	A803	C540	C475	G411	A342	C275	C211
A1194	A1126	G1062	G993	A928	G862	G797	G729	U665	G604	A541	G476	A412	C343	U276	G212
G1196	U1130	G1063	U929	U928	A863		A730	A666	A542	C542	G477		A346	G277	A213
G1197	G1131	C1064	G930	U931	G864	A800	G731	U667	U606	G543	A478	U416	A347	A278	G214
U1198	U1132	U1066	A995	U931	C865	G801	C732	A668	U607	C544	A479	U417	A352	A279	G215
U1199	A1133	A1067	G997	U932	A866	A802	G733	G669	A608	U545	A480	C417	C352	U280	A216
C1200	G1134	G1068	C998	A933	C867		A734	A670	A609	U546	G481	C418	C353	C281	A217
		C1135	U999	U934	U868	G805	A735	C671	C610	G548	A482	U419	C354	G283	A218
		A1070	A1001	C937	U870	U807	C737	C672	C611	G549	A483	C420	U355	U284	A219
		G1071	G1002	G938	U871	G808	G738	C673	A613	C550	C485	A422	G356	G220	
A1203	G1136	C1072		G939	U872	G809	A739	A675	A614		C486	A423	G359	U286	A221
A1204	G1137	G1073	G1005	G940		U810	C740	A676	U615	U554	C487	G424	U360	G287	A223
G1206	G1138	A1074	C1006	A941	G875	U811	U741	A677	A616	G555		G425	U361	G288	U224
C1207	U1140	G1075	C1007	G942	C876	C812	A742	C678	G617	A556	G491	C426	A362	U289	
C1208	U1141	C1076	G1008	A943	A877	U813	A743	C679	G618	C557	A492	U427	G363		A226
U1209	A1142	A1077	A1009	C944	A878	C814		C680	G619	U558	A493		C364	U292	A227
G1210	A1143	C1078	A1010	A945	G879	C815	U746	G681	G620	G559	G494	A430	U365	U283	C228
C1211	A1144	U1078	G1011	C946	G880	G816	U747	G682	A821	C580	G495	U431	G366	G230	
G1212	C1145	C1079	G1012	A947	G881	C817	G748	U683	G622	A563	G496	A432	G367	G296	G231
G1213	A1146	U1080	U1012	G948	G882	G818	A749	G684	C823	C564	A497	C433	U368	G297	A232
A1214	U1147	U1081	A1014		G883	A819	A750	A685	G624	C565	A498	U434	U369	G298	A233
G1215	U1148	U1082	C948		U884	A820	A751	U686	G625	C566	U499	C435	G370	A299	
U1216	G1149	A1075	C951	G951	C885	A821	A752	C687	A626	U566	G500	C436	A371	G299	
G1217	C1150	U1083	G952	G953	A	G822	A753	U688	A627	U567	G512	U437	G372	A300	U235
A1218	A1151	A1086	G954	G954	U	C823	U754	A689	G628	U568	A502	G438	U373	G301	
U1219	C1152	G1087	U955	U955	C	U824	U755	G690	G629	U569	A503	A439	A374	C302	C238
G1220	G1153	A1088	G956	G956	C	A825	A756	C691	G630	G570	A504	C440	U375	G303	C239
C1221	A1154	A1089	C957	C957	C	U826	G757	C692	G631	U571	A505	U441	G377	U304	
U1222	A1155	U1090	U1023	U958	G	U827		A693	A633	A572	G506	G442	C378	C305	G242
G1223	A1156	G1091	G1024	A958	A892	U828	A761	U694	C634	U573	A507	A443	G379	U306	U243
U1224	G1157	C1092	G1025	A959	C893	A829	U762	G695	C635	A574	A508	C444	G380	G307	A244
G1225		G1093	G1026	A960	U894	G830	G763	G696	G636	A575	C509	C445	G381	G308	A245
A1226	G1162	U1094	A1027	C961	U895	G831	A764	G697	A637	U576	C510	G446	A382	A309	G246
G1227	G1163	A1095	G1028	U962	A896	U832	C765	C698	G638	G577	U511	A447	C383	A310	G247
G1228	C1164	U1096	A1029	U963	C897	A833		A699	U639	G578	G512		G383	A311	G248
C1229	A1165	U1097	C964	C965	C898	G834	G770	G700	C640	G579	A513	G450	G386	G312	C249
		G1030	C964	C965	A899	C835			U641	U580	A514	U451	U387	G250	
G1232	G1168	A900	G969	G969	A900	C839	U773	G704	A642	C581	C517	G452	G388	G319	A251
U1233	U1169	C901	U970	U970	C901		G774	G775	A643	A582	C517	A453	G389	A320	G252
G1235	G1170	G971	G971	G971			G776	G777	A644	A583	C517	U321	U390	U321	
A1236	U1171	A1039	A972	A972	G907	U842	G777	U709	C645	C584	G520	C455	G380	A322	A255
G1237	C1172	A1040	A973	A973	C908	G843	G778	U710	G646	C585	G521	C456	G379	C323	G256
U1238	U1173	G1041	G974	G974	A909	A844	G779	G711	G847	A586	A522	A457	C393	A324	C257
G1239	U1176	U1105	G975	G975	A910	A945	U779	G712	G648	C587	C523	G458	C394	G325	G258
U1240	C1177	G1106	A911	A911	A911	U846	G780	G713	G649	U588	C523	U459	U395	G326	
A1241	G1179	C912	G977	G977	C912	U847	A781	U714	C650	U589	A526	A460	G396	U328	G260





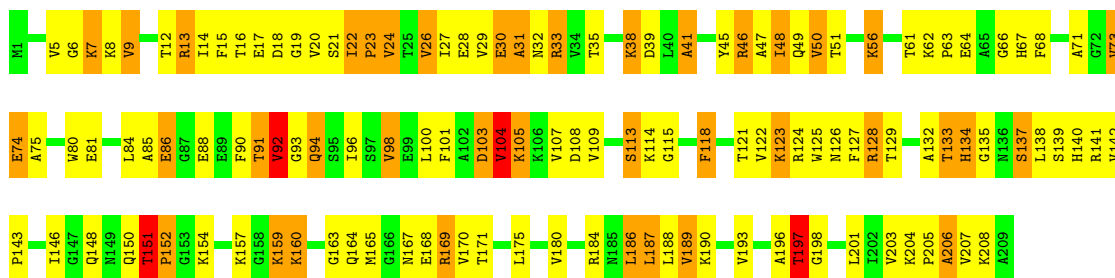






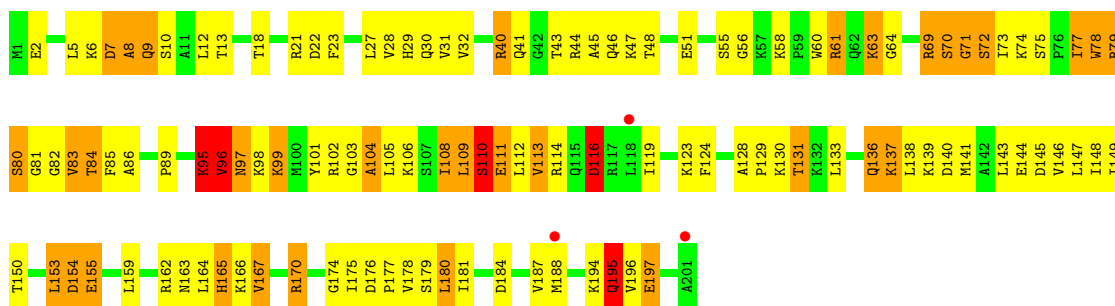






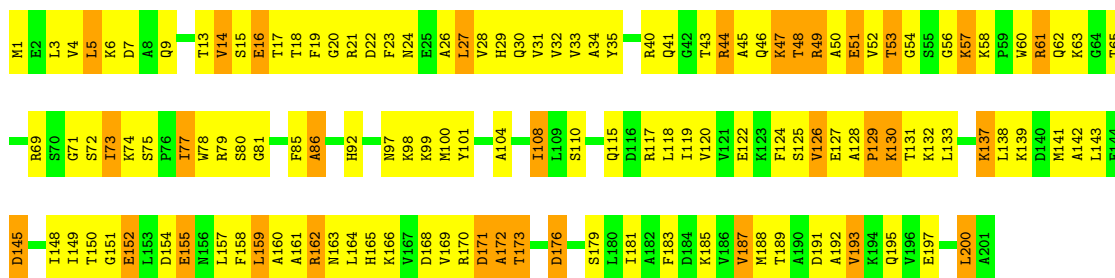
• Molecule 28: 50S ribosomal protein L4

Chain BE:



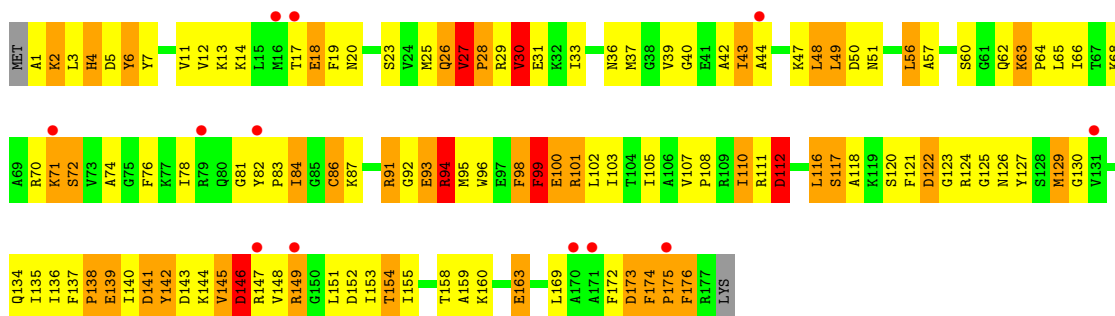
• Molecule 28: 50S ribosomal protein L4

Chain DE:



• Molecule 29: 50S ribosomal protein L5

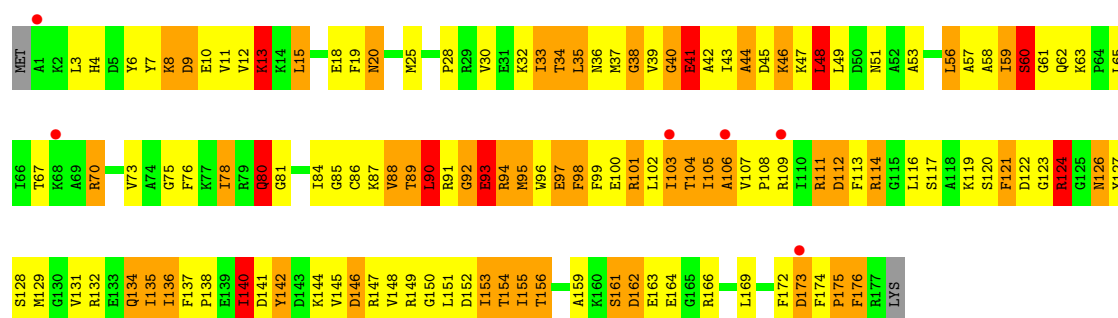
Chain BF:



• Molecule 29: 50S ribosomal protein L5

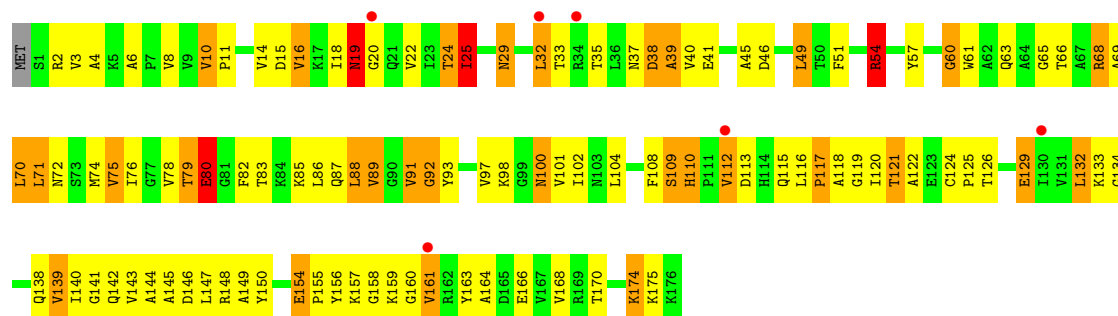
Chain DF:





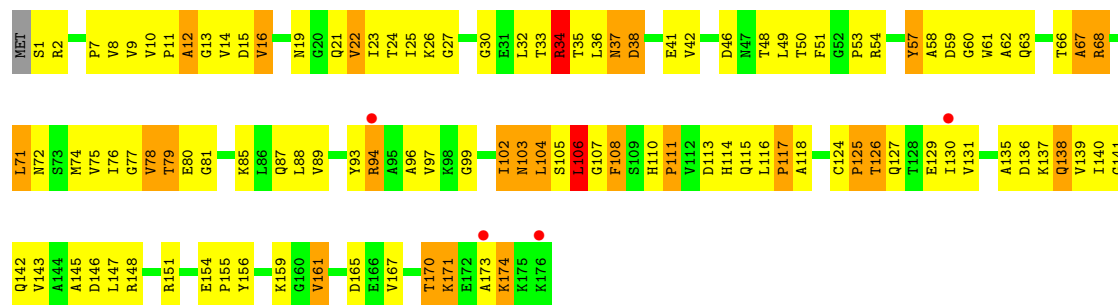
- Molecule 30: 50S ribosomal protein L6

Chain BG:



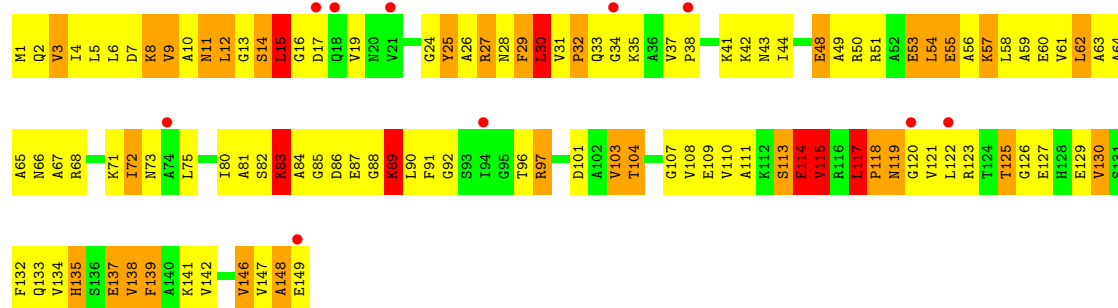
- Molecule 30: 50S ribosomal protein L6

Chain DG:



- Molecule 31: 50S ribosomal protein L9

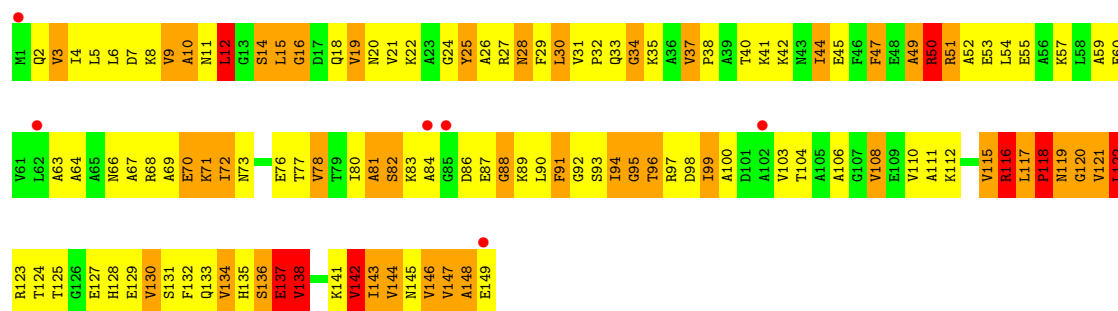
Chain BH:



- Molecule 31: 50S ribosomal protein L9

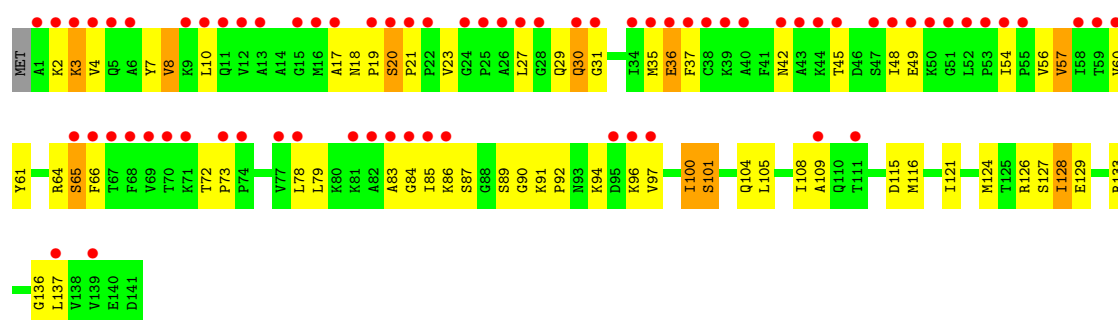


Chain DH:



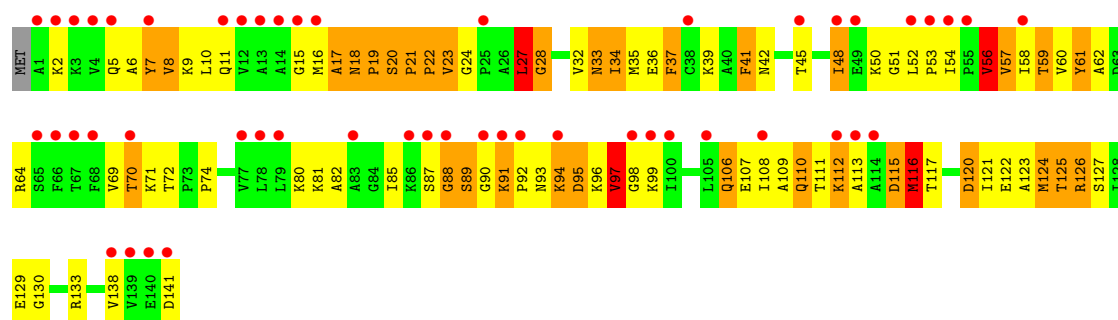
- Molecule 32: 50S ribosomal protein L11

Chain BI:



- Molecule 32: 50S ribosomal protein L11

Chain DI:



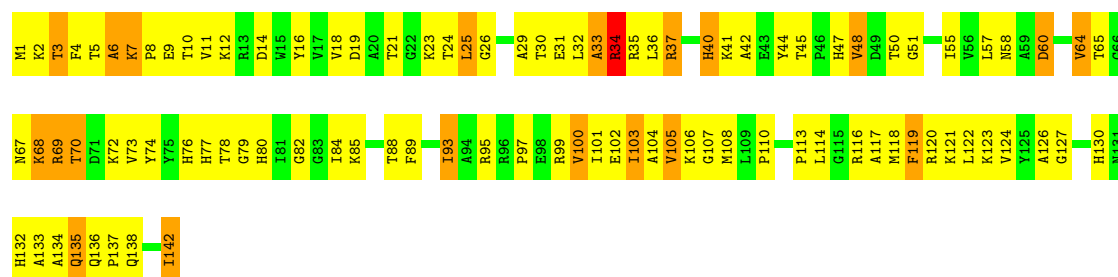
- Molecule 33: 50S ribosomal protein L13

Chain BJ:

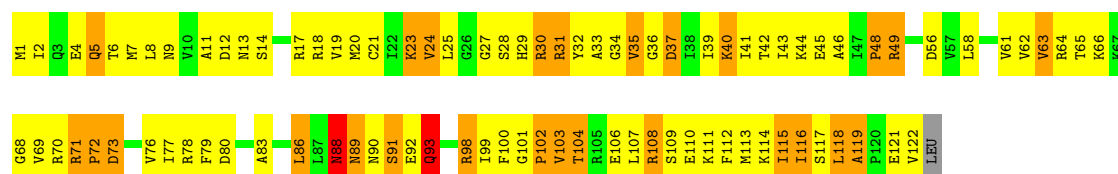


- Molecule 33: 50S ribosomal protein L13

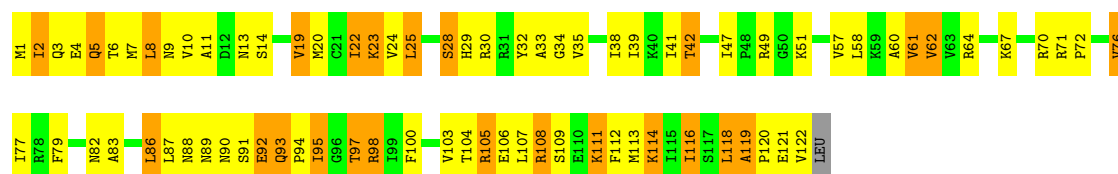


Chain DJ: 

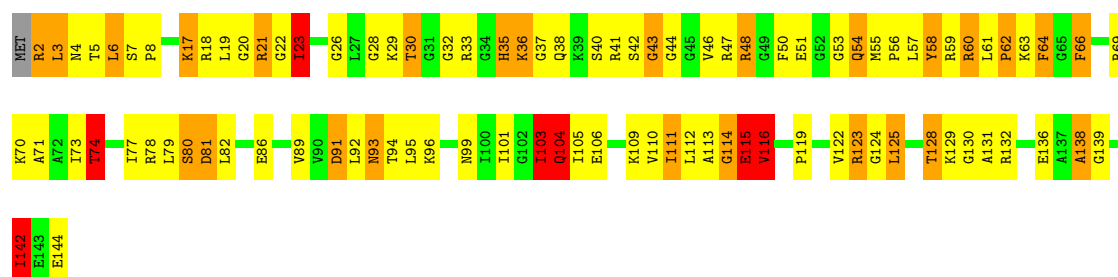
- Molecule 34: 50S ribosomal protein L14

Chain BK: 

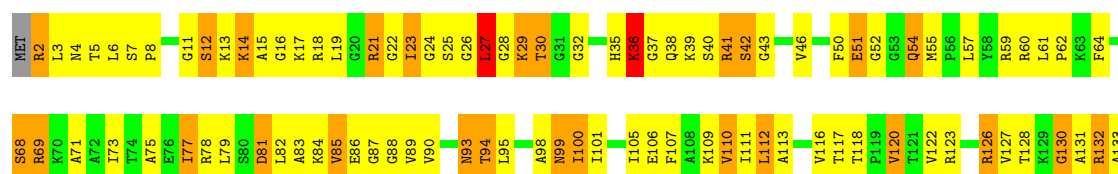
- Molecule 34: 50S ribosomal protein L14

Chain DK: 

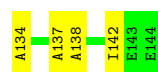
- Molecule 35: 50S ribosomal protein L15

Chain BL: 

- Molecule 35: 50S ribosomal protein L15

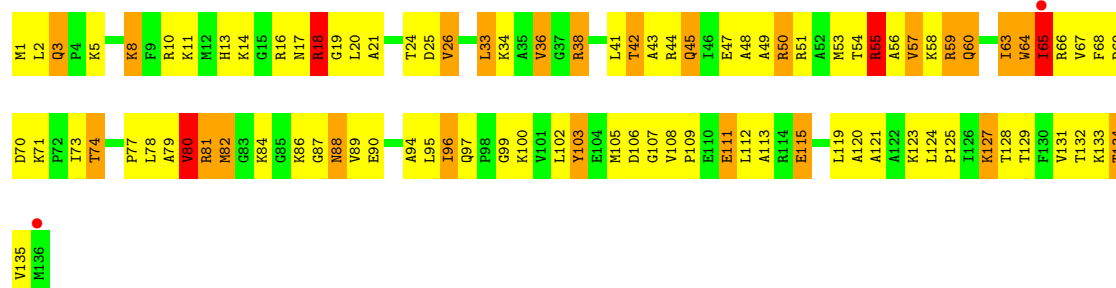
Chain DL: 





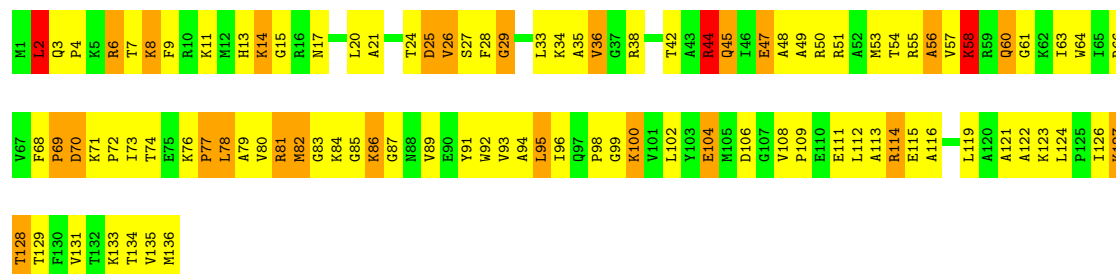
- Molecule 36: 50S ribosomal protein L16

Chain BM:



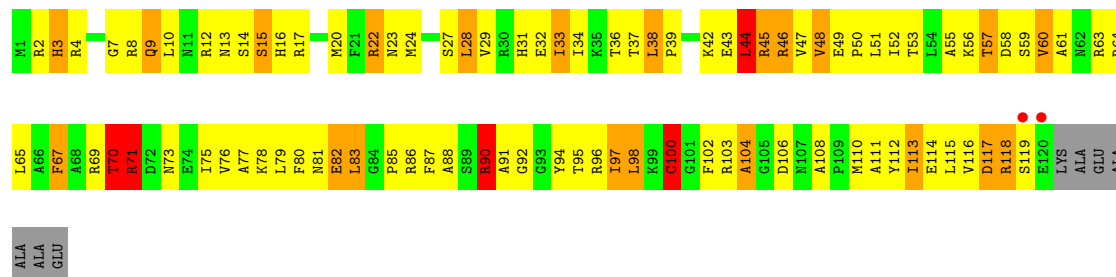
- Molecule 36: 50S ribosomal protein L16

Chain DM:



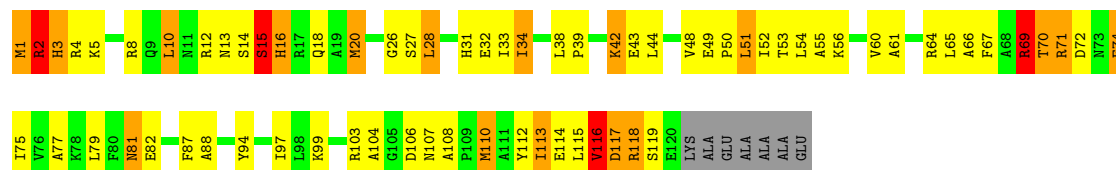
- Molecule 37: 50S ribosomal protein L17

Chain BN:



- Molecule 37: 50S ribosomal protein L17

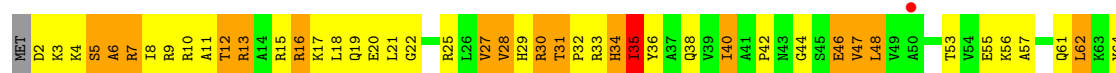
Chain DN:



- Molecule 38: 50S ribosomal protein L18



Chain BO: 



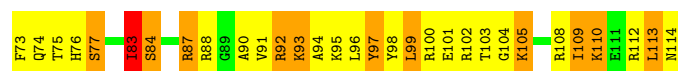
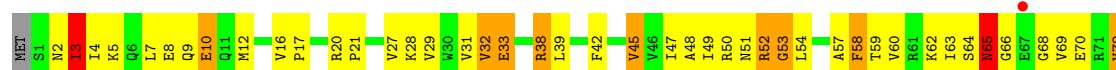
- Molecule 38: 50S ribosomal protein L18

Chain DO: 



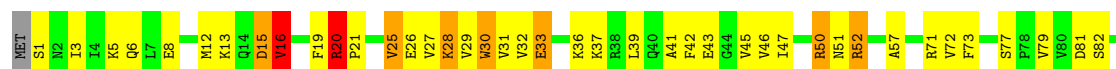
- Molecule 39: 50S ribosomal protein L19

Chain BP: 



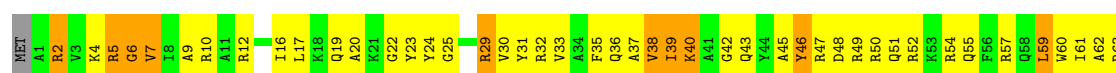
- Molecule 39: 50S ribosomal protein L19

Chain DP: 



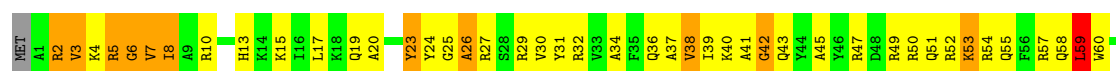
- Molecule 40: 50S ribosomal protein L20

Chain BQ: 



- Molecule 40: 50S ribosomal protein L20

Chain DQ: 







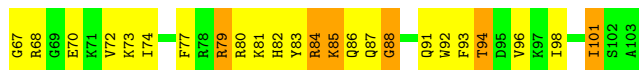
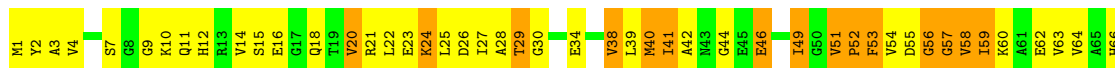
- Molecule 41: 50S ribosomal protein L21

Chain BR:



- Molecule 41: 50S ribosomal protein L21

Chain DR:



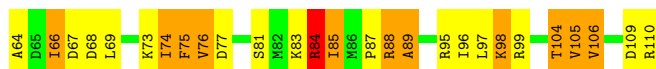
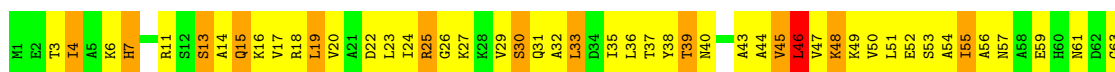
- Molecule 42: 50S ribosomal protein L22

Chain BS:



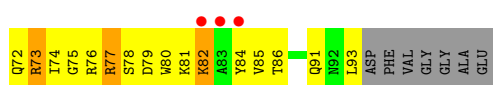
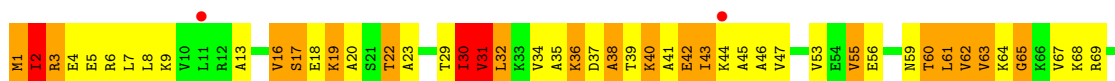
- Molecule 42: 50S ribosomal protein L22

Chain DS:



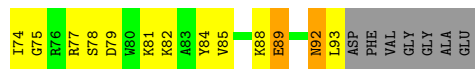
- Molecule 43: 50S ribosomal protein L23

Chain BT:



- Molecule 43: 50S ribosomal protein L23

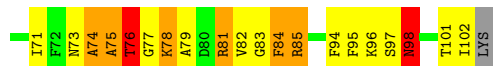




- 



- 



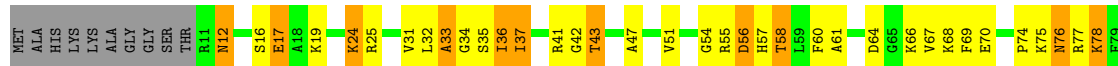
- 



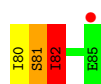
- 
- | Frequency | Percentage |
|-----------|------------|
| Daily     | 45%        |
| Weekly    | 35%        |
| Monthly   | 20%        |



- 

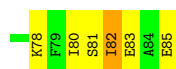
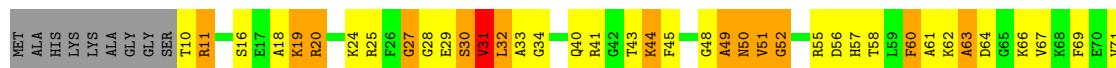






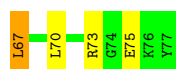
- Molecule 46: 50S ribosomal protein L27

Chain DW:



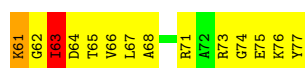
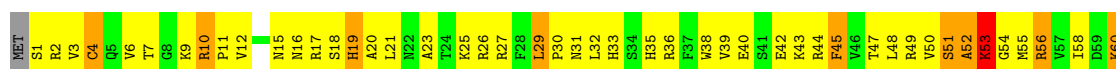
- Molecule 47: 50S ribosomal protein L28

Chain BX:



- Molecule 47: 50S ribosomal protein L28

Chain DX:



- Molecule 48: 50S ribosomal protein L29

Chain BY:



- Molecule 48: 50S ribosomal protein L29

Chain DY:



- Molecule 49: 50S ribosomal protein L30

Chain BZ:



- Molecule 49: 50S ribosomal protein L30

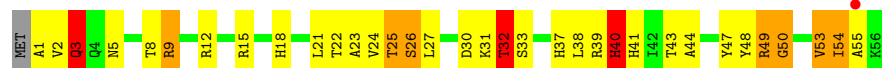


Chain DZ: 



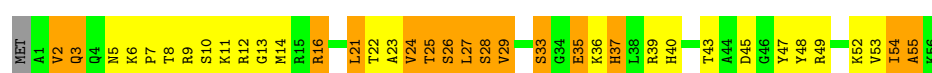
- Molecule 50: 50S ribosomal protein L32

Chain B0: 



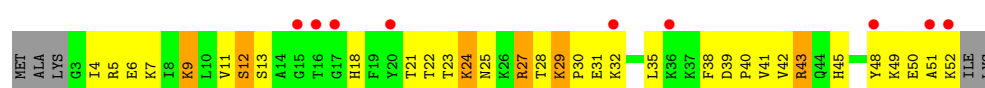
- Molecule 50: 50S ribosomal protein L32

Chain D0: 



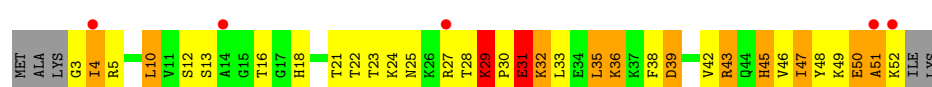
- Molecule 51: 50S ribosomal protein L33

Chain B1: 



- Molecule 51: 50S ribosomal protein L33

Chain D1: 



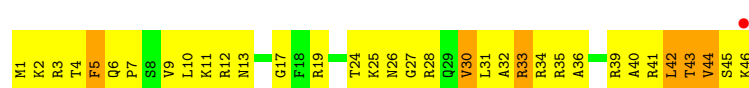
- Molecule 52: 50S ribosomal protein L34

Chain B2: 



- Molecule 52: 50S ribosomal protein L34

Chain D2: 



- Molecule 53: 50S ribosomal protein L35

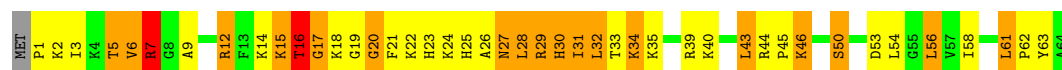
Chain B3: 



A64



- Molecule 53: 50S ribosomal protein L35

Chain D3: 

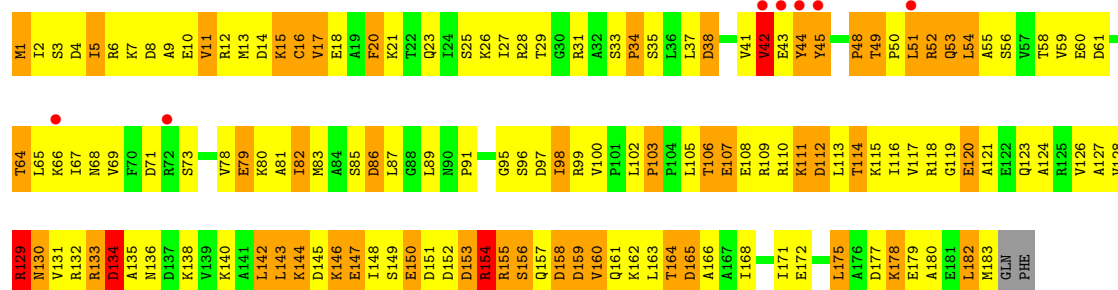
- Molecule 54: 50S ribosomal protein L36

Chain B4: 

- Molecule 54: 50S ribosomal protein L36

Chain D4: 

- Molecule 55: Ribosome recycling factor, RRF

Chain CY: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.18Å 433.90Å 608.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.30 69.81 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.30) 95.0 (69.81-3.30)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.206 , 0.255 0.208 , 0.259	Depositor DCC
$R_{free}$ test set	2000 reflections (0.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.3	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 75.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 793808 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	293103	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, NMY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	AA	0.34	0/36966	0.95	39/57666 (0.1%)
1	CA	0.33	0/36944	0.93	15/57632 (0.0%)
2	AB	0.28	0/1735	0.61	0/2338
2	CB	0.26	0/1735	0.57	0/2338
3	AC	0.29	0/1651	0.61	0/2225
3	CC	0.30	0/1651	0.58	0/2225
4	AD	0.35	0/1665	0.69	0/2227
4	CD	0.29	0/1665	0.65	0/2227
5	AE	0.28	0/1118	0.66	0/1504
5	CE	0.30	0/1118	0.63	0/1504
6	AF	0.33	0/835	0.67	0/1128
6	CF	0.32	0/835	0.62	0/1128
7	AG	0.25	0/1195	0.52	0/1602
7	CG	0.27	0/1195	0.56	0/1602
8	AH	0.30	0/989	0.66	0/1326
8	CH	0.29	0/989	0.60	0/1326
9	AI	0.25	0/1034	0.59	0/1375
9	CI	0.27	0/1034	0.58	0/1375
10	AJ	0.26	0/796	0.60	0/1077
10	CJ	0.24	0/796	0.53	0/1077
11	AK	0.33	0/893	0.68	0/1205
11	CK	0.30	0/893	0.63	0/1205
12	AL	0.30	0/969	0.71	0/1300
12	CL	0.35	0/969	0.71	1/1300 (0.1%)
13	AM	0.25	0/892	0.57	0/1193
13	CM	0.26	0/892	0.64	0/1193
14	AN	0.26	0/785	0.55	0/1043
14	CN	0.25	0/785	0.56	0/1043
15	AO	0.35	0/722	0.58	0/964
15	CO	0.27	0/722	0.60	0/964
16	AP	0.32	0/659	0.74	2/884 (0.2%)
16	CP	0.29	0/659	0.63	0/884



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.28	0/657	0.61	0/881
17	CQ	0.34	0/657	0.71	0/881
18	AR	0.31	0/462	0.69	0/621
18	CR	0.30	0/462	0.60	0/621
19	AS	0.26	0/652	0.57	0/877
19	CS	0.27	0/652	0.65	0/877
20	AT	0.27	0/671	0.59	0/888
20	CT	0.25	0/671	0.58	0/888
21	AU	0.37	0/430	0.76	0/570
21	CU	0.30	0/430	0.61	0/570
22	AV	0.40	1/1813 (0.1%)	0.89	0/2823
22	CV	0.32	1/1813 (0.1%)	0.77	0/2823
23	AX	0.32	0/388	0.88	0/603
23	CX	0.28	0/363	0.85	0/564
24	BA	0.36	0/69659	0.97	72/108672 (0.1%)
24	DA	0.43	3/69659 (0.0%)	1.07	120/108672 (0.1%)
25	BB	0.28	0/2828	0.84	0/4410
25	DB	0.36	0/2850	0.96	2/4444 (0.0%)
26	BC	0.29	0/2121	0.67	0/2852
26	DC	0.34	0/2121	0.75	2/2852 (0.1%)
27	BD	0.31	0/1586	0.66	0/2134
27	DD	0.36	0/1586	0.68	0/2134
28	BE	0.29	0/1571	0.59	0/2113
28	DE	0.32	0/1571	0.67	1/2113 (0.0%)
29	BF	0.26	0/1434	0.53	0/1926
29	DF	0.29	0/1434	0.66	0/1926
30	BG	0.27	0/1343	0.57	0/1816
30	DG	0.31	0/1343	0.67	1/1816 (0.1%)
31	BH	0.31	0/1121	0.57	1/1515 (0.1%)
31	DH	0.34	1/1121 (0.1%)	0.60	1/1515 (0.1%)
32	BI	0.23	0/1046	0.47	0/1410
32	DI	0.24	0/1046	0.56	0/1410
33	BJ	0.32	0/1152	0.66	0/1551
33	DJ	0.35	0/1152	0.67	0/1551
34	BK	0.32	0/947	0.68	0/1268
34	DK	0.37	0/947	0.71	0/1268
35	BL	0.29	0/1054	0.66	0/1403
35	DL	0.33	0/1054	0.73	0/1403
36	BM	0.28	0/1093	0.61	0/1460
36	DM	0.36	0/1093	0.77	2/1460 (0.1%)
37	BN	0.28	0/973	0.63	0/1301
37	DN	0.36	0/973	0.70	0/1301
38	BO	0.27	0/902	0.55	0/1209



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DO	0.33	0/902	0.62	0/1209
39	BP	0.33	0/929	0.67	0/1242
39	DP	0.37	0/929	0.74	1/1242 (0.1%)
40	BQ	0.32	0/960	0.60	0/1278
40	DQ	0.34	0/960	0.69	0/1278
41	BR	0.32	0/829	0.66	0/1107
41	DR	0.38	0/829	0.75	0/1107
42	BS	0.31	0/864	0.69	0/1156
42	DS	0.35	0/864	0.70	0/1156
43	BT	0.30	0/744	0.63	1/994 (0.1%)
43	DT	0.34	0/744	0.70	2/994 (0.2%)
44	BU	0.29	0/787	0.59	0/1051
44	DU	0.32	0/787	0.68	0/1051
45	BV	0.26	0/766	0.57	0/1025
45	DV	0.32	0/766	0.68	0/1025
46	BW	0.30	0/576	0.58	0/762
46	DW	0.35	0/587	0.72	0/776
47	BX	0.33	0/635	0.65	0/848
47	DX	0.32	0/635	0.65	0/848
48	BY	0.25	0/510	0.59	0/677
48	DY	0.28	0/510	0.70	0/677
49	BZ	0.29	0/453	0.59	0/605
49	DZ	0.29	0/453	0.73	0/605
50	B0	0.29	0/450	0.62	0/599
50	D0	0.32	0/450	0.67	0/599
51	B1	0.33	0/416	0.57	0/554
51	D1	0.29	0/416	0.63	0/554
52	B2	0.28	0/380	0.58	0/498
52	D2	0.31	0/380	0.67	0/498
53	B3	0.29	0/513	0.63	0/676
53	D3	0.33	0/513	0.71	0/676
54	B4	0.31	0/303	0.62	0/397
54	D4	0.34	0/303	0.75	0/397
55	CY	0.28	0/1434	0.66	1/1929 (0.1%)
All	All	0.36	6/315264 (0.0%)	0.91	264/471562 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	CB	0	1
3	CC	0	1
4	CD	0	2
5	AE	0	1
8	AH	0	3
9	CI	0	1
12	AL	0	1
13	CM	0	1
16	AP	0	1
16	CP	0	1
26	BC	0	1
26	DC	0	3
27	BD	0	1
27	DD	0	1
31	BH	0	1
31	DH	0	2
33	DJ	0	1
37	BN	0	1
37	DN	0	1
39	DP	0	1
42	DS	0	1
50	D0	0	1
All	All	0	29

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CV	1	G	OP3-P	-10.55	1.48	1.61
22	AV	1	G	OP3-P	-10.36	1.48	1.61
24	DA	2204	G	N9-C8	7.67	1.43	1.37
24	DA	733	G	N3-C4	-5.30	1.31	1.35
31	DH	118	PRO	N-CD	5.25	1.55	1.47

The worst 5 of 264 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	DA	2204	G	C8-N9-C4	-13.18	101.13	106.40
24	DA	733	G	N3-C4-N9	-11.80	118.92	126.00
24	DA	733	G	C6-C5-N7	10.61	136.76	130.40
24	DA	733	G	N9-C4-C5	10.19	109.47	105.40
1	AA	890	G	O4'-C1'-N9	9.65	115.92	108.20



There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	162	PHE	Peptide
5	AE	157	ARG	Peptide
8	AH	125	ILE	Peptide
8	AH	87	LYS	Peptide
8	AH	88	ARG	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	33015	0	16617	2761	0
1	CA	32995	0	16607	2603	2
2	AB	1704	0	1732	275	0
2	CB	1704	0	1732	227	0
3	AC	1624	0	1696	188	0
3	CC	1624	0	1696	185	0
4	AD	1643	0	1707	369	0
4	CD	1643	0	1707	356	0
5	AE	1105	0	1148	164	0
5	CE	1105	0	1148	126	0
6	AF	817	0	808	119	0
6	CF	817	0	808	113	0
7	AG	1181	0	1238	102	0
7	CG	1181	0	1238	150	0
8	AH	979	0	1031	209	0
8	CH	979	0	1031	127	0
9	AI	1022	0	1070	143	0
9	CI	1022	0	1070	161	0
10	AJ	786	0	828	71	0
10	CJ	786	0	828	89	0
11	AK	877	0	887	145	0
11	CK	877	0	887	203	0
12	AL	955	0	1016	153	0
12	CL	955	0	1016	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	AM	883	0	941	137	0
13	CM	883	0	941	173	0
14	AN	774	0	827	114	0
14	CN	774	0	827	142	0
15	AO	714	0	734	72	0
15	CO	714	0	734	128	0
16	AP	649	0	666	101	0
16	CP	649	0	666	96	0
17	AQ	648	0	691	78	0
17	CQ	648	0	691	97	0
18	AR	455	0	478	67	0
18	CR	455	0	478	65	0
19	AS	637	0	665	116	0
19	CS	637	0	665	130	0
20	AT	665	0	714	125	0
20	CT	665	0	714	103	0
21	AU	425	0	449	95	0
21	CU	425	0	449	88	0
22	AV	1623	0	821	70	0
22	CV	1623	0	821	171	0
23	AX	346	0	173	39	0
23	CX	324	0	162	15	0
24	BA	62195	0	31280	4102	1
24	DA	62195	0	31280	3371	1
25	BB	2529	0	1281	202	0
25	DB	2549	0	1291	111	0
26	BC	2082	0	2157	284	0
26	DC	2082	0	2157	277	0
27	BD	1565	0	1616	178	0
27	DD	1565	0	1616	153	0
28	BE	1552	0	1619	176	0
28	DE	1552	0	1619	153	0
29	BF	1410	0	1447	208	0
29	DF	1410	0	1447	252	0
30	BG	1323	0	1374	137	0
30	DG	1323	0	1374	105	0
31	BH	1110	0	1148	131	1
31	DH	1110	0	1148	237	0
32	BI	1032	0	1088	42	0
32	DI	1032	0	1088	87	0
33	BJ	1129	0	1162	133	0
33	DJ	1129	0	1162	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	BK	938	0	1012	122	0
34	DK	938	0	1012	99	0
35	BL	1045	0	1117	138	0
35	DL	1045	0	1117	115	0
36	BM	1074	0	1157	117	0
36	DM	1074	0	1157	116	0
37	BN	960	0	1000	133	0
37	DN	960	0	1000	98	0
38	BO	892	0	923	147	0
38	DO	892	0	923	123	0
39	BP	917	0	965	102	0
39	DP	917	0	965	72	0
40	BQ	947	0	1022	96	0
40	DQ	947	0	1022	128	0
41	BR	816	0	839	82	0
41	DR	816	0	839	121	0
42	BS	857	0	922	116	0
42	DS	857	0	922	89	0
43	BT	738	0	807	89	0
43	DT	738	0	807	74	0
44	BU	779	0	834	108	0
44	DU	779	0	834	106	0
45	BV	753	0	780	77	0
45	DV	753	0	780	63	1
46	BW	569	0	581	55	0
46	DW	580	0	594	78	0
47	BX	625	0	655	76	0
47	DX	625	0	655	82	0
48	BY	509	0	543	59	0
48	DY	509	0	543	75	0
49	BZ	449	0	491	53	0
49	DZ	449	0	491	32	0
50	B0	444	0	461	43	0
50	D0	444	0	461	39	0
51	B1	409	0	440	50	0
51	D1	409	0	440	38	0
52	B2	377	0	418	52	0
52	D2	377	0	418	40	0
53	B3	504	0	574	66	0
53	D3	504	0	574	69	0
54	B4	302	0	340	33	0
54	D4	302	0	340	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	CY	1423	0	1476	166	0
56	AA	54	0	0	0	0
56	AD	1	0	0	0	0
56	AN	1	0	0	0	0
56	BA	163	0	0	0	0
56	BB	3	0	0	0	0
56	BC	1	0	0	0	0
56	BQ	1	0	0	0	0
56	CA	71	0	0	0	0
56	CX	1	0	0	0	0
56	DA	187	0	0	0	0
56	DB	4	0	0	0	0
56	DE	1	0	0	0	0
56	DL	1	0	0	0	0
56	DO	1	0	0	0	0
57	AA	126	0	135	48	0
57	BA	294	0	317	87	0
57	CA	42	0	46	6	0
57	DA	294	0	311	107	0
58	B4	1	0	0	0	0
58	D4	1	0	0	0	0
59	AA	188	0	0	29	0
59	AD	2	0	0	2	0
59	AK	1	0	0	1	0
59	AN	4	0	0	1	0
59	AT	2	0	0	0	0
59	AU	1	0	0	0	0
59	B0	1	0	0	0	0
59	B3	1	0	0	0	0
59	B4	1	0	0	0	0
59	BA	616	0	0	116	0
59	BB	13	0	0	2	0
59	BC	10	0	0	6	0
59	BD	4	0	0	0	0
59	BL	4	0	0	2	0
59	BN	1	0	0	0	0
59	BT	3	0	0	2	0
59	BU	3	0	0	0	0
59	BV	1	0	0	0	0
59	CA	192	0	0	32	0
59	CC	1	0	0	1	0
59	CE	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	CL	1	0	0	1	0
59	CN	6	0	0	0	0
59	CT	2	0	0	1	0
59	D3	2	0	0	0	0
59	D4	1	0	0	0	0
59	DA	627	0	0	120	0
59	DB	13	0	0	4	0
59	DC	4	0	0	0	0
59	DD	2	0	0	1	0
59	DE	4	0	0	2	0
59	DF	1	0	0	0	0
59	DL	7	0	0	4	0
59	DN	2	0	0	0	0
59	DQ	1	0	0	0	0
59	DS	1	0	0	0	0
59	DT	1	0	0	0	0
59	DU	1	0	0	0	0
59	DV	1	0	0	0	0
All	All	293103	0	196267	22971	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 48.

The worst 5 of 22971 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:BF:96:TRP:CE3	29:BF:99:PHE:CE2	1.79	1.66
29:BF:96:TRP:CZ3	29:BF:99:PHE:HE2	1.31	1.48
31:BH:121:VAL:HB	31:BH:122:LEU:CD2	1.41	1.47
29:BF:96:TRP:CD2	29:BF:99:PHE:CZ	2.03	1.47
31:BH:121:VAL:CB	31:BH:122:LEU:HD23	1.49	1.42

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:BH:123:ARG:NH2	1:CA:358:U:OP1[4_555]	2.07	0.13
24:BA:2152:G:N2	1:CA:416:G:OP1[4_555]	2.15	0.05
24:DA:544:C:OP2	45:DV:34:LYS:NZ[4_545]	2.16	0.04



## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/241 (90%)	106 (49%)	51 (24%)	59 (27%)	0	0
2	CB	216/241 (90%)	110 (51%)	51 (24%)	55 (26%)	0	0
3	AC	204/233 (88%)	124 (61%)	46 (22%)	34 (17%)	0	1
3	CC	204/233 (88%)	122 (60%)	48 (24%)	34 (17%)	0	1
4	AD	203/206 (98%)	100 (49%)	48 (24%)	55 (27%)	0	0
4	CD	203/206 (98%)	92 (45%)	49 (24%)	62 (30%)	0	0
5	AE	148/167 (89%)	86 (58%)	30 (20%)	32 (22%)	0	1
5	CE	148/167 (89%)	106 (72%)	22 (15%)	20 (14%)	0	3
6	AF	98/135 (73%)	53 (54%)	27 (28%)	18 (18%)	0	1
6	CF	98/135 (73%)	47 (48%)	22 (22%)	29 (30%)	0	0
7	AG	149/179 (83%)	92 (62%)	33 (22%)	24 (16%)	0	1
7	CG	149/179 (83%)	65 (44%)	46 (31%)	38 (26%)	0	0
8	AH	127/130 (98%)	62 (49%)	37 (29%)	28 (22%)	0	0
8	CH	127/130 (98%)	80 (63%)	28 (22%)	19 (15%)	0	2
9	AI	125/130 (96%)	60 (48%)	36 (29%)	29 (23%)	0	0
9	CI	125/130 (96%)	61 (49%)	36 (29%)	28 (22%)	0	0
10	AJ	96/103 (93%)	62 (65%)	22 (23%)	12 (12%)	1	4
10	CJ	96/103 (93%)	55 (57%)	21 (22%)	20 (21%)	0	1
11	AK	115/129 (89%)	76 (66%)	19 (16%)	20 (17%)	0	1
11	CK	115/129 (89%)	52 (45%)	40 (35%)	23 (20%)	0	1
12	AL	121/124 (98%)	58 (48%)	28 (23%)	35 (29%)	0	0
12	CL	121/124 (98%)	72 (60%)	26 (22%)	23 (19%)	0	1
13	AM	112/118 (95%)	65 (58%)	19 (17%)	28 (25%)	0	0
13	CM	112/118 (95%)	55 (49%)	22 (20%)	35 (31%)	0	0
14	AN	92/101 (91%)	50 (54%)	21 (23%)	21 (23%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	92/101 (91%)	64 (70%)	11 (12%)	17 (18%)	0	1
15	AO	86/89 (97%)	52 (60%)	20 (23%)	14 (16%)	0	1
15	CO	86/89 (97%)	42 (49%)	23 (27%)	21 (24%)	0	0
16	AP	80/82 (98%)	35 (44%)	27 (34%)	18 (22%)	0	0
16	CP	80/82 (98%)	39 (49%)	23 (29%)	18 (22%)	0	0
17	AQ	78/84 (93%)	40 (51%)	20 (26%)	18 (23%)	0	0
17	CQ	78/84 (93%)	51 (65%)	12 (15%)	15 (19%)	0	1
18	AR	53/75 (71%)	31 (58%)	8 (15%)	14 (26%)	0	0
18	CR	53/75 (71%)	28 (53%)	12 (23%)	13 (24%)	0	0
19	AS	77/92 (84%)	43 (56%)	23 (30%)	11 (14%)	0	2
19	CS	77/92 (84%)	35 (46%)	23 (30%)	19 (25%)	0	0
20	AT	83/87 (95%)	45 (54%)	23 (28%)	15 (18%)	0	1
20	CT	83/87 (95%)	42 (51%)	22 (26%)	19 (23%)	0	0
21	AU	49/71 (69%)	18 (37%)	16 (33%)	15 (31%)	0	0
21	CU	49/71 (69%)	23 (47%)	14 (29%)	12 (24%)	0	0
26	BC	269/273 (98%)	171 (64%)	48 (18%)	50 (19%)	0	1
26	DC	269/273 (98%)	187 (70%)	51 (19%)	31 (12%)	1	5
27	BD	207/209 (99%)	159 (77%)	29 (14%)	19 (9%)	1	9
27	DD	207/209 (99%)	159 (77%)	33 (16%)	15 (7%)	2	16
28	BE	199/201 (99%)	126 (63%)	49 (25%)	24 (12%)	1	4
28	DE	199/201 (99%)	131 (66%)	53 (27%)	15 (8%)	2	15
29	BF	175/179 (98%)	104 (59%)	44 (25%)	27 (15%)	0	1
29	DF	175/179 (98%)	96 (55%)	39 (22%)	40 (23%)	0	0
30	BG	174/177 (98%)	107 (62%)	43 (25%)	24 (14%)	0	2
30	DG	174/177 (98%)	127 (73%)	27 (16%)	20 (12%)	1	5
31	BH	147/149 (99%)	82 (56%)	39 (26%)	26 (18%)	0	1
31	DH	147/149 (99%)	67 (46%)	37 (25%)	43 (29%)	0	0
32	BI	139/142 (98%)	77 (55%)	45 (32%)	17 (12%)	1	4
32	DI	139/142 (98%)	65 (47%)	39 (28%)	35 (25%)	0	0
33	BJ	140/142 (99%)	108 (77%)	19 (14%)	13 (9%)	1	9
33	DJ	140/142 (99%)	110 (79%)	25 (18%)	5 (4%)	5	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	BK	120/123 (98%)	77 (64%)	29 (24%)	14 (12%)	1	5
34	DK	120/123 (98%)	95 (79%)	18 (15%)	7 (6%)	3	23
35	BL	141/144 (98%)	84 (60%)	35 (25%)	22 (16%)	0	1
35	DL	141/144 (98%)	98 (70%)	29 (21%)	14 (10%)	1	8
36	BM	134/136 (98%)	94 (70%)	27 (20%)	13 (10%)	1	8
36	DM	134/136 (98%)	94 (70%)	28 (21%)	12 (9%)	1	10
37	BN	118/127 (93%)	72 (61%)	30 (25%)	16 (14%)	0	3
37	DN	118/127 (93%)	84 (71%)	22 (19%)	12 (10%)	1	7
38	BO	114/117 (97%)	65 (57%)	30 (26%)	19 (17%)	0	1
38	DO	114/117 (97%)	64 (56%)	25 (22%)	25 (22%)	0	0
39	BP	112/115 (97%)	80 (71%)	18 (16%)	14 (12%)	1	4
39	DP	112/115 (97%)	92 (82%)	12 (11%)	8 (7%)	2	17
40	BQ	115/118 (98%)	98 (85%)	13 (11%)	4 (4%)	6	41
40	DQ	115/118 (98%)	89 (77%)	16 (14%)	10 (9%)	1	11
41	BR	101/103 (98%)	76 (75%)	18 (18%)	7 (7%)	2	17
41	DR	101/103 (98%)	67 (66%)	23 (23%)	11 (11%)	1	6
42	BS	108/110 (98%)	68 (63%)	22 (20%)	18 (17%)	0	1
42	DS	108/110 (98%)	77 (71%)	21 (19%)	10 (9%)	1	9
43	BT	91/100 (91%)	54 (59%)	26 (29%)	11 (12%)	1	4
43	DT	91/100 (91%)	60 (66%)	18 (20%)	13 (14%)	0	2
44	BU	100/104 (96%)	55 (55%)	21 (21%)	24 (24%)	0	0
44	DU	100/104 (96%)	73 (73%)	12 (12%)	15 (15%)	0	2
45	BV	92/94 (98%)	50 (54%)	26 (28%)	16 (17%)	0	1
45	DV	92/94 (98%)	79 (86%)	4 (4%)	9 (10%)	1	8
46	BW	73/85 (86%)	56 (77%)	9 (12%)	8 (11%)	1	6
46	DW	74/85 (87%)	51 (69%)	14 (19%)	9 (12%)	1	4
47	BX	75/78 (96%)	55 (73%)	10 (13%)	10 (13%)	0	3
47	DX	75/78 (96%)	51 (68%)	14 (19%)	10 (13%)	0	3
48	BY	61/63 (97%)	38 (62%)	17 (28%)	6 (10%)	1	8
48	DY	61/63 (97%)	31 (51%)	19 (31%)	11 (18%)	0	1
49	BZ	56/59 (95%)	42 (75%)	12 (21%)	2 (4%)	5	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	DZ	56/59 (95%)	37 (66%)	16 (29%)	3 (5%)	3	26
50	B0	54/57 (95%)	34 (63%)	9 (17%)	11 (20%)	0	1
50	D0	54/57 (95%)	36 (67%)	10 (18%)	8 (15%)	0	2
51	B1	48/55 (87%)	29 (60%)	15 (31%)	4 (8%)	1	12
51	D1	48/55 (87%)	28 (58%)	10 (21%)	10 (21%)	0	1
52	B2	44/46 (96%)	29 (66%)	8 (18%)	7 (16%)	0	1
52	D2	44/46 (96%)	31 (70%)	10 (23%)	3 (7%)	2	18
53	B3	62/65 (95%)	47 (76%)	9 (14%)	6 (10%)	1	8
53	D3	62/65 (95%)	47 (76%)	7 (11%)	8 (13%)	0	3
54	B4	36/38 (95%)	27 (75%)	7 (19%)	2 (6%)	3	25
54	D4	36/38 (95%)	26 (72%)	7 (19%)	3 (8%)	1	12
55	CY	181/185 (98%)	99 (55%)	52 (29%)	30 (17%)	0	1
All	All	11416/12155 (94%)	7014 (61%)	2503 (22%)	1899 (17%)	0	1

5 of 1899 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	11	LYS
2	AB	16	PHE
2	AB	23	TRP
2	AB	58	ASN
2	AB	64	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/199 (90%)	128 (71%)	52 (29%)	0	2
2	CB	180/199 (90%)	137 (76%)	43 (24%)	1	4
3	AC	170/190 (90%)	138 (81%)	32 (19%)	2	11
3	CC	170/190 (90%)	130 (76%)	40 (24%)	1	4
4	AD	172/173 (99%)	116 (67%)	56 (33%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	172/173 (99%)	125 (73%)	47 (27%)	0	2
5	AE	113/126 (90%)	91 (80%)	22 (20%)	2	9
5	CE	113/126 (90%)	94 (83%)	19 (17%)	3	16
6	AF	87/116 (75%)	72 (83%)	15 (17%)	3	15
6	CF	87/116 (75%)	65 (75%)	22 (25%)	1	3
7	AG	124/147 (84%)	96 (77%)	28 (23%)	1	5
7	CG	124/147 (84%)	101 (82%)	23 (18%)	2	11
8	AH	104/105 (99%)	81 (78%)	23 (22%)	1	6
8	CH	104/105 (99%)	87 (84%)	17 (16%)	3	17
9	AI	105/107 (98%)	81 (77%)	24 (23%)	1	5
9	CI	105/107 (98%)	84 (80%)	21 (20%)	2	9
10	AJ	86/90 (96%)	73 (85%)	13 (15%)	4	21
10	CJ	86/90 (96%)	67 (78%)	19 (22%)	1	6
11	AK	90/99 (91%)	74 (82%)	16 (18%)	2	13
11	CK	90/99 (91%)	67 (74%)	23 (26%)	1	3
12	AL	103/104 (99%)	69 (67%)	34 (33%)	0	1
12	CL	103/104 (99%)	77 (75%)	26 (25%)	1	3
13	AM	92/96 (96%)	77 (84%)	15 (16%)	3	17
13	CM	92/96 (96%)	63 (68%)	29 (32%)	0	1
14	AN	79/84 (94%)	64 (81%)	15 (19%)	2	11
14	CN	79/84 (94%)	60 (76%)	19 (24%)	1	4
15	AO	76/77 (99%)	55 (72%)	21 (28%)	0	2
15	CO	76/77 (99%)	57 (75%)	19 (25%)	1	3
16	AP	65/65 (100%)	51 (78%)	14 (22%)	1	7
16	CP	65/65 (100%)	41 (63%)	24 (37%)	0	0
17	AQ	74/78 (95%)	59 (80%)	15 (20%)	2	8
17	CQ	74/78 (95%)	54 (73%)	20 (27%)	1	2
18	AR	48/65 (74%)	36 (75%)	12 (25%)	1	3
18	CR	48/65 (74%)	36 (75%)	12 (25%)	1	3
19	AS	70/79 (89%)	53 (76%)	17 (24%)	1	3
19	CS	70/79 (89%)	53 (76%)	17 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AT	65/66 (98%)	50 (77%)	15 (23%)	1	5
20	CT	65/66 (98%)	50 (77%)	15 (23%)	1	5
21	AU	44/61 (72%)	30 (68%)	14 (32%)	0	1
21	CU	44/61 (72%)	29 (66%)	15 (34%)	0	1
26	BC	216/218 (99%)	164 (76%)	52 (24%)	1	4
26	DC	216/218 (99%)	147 (68%)	69 (32%)	0	1
27	BD	164/164 (100%)	131 (80%)	33 (20%)	2	8
27	DD	164/164 (100%)	125 (76%)	39 (24%)	1	4
28	BE	165/165 (100%)	133 (81%)	32 (19%)	2	10
28	DE	165/165 (100%)	130 (79%)	35 (21%)	1	7
29	BF	148/150 (99%)	115 (78%)	33 (22%)	1	6
29	DF	148/150 (99%)	114 (77%)	34 (23%)	1	5
30	BG	137/138 (99%)	108 (79%)	29 (21%)	1	7
30	DG	137/138 (99%)	111 (81%)	26 (19%)	2	11
31	BH	114/114 (100%)	83 (73%)	31 (27%)	0	2
31	DH	114/114 (100%)	92 (81%)	22 (19%)	2	10
32	BI	109/110 (99%)	101 (93%)	8 (7%)	20	63
32	DI	109/110 (99%)	89 (82%)	20 (18%)	2	12
33	BJ	116/116 (100%)	90 (78%)	26 (22%)	1	6
33	DJ	116/116 (100%)	95 (82%)	21 (18%)	2	12
34	BK	103/104 (99%)	81 (79%)	22 (21%)	1	7
34	DK	103/104 (99%)	77 (75%)	26 (25%)	1	3
35	BL	102/103 (99%)	76 (74%)	26 (26%)	1	3
35	DL	102/103 (99%)	74 (72%)	28 (28%)	0	2
36	BM	109/109 (100%)	80 (73%)	29 (27%)	1	2
36	DM	109/109 (100%)	86 (79%)	23 (21%)	1	7
37	BN	100/103 (97%)	81 (81%)	19 (19%)	2	11
37	DN	100/103 (97%)	83 (83%)	17 (17%)	3	15
38	BO	86/87 (99%)	67 (78%)	19 (22%)	1	6
38	DO	86/87 (99%)	61 (71%)	25 (29%)	0	2
39	BP	99/100 (99%)	81 (82%)	18 (18%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	DP	99/100 (99%)	80 (81%)	19 (19%)	2	10
40	BQ	89/90 (99%)	66 (74%)	23 (26%)	1	3
40	DQ	89/90 (99%)	69 (78%)	20 (22%)	1	6
41	BR	84/84 (100%)	66 (79%)	18 (21%)	1	7
41	DR	84/84 (100%)	70 (83%)	14 (17%)	3	16
42	BS	93/93 (100%)	70 (75%)	23 (25%)	1	3
42	DS	93/93 (100%)	68 (73%)	25 (27%)	1	2
43	BT	80/84 (95%)	57 (71%)	23 (29%)	0	2
43	DT	80/84 (95%)	62 (78%)	18 (22%)	1	6
44	BU	83/85 (98%)	61 (74%)	22 (26%)	1	2
44	DU	83/85 (98%)	63 (76%)	20 (24%)	1	4
45	BV	78/78 (100%)	60 (77%)	18 (23%)	1	5
45	DV	78/78 (100%)	63 (81%)	15 (19%)	2	10
46	BW	56/63 (89%)	45 (80%)	11 (20%)	2	9
46	DW	57/63 (90%)	48 (84%)	9 (16%)	4	18
47	BX	67/68 (98%)	47 (70%)	20 (30%)	0	1
47	DX	67/68 (98%)	56 (84%)	11 (16%)	3	16
48	BY	55/55 (100%)	47 (86%)	8 (14%)	5	23
48	DY	55/55 (100%)	43 (78%)	12 (22%)	1	7
49	BZ	48/49 (98%)	40 (83%)	8 (17%)	3	16
49	DZ	48/49 (98%)	42 (88%)	6 (12%)	7	31
50	B0	47/48 (98%)	39 (83%)	8 (17%)	3	15
50	D0	47/48 (98%)	38 (81%)	9 (19%)	2	10
51	B1	45/49 (92%)	39 (87%)	6 (13%)	6	27
51	D1	45/49 (92%)	36 (80%)	9 (20%)	2	9
52	B2	38/38 (100%)	26 (68%)	12 (32%)	0	1
52	D2	38/38 (100%)	33 (87%)	5 (13%)	6	28
53	B3	51/52 (98%)	37 (72%)	14 (28%)	0	2
53	D3	51/52 (98%)	36 (71%)	15 (29%)	0	2
54	B4	34/34 (100%)	27 (79%)	7 (21%)	2	8
54	D4	34/34 (100%)	23 (68%)	11 (32%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	CY	158/160 (99%)	122 (77%)	36 (23%)	<b>1</b> <b>5</b>
All	All	9485/9916 (96%)	7325 (77%)	2160 (23%)	<b>1</b> <b>5</b>

5 of 2160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BX	45	PHE
6	CF	42	TRP
42	DS	4	ILE
50	B0	5	ASN
3	CC	16	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
50	B0	37	HIS
5	CE	121	HIS
40	DQ	43	GLN
51	B1	25	ASN
3	CC	176	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1538/1542 (99%)	503 (32%)	31 (2%)
1	CA	1537/1542 (99%)	498 (32%)	37 (2%)
22	AV	75/76 (98%)	19 (25%)	1 (1%)
22	CV	75/76 (98%)	27 (36%)	6 (8%)
23	AX	15/24 (62%)	7 (46%)	0
23	CX	14/24 (58%)	6 (42%)	1 (7%)
24	BA	2896/2904 (99%)	884 (30%)	70 (2%)
24	DA	2896/2904 (99%)	826 (28%)	71 (2%)
25	BB	117/120 (97%)	29 (24%)	1 (0%)
25	DB	118/120 (98%)	24 (20%)	0
All	All	9281/9332 (99%)	2823 (30%)	218 (2%)

5 of 2823 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	3	A

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Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	8	A
1	AA	9	G

5 of 218 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	2756	U
1	CA	793	U
24	DA	2326	C
24	BA	2849	U
1	CA	251	G

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 510 ligands modelled in this entry, 492 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	NMY	AA	1655	-	45,45,45	0.55	0	67,67,67	0.97	4 (5%)
57	NMY	AA	1656	-	45,45,45	2.14	11 (24%)	67,67,67	1.80	20 (29%)
57	NMY	AA	1657	-	45,45,45	2.18	11 (24%)	67,67,67	1.77	17 (25%)
57	NMY	BA	3161	-	45,45,45	0.50	0	67,67,67	0.99	4 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	NMY	BA	3162	-	45,45,45	0.50	0	67,67,67	1.02	5 (7%)
57	NMY	BA	3163	-	45,45,45	2.18	10 (22%)	67,67,67	2.35	27 (40%)
57	NMY	BA	3164	-	45,45,45	2.12	10 (22%)	67,67,67	2.33	25 (37%)
57	NMY	BA	3165	-	45,45,45	0.51	0	67,67,67	1.08	7 (10%)
57	NMY	BA	3166	-	45,45,45	2.04	10 (22%)	67,67,67	2.35	17 (25%)
57	NMY	BA	3167	-	45,45,45	2.14	11 (24%)	67,67,67	1.86	14 (20%)
57	NMY	CA	1672	-	45,45,45	0.52	0	67,67,67	0.94	3 (4%)
57	NMY	DA	3184	-	45,45,45	0.57	0	67,67,67	1.19	5 (7%)
57	NMY	DA	3185	-	45,45,45	2.18	12 (26%)	67,67,67	1.70	16 (23%)
57	NMY	DA	3186	-	45,45,45	2.22	11 (24%)	67,67,67	2.30	16 (23%)
57	NMY	DA	3187	-	45,45,45	2.16	11 (24%)	67,67,67	1.47	14 (20%)
57	NMY	DA	3188	-	45,45,45	2.08	13 (28%)	67,67,67	1.91	22 (32%)
57	NMY	DA	3189	-	45,45,45	2.08	12 (26%)	67,67,67	2.31	25 (37%)
57	NMY	DA	3190	-	45,45,45	2.13	10 (22%)	67,67,67	2.53	27 (40%)

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
57	NMY	AA	1655	-	-	1/18/94/94	0/4/4/4
57	NMY	AA	1656	-	-	0/18/94/94	0/4/4/4
57	NMY	AA	1657	-	-	1/18/94/94	0/4/4/4
57	NMY	BA	3161	-	-	0/18/94/94	0/4/4/4
57	NMY	BA	3162	-	-	0/18/94/94	0/4/4/4
57	NMY	BA	3163	-	-	0/18/94/94	0/4/4/4
57	NMY	BA	3164	-	-	0/18/94/94	0/4/4/4
57	NMY	BA	3165	-	-	0/18/94/94	0/4/4/4
57	NMY	BA	3166	-	-	0/18/94/94	0/4/4/4
57	NMY	BA	3167	-	-	0/18/94/94	0/4/4/4
57	NMY	CA	1672	-	-	0/18/94/94	0/4/4/4
57	NMY	DA	3184	-	-	0/18/94/94	0/4/4/4
57	NMY	DA	3185	-	-	0/18/94/94	0/4/4/4
57	NMY	DA	3186	-	-	0/18/94/94	0/4/4/4
57	NMY	DA	3187	-	-	0/18/94/94	0/4/4/4
57	NMY	DA	3188	-	-	0/18/94/94	0/4/4/4
57	NMY	DA	3189	-	-	0/18/94/94	0/4/4/4
57	NMY	DA	3190	-	-	1/18/94/94	0/4/4/4



The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	DA	3187	NMY	C20-C19	-9.18	1.40	1.53
57	DA	3186	NMY	C20-C19	-9.02	1.41	1.53
57	AA	1657	NMY	C20-C19	-9.00	1.41	1.53
57	DA	3190	NMY	C20-C19	-8.94	1.41	1.53
57	DA	3185	NMY	C20-C19	-8.90	1.41	1.53

The worst 5 of 268 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	DA	3186	NMY	O11-C13-O16	11.17	122.39	111.57
57	BA	3166	NMY	O11-C13-C14	8.36	122.43	107.50
57	DA	3186	NMY	C8-C7-C12	6.39	119.85	110.13
57	BA	3163	NMY	C8-C7-C12	6.18	119.52	110.13
57	BA	3163	NMY	C1-O1-C10	-6.13	102.42	118.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	AA	1655	NMY	C15-O18-C18-C19
57	DA	3190	NMY	C18-O18-C15-C16
57	AA	1657	NMY	C15-O18-C18-C19

There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1539/1542 (99%)	-0.55	2 (0%) 93 77	67, 121, 207, 543	0
1	CA	1538/1542 (99%)	-0.54	2 (0%) 93 77	63, 120, 240, 527	0
2	AB	218/241 (90%)	0.40	5 (2%) 57 15	86, 172, 404, 542	0
2	CB	218/241 (90%)	0.27	8 (3%) 39 9	96, 215, 508, 545	0
3	AC	206/233 (88%)	0.27	4 (1%) 64 20	81, 139, 325, 514	0
3	CC	206/233 (88%)	0.08	2 (0%) 79 33	80, 120, 286, 513	0
4	AD	205/206 (99%)	0.42	15 (7%) 15 4	83, 161, 372, 537	0
4	CD	205/206 (99%)	0.31	9 (4%) 33 7	81, 148, 442, 537	0
5	AE	150/167 (89%)	-0.00	1 (0%) 84 42	79, 130, 272, 478	0
5	CE	150/167 (89%)	0.22	2 (1%) 74 27	68, 114, 292, 527	0
6	AF	100/135 (74%)	0.02	0 100 100	85, 142, 331, 528	0
6	CF	100/135 (74%)	0.24	4 (4%) 36 8	87, 178, 386, 531	0
7	AG	151/179 (84%)	0.13	3 (1%) 62 19	93, 161, 365, 539	0
7	CG	151/179 (84%)	0.43	10 (6%) 18 4	112, 234, 452, 540	0
8	AH	129/130 (99%)	0.09	0 100 100	79, 145, 341, 424	0
8	CH	129/130 (99%)	0.28	3 (2%) 57 15	81, 121, 307, 437	0
9	AI	127/130 (97%)	0.32	6 (4%) 30 7	101, 180, 459, 535	0
9	CI	127/130 (97%)	0.49	6 (4%) 30 7	97, 216, 478, 540	0
10	AJ	98/103 (95%)	0.42	4 (4%) 35 8	95, 165, 363, 543	0
10	CJ	98/103 (95%)	0.95	15 (15%) 3 1	101, 202, 530, 543	0
11	AK	117/129 (90%)	0.12	1 (0%) 81 37	75, 112, 337, 492	0
11	CK	117/129 (90%)	0.59	5 (4%) 34 8	83, 243, 494, 531	0
12	AL	123/124 (99%)	0.29	1 (0%) 83 39	75, 109, 299, 403	0
12	CL	123/124 (99%)	-0.05	3 (2%) 56 15	62, 93, 294, 386	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/118 (96%)	0.33	5 (4%) 33 7	106, 239, 498, 530	0
13	CM	114/118 (96%)	0.71	11 (9%) 8 2	122, 312, 536, 547	0
14	AN	96/101 (95%)	0.20	0 100 100	89, 175, 381, 527	0
14	CN	96/101 (95%)	0.41	5 (5%) 26 6	95, 183, 535, 545	0
15	AO	88/89 (98%)	0.15	1 (1%) 77 30	90, 136, 315, 374	0
15	CO	88/89 (98%)	0.17	2 (2%) 57 15	94, 176, 350, 510	0
16	AP	82/82 (100%)	0.80	8 (9%) 8 2	76, 125, 380, 528	0
16	CP	82/82 (100%)	0.67	5 (6%) 21 5	75, 115, 387, 524	0
17	AQ	80/84 (95%)	0.58	4 (5%) 28 6	88, 162, 370, 434	0
17	CQ	80/84 (95%)	0.18	0 100 100	75, 141, 337, 496	0
18	AR	55/75 (73%)	0.17	2 (3%) 41 9	84, 115, 320, 391	0
18	CR	55/75 (73%)	0.07	0 100 100	107, 159, 370, 440	0
19	AS	79/92 (85%)	0.78	9 (11%) 6 2	118, 215, 454, 530	0
19	CS	79/92 (85%)	0.96	13 (16%) 2 1	133, 302, 496, 542	0
20	AT	85/87 (97%)	0.18	1 (1%) 75 29	93, 158, 363, 497	0
20	CT	85/87 (97%)	0.46	3 (3%) 42 10	82, 128, 351, 491	0
21	AU	51/71 (71%)	0.18	1 (1%) 62 19	83, 133, 326, 395	0
21	CU	51/71 (71%)	0.29	1 (1%) 62 19	108, 193, 374, 512	0
22	AV	76/76 (100%)	-0.29	1 (1%) 74 27	63, 117, 160, 255	0
22	CV	76/76 (100%)	1.00	15 (19%) 2 1	61, 257, 424, 542	0
23	AX	16/24 (66%)	-0.13	1 (6%) 19 5	76, 139, 214, 261	0
23	CX	15/24 (62%)	0.05	1 (6%) 17 4	83, 191, 269, 339	0
24	BA	2897/2904 (99%)	-0.50	21 (0%) 84 42	54, 96, 294, 544	0
24	DA	2897/2904 (99%)	-0.38	87 (3%) 48 11	37, 67, 231, 547	0
25	BB	118/120 (98%)	-0.83	0 100 100	78, 151, 201, 231	0
25	DB	119/120 (99%)	-0.71	0 100 100	47, 88, 129, 188	0
26	BC	271/273 (99%)	0.15	2 (0%) 84 42	56, 106, 196, 362	0
26	DC	271/273 (99%)	-0.01	0 100 100	46, 81, 188, 348	0
27	BD	209/209 (100%)	0.00	0 100 100	58, 88, 195, 401	0
27	DD	209/209 (100%)	-0.15	0 100 100	38, 57, 129, 253	0
28	BE	201/201 (100%)	0.19	3 (1%) 70 24	59, 105, 224, 424	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DE	201/201 (100%)	-0.05	0 100 100	40, 72, 155, 487	0
29	BF	177/179 (98%)	0.62	12 (6%) 17 4	125, 257, 446, 539	0
29	DF	177/179 (98%)	0.50	6 (3%) 43 10	76, 147, 367, 520	0
30	BG	176/177 (99%)	0.47	6 (3%) 43 10	93, 155, 360, 507	0
30	DG	176/177 (99%)	0.18	4 (2%) 57 15	54, 94, 190, 439	0
31	BH	149/149 (100%)	0.49	10 (6%) 17 4	15, 223, 436, 532	0
31	DH	149/149 (100%)	0.31	6 (4%) 36 8	25, 213, 475, 538	0
32	BI	141/142 (99%)	2.14	72 (51%) 0 0	126, 471, 546, 549	0
32	DI	141/142 (99%)	1.64	50 (35%) 1 0	123, 380, 542, 548	0
33	BJ	142/142 (100%)	0.09	0 100 100	56, 83, 169, 348	0
33	DJ	142/142 (100%)	-0.09	0 100 100	38, 60, 146, 265	0
34	BK	122/123 (99%)	0.24	0 100 100	65, 93, 197, 357	0
34	DK	122/123 (99%)	-0.03	0 100 100	43, 63, 112, 229	0
35	BL	143/144 (99%)	0.02	0 100 100	55, 110, 265, 507	0
35	DL	143/144 (99%)	-0.17	0 100 100	41, 68, 170, 291	0
36	BM	136/136 (100%)	0.42	2 (1%) 70 24	65, 99, 208, 340	0
36	DM	136/136 (100%)	-0.04	0 100 100	47, 67, 153, 262	0
37	BN	120/127 (94%)	0.04	2 (1%) 67 21	66, 107, 190, 466	0
37	DN	120/127 (94%)	-0.07	0 100 100	40, 61, 151, 420	0
38	BO	116/117 (99%)	0.42	2 (1%) 67 21	96, 193, 363, 537	0
38	DO	116/117 (99%)	0.19	0 100 100	66, 94, 183, 322	0
39	BP	114/115 (99%)	0.14	1 (0%) 81 37	71, 109, 288, 356	0
39	DP	114/115 (99%)	-0.11	0 100 100	47, 69, 178, 330	0
40	BQ	117/118 (99%)	-0.05	0 100 100	55, 76, 170, 304	0
40	DQ	117/118 (99%)	-0.24	0 100 100	38, 54, 156, 310	0
41	BR	103/103 (100%)	0.02	1 (0%) 79 33	57, 92, 180, 286	0
41	DR	103/103 (100%)	-0.09	0 100 100	42, 68, 152, 458	0
42	BS	110/110 (100%)	0.05	1 (0%) 81 37	60, 92, 175, 299	0
42	DS	110/110 (100%)	0.00	0 100 100	38, 56, 115, 161	0
43	BT	93/100 (93%)	0.59	5 (5%) 25 6	93, 155, 337, 441	0
43	DT	93/100 (93%)	0.24	0 100 100	56, 90, 192, 530	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BU	102/104 (98%)	0.51	4 (3%) 37 8	78, 133, 337, 443	0
44	DU	102/104 (98%)	-0.12	0 100 100	52, 82, 226, 299	0
45	BV	94/94 (100%)	0.27	0 100 100	86, 144, 310, 421	0
45	DV	94/94 (100%)	0.22	0 100 100	60, 94, 183, 336	0
46	BW	75/85 (88%)	0.30	1 (1%) 74 27	70, 113, 202, 321	0
46	DW	76/85 (89%)	0.09	0 100 100	46, 70, 156, 244	0
47	BX	77/78 (98%)	0.14	0 100 100	62, 110, 268, 318	0
47	DX	77/78 (98%)	0.18	0 100 100	48, 83, 165, 320	0
48	BY	63/63 (100%)	0.32	0 100 100	95, 176, 353, 521	0
48	DY	63/63 (100%)	0.19	1 (1%) 68 22	58, 106, 283, 388	0
49	BZ	58/59 (98%)	0.26	1 (1%) 67 21	67, 93, 170, 515	0
49	DZ	58/59 (98%)	-0.06	0 100 100	44, 59, 141, 198	0
50	B0	56/57 (98%)	-0.04	1 (1%) 65 20	59, 98, 294, 405	0
50	D0	56/57 (98%)	-0.24	0 100 100	33, 64, 166, 282	0
51	B1	50/55 (90%)	1.30	9 (18%) 2 1	88, 147, 326, 377	0
51	D1	50/55 (90%)	0.98	5 (10%) 8 2	78, 120, 326, 532	0
52	B2	46/46 (100%)	0.10	0 100 100	70, 95, 239, 293	0
52	D2	46/46 (100%)	0.09	1 (2%) 59 16	54, 67, 171, 292	0
53	B3	64/65 (98%)	-0.00	0 100 100	67, 91, 201, 286	0
53	D3	64/65 (98%)	-0.05	0 100 100	47, 61, 161, 254	0
54	B4	38/38 (100%)	0.04	0 100 100	78, 108, 174, 322	0
54	D4	38/38 (100%)	0.05	0 100 100	53, 67, 150, 295	0
55	CY	183/185 (98%)	0.17	7 (3%) 38 9	53, 148, 442, 539	0
All	All	20909/21487 (97%)	-0.06	523 (2%) 54 14	15, 110, 357, 549	0

The worst 5 of 523 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	DA	2145	C	11.2
16	AP	47	GLU	9.9
22	CV	71	G	9.7
32	BI	2	LYS	9.5
24	DA	2140	G	9.4



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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	BA	3024	1/1	0.55	831.00	114,114,114,114	0
56	MG	BA	3007	1/1	0.63	344.36	127,127,127,127	0
56	MG	BA	3157	1/1	1.21	293.06	97,97,97,97	0
56	MG	DA	3073	1/1	0.26	251.00	99,99,99,99	0
56	MG	AA	1650	1/1	2.89	196.96	118,118,118,118	0
56	MG	DA	3165	1/1	0.72	152.21	78,78,78,78	0
56	MG	CA	1652	1/1	0.41	149.00	106,106,106,106	0
56	MG	BA	3143	1/1	0.53	142.67	103,103,103,103	0
56	MG	BA	3059	1/1	1.32	126.31	122,122,122,122	0
56	MG	BA	3135	1/1	0.72	110.89	74,74,74,74	0
56	MG	BA	3152	1/1	0.78	105.01	115,115,115,115	0
56	MG	CA	1668	1/1	0.90	98.69	107,107,107,107	0
56	MG	AA	1639	1/1	1.04	92.82	113,113,113,113	0
56	MG	BA	3053	1/1	0.69	89.82	98,98,98,98	0
56	MG	BA	3097	1/1	1.16	87.74	111,111,111,111	0
56	MG	DA	3166	1/1	0.89	86.26	87,87,87,87	0
56	MG	DA	3143	1/1	1.25	85.51	79,79,79,79	0
56	MG	BA	3058	1/1	0.98	84.41	108,108,108,108	0
56	MG	BA	3151	1/1	0.69	83.40	92,92,92,92	0
56	MG	DB	202	1/1	0.71	76.57	122,122,122,122	0
56	MG	BA	3159	1/1	0.71	75.81	109,109,109,109	0
56	MG	CA	1633	1/1	0.81	73.61	116,116,116,116	0
56	MG	DA	3081	1/1	1.17	71.41	110,110,110,110	0
56	MG	DA	3160	1/1	0.89	69.90	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3151	1/1	1.02	68.62	101,101,101,101	0
56	MG	BA	3155	1/1	0.94	68.58	114,114,114,114	0
56	MG	DA	3141	1/1	0.68	66.04	73,73,73,73	0
56	MG	DA	3025	1/1	0.78	63.88	118,118,118,118	0
56	MG	CA	1651	1/1	1.05	63.63	103,103,103,103	0
56	MG	DA	3057	1/1	0.88	61.51	114,114,114,114	0
56	MG	DA	3137	1/1	0.55	59.50	93,93,93,93	0
56	MG	DA	3015	1/1	0.77	59.48	124,124,124,124	0
56	MG	DA	3154	1/1	0.76	57.99	86,86,86,86	0
56	MG	DA	3068	1/1	0.78	57.51	117,117,117,117	0
56	MG	CA	1644	1/1	1.09	57.28	118,118,118,118	0
56	MG	BA	3149	1/1	0.68	56.95	85,85,85,85	0
56	MG	AA	1649	1/1	1.05	56.72	90,90,90,90	0
56	MG	CA	1650	1/1	0.67	56.69	102,102,102,102	0
56	MG	DA	3169	1/1	0.76	56.56	94,94,94,94	0
56	MG	BA	3154	1/1	0.78	56.05	97,97,97,97	0
56	MG	CA	1645	1/1	0.42	55.91	96,96,96,96	0
56	MG	DA	3042	1/1	0.76	55.91	105,105,105,105	0
56	MG	CA	1654	1/1	1.13	53.25	116,116,116,116	0
56	MG	DL	201	1/1	0.84	52.18	110,110,110,110	0
56	MG	DA	3164	1/1	0.72	49.33	94,94,94,94	0
56	MG	DA	3152	1/1	0.83	48.55	105,105,105,105	0
56	MG	CA	1637	1/1	1.04	48.04	139,139,139,139	0
56	MG	BA	3156	1/1	0.74	47.71	106,106,106,106	0
56	MG	CA	1636	1/1	1.03	47.37	134,134,134,134	0
56	MG	BA	3026	1/1	0.86	46.99	134,134,134,134	0
56	MG	CA	1647	1/1	0.62	46.40	112,112,112,112	0
56	MG	AA	1654	1/1	0.70	46.34	110,110,110,110	0
56	MG	CA	1632	1/1	1.14	46.18	128,128,128,128	0
56	MG	CA	1629	1/1	1.02	46.16	123,123,123,123	0
56	MG	DA	3172	1/1	0.62	45.09	109,109,109,109	0
56	MG	CA	1664	1/1	0.29	45.00	112,112,112,112	0
56	MG	BA	3168	1/1	0.92	44.68	114,114,114,114	0
56	MG	CA	1640	1/1	0.87	44.68	114,114,114,114	0
56	MG	DA	3052	1/1	0.60	44.63	95,95,95,95	0
56	MG	DA	3023	1/1	0.60	43.36	120,120,120,120	0
56	MG	CA	1656	1/1	0.60	43.27	106,106,106,106	0
56	MG	BA	3096	1/1	0.84	42.79	118,118,118,118	0
56	MG	CX	101	1/1	1.03	42.70	112,112,112,112	0
56	MG	CA	1642	1/1	0.36	42.44	106,106,106,106	0
56	MG	BA	3014	1/1	0.73	41.83	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	DA	3095	1/1	1.75	40.69	116,116,116,116	0
56	MG	BA	3025	1/1	0.47	40.37	103,103,103,103	0
56	MG	DA	3105	1/1	0.39	39.14	90,90,90,90	0
56	MG	AA	1653	1/1	0.60	38.46	106,106,106,106	0
56	MG	DB	204	1/1	0.86	38.10	109,109,109,109	0
56	MG	AA	1628	1/1	0.38	37.71	116,116,116,116	0
56	MG	AA	1648	1/1	1.21	35.43	116,116,116,116	0
56	MG	BA	3103	1/1	0.89	35.18	105,105,105,105	0
56	MG	DA	3167	1/1	0.74	34.97	84,84,84,84	0
56	MG	DA	3058	1/1	0.41	34.66	96,96,96,96	0
56	MG	BA	3107	1/1	0.45	34.40	106,106,106,106	0
56	MG	DA	3113	1/1	0.52	33.80	106,106,106,106	0
56	MG	DA	3150	1/1	0.64	33.64	78,78,78,78	0
56	MG	BA	3060	1/1	0.53	33.59	106,106,106,106	0
56	MG	DA	3159	1/1	0.63	33.27	90,90,90,90	0
56	MG	BA	3037	1/1	0.76	32.74	97,97,97,97	0
56	MG	BA	3069	1/1	0.45	32.71	129,129,129,129	0
56	MG	BA	3054	1/1	1.66	32.45	119,119,119,119	0
56	MG	DA	3179	1/1	0.45	32.38	113,113,113,113	0
56	MG	BA	3032	1/1	0.64	31.99	110,110,110,110	0
56	MG	BA	3158	1/1	0.60	31.54	106,106,106,106	0
56	MG	CA	1653	1/1	0.54	31.07	99,99,99,99	0
56	MG	DA	3163	1/1	0.24	30.71	99,99,99,99	0
56	MG	AA	1625	1/1	0.82	30.67	117,117,117,117	0
56	MG	DA	3175	1/1	0.72	30.58	75,75,75,75	0
56	MG	AA	1631	1/1	0.59	30.11	126,126,126,126	0
56	MG	CA	1665	1/1	0.43	29.97	112,112,112,112	0
56	MG	CA	1663	1/1	0.43	29.84	82,82,82,82	0
56	MG	DA	3103	1/1	0.35	29.72	81,81,81,81	0
56	MG	DA	3129	1/1	1.80	29.70	124,124,124,124	0
56	MG	BA	3013	1/1	0.52	29.45	114,114,114,114	0
56	MG	BA	3150	1/1	0.60	28.28	95,95,95,95	0
56	MG	DA	3192	1/1	0.47	28.17	95,95,95,95	0
56	MG	BA	3104	1/1	0.56	28.14	106,106,106,106	0
56	MG	DA	3170	1/1	0.46	27.94	94,94,94,94	0
56	MG	DA	3138	1/1	0.74	27.71	81,81,81,81	0
56	MG	BQ	201	1/1	1.37	26.86	93,93,93,93	0
56	MG	AD	301	1/1	0.80	26.83	119,119,119,119	0
56	MG	CA	1643	1/1	0.43	26.80	103,103,103,103	0
56	MG	BA	3012	1/1	1.00	26.69	118,118,118,118	0
56	MG	BA	3139	1/1	0.79	26.66	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	DA	3102	1/1	0.61	26.06	94,94,94,94	0
56	MG	AA	1638	1/1	0.78	26.00	104,104,104,104	0
56	MG	BA	3062	1/1	0.48	26.00	91,91,91,91	0
56	MG	DA	3061	1/1	0.64	25.75	106,106,106,106	0
56	MG	BA	3087	1/1	0.57	25.44	112,112,112,112	0
56	MG	CA	1670	1/1	0.70	25.06	102,102,102,102	0
56	MG	BA	3129	1/1	0.63	25.06	107,107,107,107	0
56	MG	BA	3102	1/1	0.57	24.98	119,119,119,119	0
56	MG	BA	3147	1/1	0.58	24.82	95,95,95,95	0
56	MG	CA	1618	1/1	0.38	24.81	83,83,83,83	0
56	MG	AA	1626	1/1	0.58	24.70	111,111,111,111	0
56	MG	BA	3123	1/1	0.48	24.47	88,88,88,88	0
56	MG	BA	3142	1/1	0.55	24.16	103,103,103,103	0
56	MG	DA	3147	1/1	0.78	23.92	107,107,107,107	0
56	MG	DA	3176	1/1	0.56	23.85	78,78,78,78	0
56	MG	DA	3026	1/1	0.55	23.55	98,98,98,98	0
56	MG	CA	1608	1/1	0.37	23.27	115,115,115,115	0
56	MG	AA	1616	1/1	0.43	23.05	113,113,113,113	0
56	MG	BA	3079	1/1	0.62	22.53	103,103,103,103	0
56	MG	CA	1602	1/1	0.47	22.52	105,105,105,105	0
56	MG	DA	3071	1/1	0.42	22.36	97,97,97,97	0
56	MG	DA	3085	1/1	0.45	22.25	108,108,108,108	0
56	MG	BA	3160	1/1	0.51	22.21	102,102,102,102	0
56	MG	BA	3093	1/1	0.54	22.06	109,109,109,109	0
56	MG	DA	3055	1/1	0.33	21.82	94,94,94,94	0
56	MG	DA	3072	1/1	0.37	21.76	93,93,93,93	0
56	MG	DA	3144	1/1	0.19	21.75	108,108,108,108	0
56	MG	CA	1628	1/1	0.37	21.68	116,116,116,116	0
56	MG	DA	3174	1/1	0.62	21.49	105,105,105,105	0
56	MG	CA	1661	1/1	0.77	21.45	101,101,101,101	0
56	MG	CA	1660	1/1	0.51	21.03	104,104,104,104	0
56	MG	DA	3018	1/1	0.74	20.86	102,102,102,102	0
56	MG	CA	1612	1/1	0.36	20.74	116,116,116,116	0
56	MG	CA	1659	1/1	0.61	20.72	110,110,110,110	0
56	MG	DA	3180	1/1	0.41	20.65	93,93,93,93	0
56	MG	AA	1610	1/1	0.27	20.57	120,120,120,120	0
56	MG	DA	3079	1/1	0.51	20.36	99,99,99,99	0
56	MG	CA	1638	1/1	0.72	20.32	113,113,113,113	0
56	MG	DA	3177	1/1	0.54	20.30	96,96,96,96	0
56	MG	BA	3027	1/1	1.45	20.16	108,108,108,108	0
56	MG	DA	3161	1/1	0.31	20.05	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	CA	1623	1/1	0.71	20.01	117,117,117,117	0
56	MG	CA	1609	1/1	0.39	19.86	117,117,117,117	0
56	MG	DA	3093	1/1	0.61	19.73	105,105,105,105	0
56	MG	CA	1607	1/1	0.51	19.68	110,110,110,110	0
56	MG	BA	3050	1/1	0.34	19.31	101,101,101,101	0
56	MG	CA	1667	1/1	0.53	19.22	111,111,111,111	0
56	MG	DA	3077	1/1	0.38	19.19	98,98,98,98	0
56	MG	DA	3139	1/1	0.55	19.16	77,77,77,77	0
56	MG	DA	3136	1/1	0.57	18.76	74,74,74,74	0
56	MG	BA	3101	1/1	0.57	18.62	102,102,102,102	0
56	MG	BA	3068	1/1	0.21	18.50	126,126,126,126	0
56	MG	CA	1648	1/1	0.43	18.43	103,103,103,103	0
56	MG	DA	3193	1/1	0.53	18.28	95,95,95,95	0
56	MG	BA	3148	1/1	0.48	18.11	101,101,101,101	0
56	MG	DA	3064	1/1	0.32	17.95	95,95,95,95	0
56	MG	BA	3144	1/1	0.46	17.93	87,87,87,87	0
56	MG	DA	3183	1/1	0.49	17.91	87,87,87,87	0
56	MG	DA	3013	1/1	0.47	17.88	107,107,107,107	0
56	MG	BA	3082	1/1	0.39	17.78	126,126,126,126	0
56	MG	DA	3182	1/1	0.48	17.51	96,96,96,96	0
56	MG	DA	3075	1/1	0.40	17.47	106,106,106,106	0
56	MG	CA	1603	1/1	0.24	17.46	120,120,120,120	0
56	MG	BA	3127	1/1	0.37	17.39	95,95,95,95	0
56	MG	BA	3138	1/1	0.69	17.35	88,88,88,88	0
56	MG	AA	1617	1/1	0.47	17.22	112,112,112,112	0
56	MG	BA	3008	1/1	0.28	16.91	107,107,107,107	0
56	MG	AA	1636	1/1	0.34	16.89	103,103,103,103	0
56	MG	BA	3118	1/1	0.47	16.77	109,109,109,109	0
56	MG	BA	3136	1/1	0.58	16.45	94,94,94,94	0
56	MG	BA	3145	1/1	0.48	16.14	99,99,99,99	0
56	MG	DA	3156	1/1	0.40	16.12	101,101,101,101	0
56	MG	AA	1602	1/1	0.49	16.10	106,106,106,106	0
56	MG	BA	3133	1/1	0.32	16.04	106,106,106,106	0
56	MG	AA	1622	1/1	0.36	15.90	107,107,107,107	0
56	MG	CA	1617	1/1	0.38	15.84	115,115,115,115	0
56	MG	DA	3044	1/1	0.39	15.70	105,105,105,105	0
56	MG	DA	3107	1/1	0.45	15.30	98,98,98,98	0
56	MG	AA	1614	1/1	0.51	15.17	123,123,123,123	0
56	MG	DA	3011	1/1	0.51	15.05	103,103,103,103	0
56	MG	CA	1626	1/1	0.37	15.01	99,99,99,99	0
56	MG	BA	3018	1/1	0.75	14.77	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	DA	3080	1/1	0.26	14.74	100,100,100,100	0
56	MG	AA	1640	1/1	0.51	14.42	110,110,110,110	0
56	MG	BA	3071	1/1	0.30	14.36	104,104,104,104	0
56	MG	DA	3016	1/1	0.23	14.27	103,103,103,103	0
56	MG	BA	3153	1/1	0.51	14.25	112,112,112,112	0
56	MG	BA	3131	1/1	0.47	14.07	114,114,114,114	0
56	MG	BA	3110	1/1	0.44	14.01	110,110,110,110	0
57	NMY	DA	3190	42/42	0.38	13.99	57,66,70,74	42
56	MG	CA	1605	1/1	0.15	13.93	97,97,97,97	0
56	MG	BA	3137	1/1	0.40	13.90	82,82,82,82	0
56	MG	BA	3109	1/1	0.42	13.84	106,106,106,106	0
56	MG	DA	3059	1/1	0.44	13.78	92,92,92,92	0
56	MG	DA	3171	1/1	0.36	13.77	108,108,108,108	0
56	MG	BA	3125	1/1	0.43	13.71	100,100,100,100	0
56	MG	DA	3146	1/1	0.36	13.70	76,76,76,76	0
56	MG	BA	3112	1/1	0.36	13.59	101,101,101,101	0
56	MG	DA	3054	1/1	0.30	13.45	93,93,93,93	0
56	MG	AA	1609	1/1	0.37	13.44	111,111,111,111	0
56	MG	BA	3115	1/1	0.28	13.26	105,105,105,105	0
56	MG	BA	3100	1/1	0.37	13.24	107,107,107,107	0
56	MG	DA	3094	1/1	0.34	13.21	87,87,87,87	0
56	MG	AA	1624	1/1	0.38	13.13	110,110,110,110	0
56	MG	BA	3033	1/1	0.50	13.01	98,98,98,98	0
56	MG	BA	3011	1/1	0.45	12.94	81,81,81,81	0
56	MG	AA	1634	1/1	0.45	12.91	120,120,120,120	0
56	MG	AA	1629	1/1	0.64	12.90	118,118,118,118	0
56	MG	DA	3007	1/1	0.22	12.55	103,103,103,103	0
56	MG	DA	3106	1/1	0.47	12.55	100,100,100,100	0
56	MG	DA	3145	1/1	0.41	12.53	91,91,91,91	0
56	MG	BA	3077	1/1	0.44	12.49	121,121,121,121	0
56	MG	DA	3157	1/1	0.40	12.46	96,96,96,96	0
56	MG	DA	3049	1/1	0.31	12.42	97,97,97,97	0
56	MG	AA	1646	1/1	0.60	12.41	95,95,95,95	0
56	MG	DA	3004	1/1	0.39	12.37	99,99,99,99	0
56	MG	BA	3061	1/1	0.27	12.34	85,85,85,85	0
56	MG	DA	3149	1/1	0.33	12.26	107,107,107,107	0
56	MG	AA	1620	1/1	0.23	12.10	118,118,118,118	0
56	MG	BA	3044	1/1	0.34	11.98	114,114,114,114	0
56	MG	DA	3134	1/1	0.35	11.95	77,77,77,77	0
56	MG	BA	3081	1/1	0.34	11.81	109,109,109,109	0
56	MG	BA	3023	1/1	0.34	11.75	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BB	201	1/1	0.20	11.57	137,137,137,137	0
56	MG	DA	3065	1/1	0.26	11.56	81,81,81,81	0
56	MG	AA	1651	1/1	0.19	11.39	119,119,119,119	0
56	MG	BA	3022	1/1	0.63	11.33	110,110,110,110	0
56	MG	CA	1655	1/1	0.33	11.27	117,117,117,117	0
56	MG	BA	3121	1/1	0.41	11.25	110,110,110,110	0
56	MG	BA	3020	1/1	0.27	11.24	95,95,95,95	0
56	MG	DB	203	1/1	0.27	11.14	100,100,100,100	0
56	MG	DA	3050	1/1	0.26	11.10	86,86,86,86	0
56	MG	DA	3173	1/1	0.45	11.09	90,90,90,90	0
56	MG	DA	3131	1/1	0.69	11.09	118,118,118,118	0
56	MG	DA	3060	1/1	0.28	11.03	89,89,89,89	0
56	MG	BA	3126	1/1	0.26	11.02	110,110,110,110	0
56	MG	DA	3101	1/1	0.36	10.90	86,86,86,86	0
56	MG	DA	3087	1/1	0.29	10.85	113,113,113,113	0
56	MG	DA	3010	1/1	0.33	10.79	106,106,106,106	0
56	MG	BA	3063	1/1	0.61	10.69	106,106,106,106	0
56	MG	BA	3072	1/1	0.29	10.64	103,103,103,103	0
56	MG	BA	3091	1/1	0.32	10.43	115,115,115,115	0
56	MG	BA	3074	1/1	0.33	10.39	115,115,115,115	0
56	MG	DO	201	1/1	0.53	10.18	109,109,109,109	0
56	MG	CA	1631	1/1	0.48	10.09	120,120,120,120	0
56	MG	DA	3051	1/1	0.26	9.85	86,86,86,86	0
56	MG	DA	3009	1/1	0.37	9.79	102,102,102,102	0
56	MG	AA	1621	1/1	0.44	9.76	116,116,116,116	0
56	MG	BA	3047	1/1	0.30	9.64	103,103,103,103	0
56	MG	AA	1645	1/1	0.28	9.54	93,93,93,93	0
56	MG	DA	3109	1/1	0.26	9.52	102,102,102,102	0
56	MG	BB	202	1/1	0.61	9.51	123,123,123,123	0
57	NMY	BA	3164	42/42	0.29	9.47	90,100,104,105	42
56	MG	AA	1613	1/1	0.24	9.47	115,115,115,115	0
56	MG	BA	3075	1/1	0.37	9.46	104,104,104,104	0
56	MG	BA	3146	1/1	0.35	9.44	98,98,98,98	0
56	MG	DA	3032	1/1	0.50	9.23	97,97,97,97	0
56	MG	DA	3116	1/1	0.21	9.08	107,107,107,107	0
56	MG	AA	1633	1/1	0.33	9.06	128,128,128,128	0
56	MG	DA	3084	1/1	0.23	8.98	104,104,104,104	0
56	MG	BA	3030	1/1	0.33	8.94	94,94,94,94	0
56	MG	AA	1606	1/1	0.30	8.91	111,111,111,111	0
56	MG	AA	1605	1/1	0.34	8.85	121,121,121,121	0
56	MG	DA	3098	1/1	0.25	8.79	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3083	1/1	0.32	8.70	82,82,82,82	0
57	NMY	AA	1656	42/42	0.27	8.65	94,99,103,104	42
56	MG	DA	3067	1/1	0.34	8.65	120,120,120,120	0
56	MG	AA	1652	1/1	0.38	8.57	101,101,101,101	0
56	MG	BA	3005	1/1	0.25	8.55	106,106,106,106	0
56	MG	BA	3083	1/1	0.27	8.53	110,110,110,110	0
56	MG	BA	3049	1/1	0.25	8.47	88,88,88,88	0
57	NMY	DA	3187	42/42	0.31	8.38	106,109,112,114	42
56	MG	DA	3006	1/1	0.20	8.36	92,92,92,92	0
56	MG	DA	3092	1/1	0.33	8.35	95,95,95,95	0
56	MG	DA	3031	1/1	0.28	8.20	108,108,108,108	0
56	MG	AA	1608	1/1	0.39	8.20	114,114,114,114	0
56	MG	BA	3070	1/1	0.33	8.12	90,90,90,90	0
56	MG	BA	3051	1/1	0.34	8.00	106,106,106,106	0
56	MG	DA	3076	1/1	0.25	7.96	100,100,100,100	0
56	MG	DA	3096	1/1	0.24	7.94	75,75,75,75	0
56	MG	DA	3029	1/1	0.25	7.91	84,84,84,84	0
56	MG	DA	3162	1/1	0.36	7.90	95,95,95,95	0
56	MG	BA	3095	1/1	0.33	7.86	107,107,107,107	0
56	MG	CA	1611	1/1	0.17	7.85	110,110,110,110	0
56	MG	BA	3028	1/1	0.32	7.75	89,89,89,89	0
56	MG	AN	201	1/1	0.63	7.74	133,133,133,133	0
56	MG	BA	3031	1/1	0.23	7.73	87,87,87,87	0
56	MG	DA	3127	1/1	0.31	7.62	77,77,77,77	0
56	MG	AA	1630	1/1	0.30	7.57	105,105,105,105	0
56	MG	BA	3066	1/1	0.23	7.56	96,96,96,96	0
56	MG	DA	3100	1/1	0.42	7.52	96,96,96,96	0
56	MG	BC	301	1/1	0.75	7.43	122,122,122,122	0
56	MG	BA	3090	1/1	0.64	7.40	130,130,130,130	0
56	MG	BA	3098	1/1	0.33	7.32	100,100,100,100	0
56	MG	DA	3121	1/1	0.29	7.27	86,86,86,86	0
56	MG	CA	1646	1/1	0.32	7.18	95,95,95,95	0
56	MG	DA	3038	1/1	0.25	7.15	81,81,81,81	0
56	MG	DA	3024	1/1	0.23	7.04	73,73,73,73	0
56	MG	DA	3158	1/1	0.28	6.93	91,91,91,91	0
57	NMY	BA	3163	42/42	0.30	6.82	89,98,100,101	42
56	MG	CA	1624	1/1	0.27	6.80	106,106,106,106	0
57	NMY	AA	1657	42/42	0.28	6.71	81,84,88,90	42
56	MG	DA	3135	1/1	0.22	6.65	71,71,71,71	0
56	MG	CA	1634	1/1	0.25	6.58	120,120,120,120	0
56	MG	DA	3048	1/1	0.29	6.55	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	BA	3094	1/1	0.23	6.53	92,92,92,92	0
56	MG	AA	1627	1/1	0.54	6.53	121,121,121,121	0
56	MG	BA	3169	1/1	0.26	6.52	101,101,101,101	0
56	MG	BA	3106	1/1	0.36	6.52	100,100,100,100	0
56	MG	DA	3069	1/1	0.28	6.45	81,81,81,81	0
56	MG	CA	1625	1/1	0.20	6.44	107,107,107,107	0
56	MG	DA	3194	1/1	0.56	6.40	90,90,90,90	0
56	MG	DA	3140	1/1	0.33	6.37	98,98,98,98	0
57	NMY	BA	3167	42/42	0.29	6.25	117,120,124,125	42
56	MG	DA	3108	1/1	0.28	6.20	100,100,100,100	0
56	MG	CA	1622	1/1	0.30	6.18	108,108,108,108	0
56	MG	DA	3020	1/1	0.26	6.13	93,93,93,93	0
56	MG	CA	1627	1/1	0.35	5.95	111,111,111,111	0
56	MG	AA	1635	1/1	0.27	5.80	105,105,105,105	0
56	MG	BA	3065	1/1	0.29	5.78	101,101,101,101	0
56	MG	BA	3122	1/1	0.32	5.74	112,112,112,112	0
56	MG	DA	3122	1/1	0.27	5.71	97,97,97,97	0
56	MG	DA	3019	1/1	0.30	5.66	78,78,78,78	0
56	MG	BA	3105	1/1	0.29	5.58	91,91,91,91	0
56	MG	BA	3003	1/1	0.21	5.57	115,115,115,115	0
56	MG	DA	3142	1/1	0.19	5.52	86,86,86,86	0
56	MG	BA	3170	1/1	0.40	5.43	88,88,88,88	0
56	MG	DA	3008	1/1	0.25	5.41	88,88,88,88	0
56	MG	DA	3097	1/1	0.55	5.38	105,105,105,105	0
56	MG	CA	1666	1/1	0.23	5.26	112,112,112,112	0
56	MG	BA	3021	1/1	0.25	5.26	108,108,108,108	0
56	MG	BA	3108	1/1	0.30	5.21	99,99,99,99	0
56	MG	DA	3181	1/1	0.40	5.20	77,77,77,77	0
56	MG	DA	3088	1/1	0.18	5.18	115,115,115,115	0
56	MG	DA	3091	1/1	0.19	5.16	104,104,104,104	0
56	MG	BA	3111	1/1	0.24	5.15	98,98,98,98	0
56	MG	BA	3134	1/1	0.26	5.13	109,109,109,109	0
56	MG	BA	3088	1/1	0.28	5.09	101,101,101,101	0
56	MG	DA	3090	1/1	0.23	5.07	107,107,107,107	0
56	MG	BA	3113	1/1	0.43	5.06	121,121,121,121	0
56	MG	AA	1644	1/1	0.41	4.99	106,106,106,106	0
56	MG	AA	1642	1/1	0.23	4.96	94,94,94,94	0
56	MG	DA	3120	1/1	0.24	4.93	98,98,98,98	0
56	MG	AA	1643	1/1	0.19	4.84	110,110,110,110	0
57	NMY	DA	3185	42/42	0.22	4.83	46,58,63,67	42
56	MG	BA	3015	1/1	0.26	4.82	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	CA	1613	1/1	0.17	4.79	103,103,103,103	0
56	MG	DA	3130	1/1	0.24	4.78	96,96,96,96	0
56	MG	CA	1669	1/1	0.35	4.68	107,107,107,107	0
56	MG	BA	3009	1/1	0.29	4.61	95,95,95,95	0
56	MG	DA	3123	1/1	0.27	4.60	102,102,102,102	0
56	MG	DA	3021	1/1	0.35	4.53	108,108,108,108	0
57	NMY	BA	3165	42/42	0.30	4.50	79,84,87,90	42
56	MG	BA	3078	1/1	0.22	4.47	119,119,119,119	0
57	NMY	BA	3162	42/42	0.27	4.46	65,79,86,93	42
56	MG	DA	3111	1/1	0.44	4.43	102,102,102,102	0
56	MG	BA	3119	1/1	0.19	4.40	106,106,106,106	0
56	MG	DA	3022	1/1	0.28	4.40	81,81,81,81	0
56	MG	BA	3130	1/1	0.61	4.40	103,103,103,103	0
56	MG	DA	3036	1/1	0.28	4.35	90,90,90,90	0
57	NMY	BA	3161	42/42	0.25	4.27	61,70,77,82	42
56	MG	DA	3124	1/1	0.25	4.13	78,78,78,78	0
57	NMY	CA	1672	42/42	0.24	4.07	54,65,74,77	42
56	MG	DA	3168	1/1	0.21	4.05	89,89,89,89	0
56	MG	DA	3035	1/1	0.24	3.99	94,94,94,94	0
56	MG	BA	3120	1/1	0.25	3.98	94,94,94,94	0
56	MG	DA	3014	1/1	0.21	3.98	90,90,90,90	0
56	MG	AA	1603	1/1	0.22	3.92	117,117,117,117	0
56	MG	DA	3148	1/1	0.36	3.76	60,60,60,60	0
57	NMY	DA	3186	42/42	0.25	3.74	53,58,64,71	42
56	MG	BA	3092	1/1	0.24	3.73	119,119,119,119	0
56	MG	DB	201	1/1	0.22	3.69	113,113,113,113	0
56	MG	DA	3017	1/1	0.24	3.63	76,76,76,76	0
56	MG	DA	3012	1/1	0.26	3.61	83,83,83,83	0
56	MG	DA	3119	1/1	0.23	3.58	82,82,82,82	0
56	MG	DA	3118	1/1	0.26	3.54	88,88,88,88	0
56	MG	CA	1615	1/1	0.18	3.46	112,112,112,112	0
56	MG	BA	3019	1/1	0.22	3.43	101,101,101,101	0
56	MG	BA	3116	1/1	0.18	3.39	99,99,99,99	0
56	MG	DA	3070	1/1	0.22	3.35	56,56,56,56	0
56	MG	DA	3110	1/1	0.26	3.29	93,93,93,93	0
56	MG	DA	3082	1/1	0.25	3.29	92,92,92,92	0
56	MG	DA	3155	1/1	0.25	3.21	115,115,115,115	0
56	MG	CA	1671	1/1	0.27	3.18	96,96,96,96	0
57	NMY	DA	3189	42/42	0.22	3.13	55,63,70,72	42
56	MG	DA	3066	1/1	0.21	3.12	90,90,90,90	0
56	MG	CA	1620	1/1	0.19	3.10	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3037	1/1	0.25	3.07	72,72,72,72	0
56	MG	DA	3178	1/1	0.23	3.04	88,88,88,88	0
56	MG	DA	3125	1/1	0.19	3.00	113,113,113,113	0
56	MG	BA	3055	1/1	0.21	2.97	101,101,101,101	0
56	MG	CA	1641	1/1	0.22	2.91	85,85,85,85	0
56	MG	CA	1614	1/1	0.18	2.89	120,120,120,120	0
57	NMY	DA	3184	42/42	0.26	2.80	57,71,80,89	42
56	MG	DA	3104	1/1	0.20	2.76	81,81,81,81	0
56	MG	DA	3028	1/1	0.31	2.70	85,85,85,85	0
56	MG	CA	1601	1/1	0.45	2.63	140,140,140,140	0
56	MG	AA	1647	1/1	0.27	2.58	109,109,109,109	0
56	MG	BA	3038	1/1	0.21	2.31	104,104,104,104	0
56	MG	CA	1658	1/1	0.44	2.26	115,115,115,115	0
56	MG	BA	3124	1/1	0.20	2.18	114,114,114,114	0
56	MG	AA	1601	1/1	0.39	2.16	132,132,132,132	0
56	MG	AA	1618	1/1	0.26	2.12	96,96,96,96	0
56	MG	BA	3099	1/1	0.38	2.12	112,112,112,112	0
56	MG	AA	1623	1/1	1.08	2.12	119,119,119,119	0
56	MG	BA	3004	1/1	0.19	2.10	120,120,120,120	0
56	MG	BA	3056	1/1	0.17	2.10	99,99,99,99	0
56	MG	DA	3078	1/1	0.19	2.07	84,84,84,84	0
56	MG	DA	3114	1/1	0.18	2.01	77,77,77,77	0
56	MG	BA	3089	1/1	0.18	2.01	109,109,109,109	0
58	ZN	D4	101	1/1	0.47	1.98	162,162,162,162	0
56	MG	AA	1637	1/1	0.24	1.94	103,103,103,103	0
56	MG	DA	3030	1/1	0.19	1.94	76,76,76,76	0
56	MG	CA	1610	1/1	0.23	1.90	102,102,102,102	0
56	MG	DA	3153	1/1	0.19	1.75	95,95,95,95	0
56	MG	BA	3076	1/1	0.36	1.73	120,120,120,120	0
56	MG	DA	3115	1/1	0.17	1.72	95,95,95,95	0
56	MG	CA	1606	1/1	0.15	1.70	99,99,99,99	0
56	MG	BA	3040	1/1	0.24	1.59	112,112,112,112	0
56	MG	BA	3064	1/1	0.16	1.56	96,96,96,96	0
56	MG	AA	1641	1/1	0.42	1.55	105,105,105,105	0
56	MG	BA	3114	1/1	0.29	1.36	120,120,120,120	0
57	NMY	BA	3166	42/42	0.24	1.36	68,77,83,90	42
56	MG	BA	3141	1/1	0.13	1.20	114,114,114,114	0
56	MG	AA	1619	1/1	0.18	1.18	95,95,95,95	0
56	MG	BA	3029	1/1	0.22	1.14	99,99,99,99	0
56	MG	BA	3034	1/1	0.17	1.10	88,88,88,88	0
56	MG	DA	3047	1/1	0.19	1.01	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
57	NMY	DA	3188	42/42	0.19	1.01	45,60,66,70	42
56	MG	DA	3133	1/1	0.25	0.99	100,100,100,100	0
56	MG	BA	3052	1/1	0.21	0.96	97,97,97,97	0
56	MG	BA	3046	1/1	0.18	0.95	109,109,109,109	0
56	MG	AA	1607	1/1	0.22	0.95	116,116,116,116	0
56	MG	DA	3040	1/1	0.18	0.94	91,91,91,91	0
57	NMY	AA	1655	42/42	0.20	0.91	61,73,90,121	0
56	MG	DA	3112	1/1	0.24	0.89	108,108,108,108	0
56	MG	DA	3056	1/1	0.16	0.87	86,86,86,86	0
56	MG	BB	203	1/1	0.12	0.87	107,107,107,107	0
56	MG	BA	3017	1/1	0.14	0.85	107,107,107,107	0
56	MG	BA	3057	1/1	0.17	0.85	98,98,98,98	0
56	MG	DA	3117	1/1	0.18	0.84	93,93,93,93	0
56	MG	AA	1632	1/1	0.17	0.83	114,114,114,114	0
56	MG	CA	1616	1/1	0.14	0.80	98,98,98,98	0
56	MG	DA	3039	1/1	0.32	0.79	117,117,117,117	0
56	MG	BA	3043	1/1	0.18	0.79	108,108,108,108	0
56	MG	BA	3140	1/1	0.18	0.79	101,101,101,101	0
56	MG	CA	1621	1/1	0.16	0.59	111,111,111,111	0
56	MG	DA	3034	1/1	0.17	0.40	84,84,84,84	0
56	MG	DA	3003	1/1	0.15	0.35	105,105,105,105	0
56	MG	DA	3053	1/1	0.18	0.33	93,93,93,93	0
56	MG	BA	3132	1/1	0.19	0.33	96,96,96,96	0
56	MG	DA	3045	1/1	0.13	0.32	95,95,95,95	0
56	MG	BA	3001	1/1	0.16	0.28	99,99,99,99	0
56	MG	DA	3005	1/1	0.14	0.22	88,88,88,88	0
56	MG	BA	3041	1/1	0.15	0.19	96,96,96,96	0
56	MG	BA	3002	1/1	0.15	0.14	89,89,89,89	0
56	MG	BA	3045	1/1	0.17	0.13	118,118,118,118	0
56	MG	AA	1615	1/1	0.13	0.10	112,112,112,112	0
56	MG	DA	3062	1/1	0.18	0.06	76,76,76,76	0
56	MG	DA	3099	1/1	0.17	0.05	90,90,90,90	0
56	MG	BA	3016	1/1	0.16	0.04	83,83,83,83	0
56	MG	BA	3084	1/1	0.19	0.04	95,95,95,95	0
58	ZN	B4	101	1/1	0.24	0.02	186,186,186,186	0
56	MG	BA	3085	1/1	0.15	0.02	95,95,95,95	0
56	MG	AA	1612	1/1	0.14	-0.06	107,107,107,107	0
56	MG	DA	3043	1/1	0.14	-0.08	90,90,90,90	0
56	MG	BA	3035	1/1	0.16	-0.09	94,94,94,94	0
56	MG	CA	1630	1/1	0.21	-0.12	118,118,118,118	0
56	MG	DA	3128	1/1	0.17	-0.14	92,92,92,92	0
56	MG	DA	3074	1/1	0.13	-0.29	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	BA	3117	1/1	0.15	-0.32	89,89,89,89	0
56	MG	DE	301	1/1	0.12	-0.39	100,100,100,100	0
56	MG	BA	3036	1/1	0.15	-0.40	95,95,95,95	0
56	MG	CA	1635	1/1	0.16	-0.42	113,113,113,113	0
56	MG	DA	3001	1/1	0.12	-0.57	91,91,91,91	0
56	MG	CA	1662	1/1	0.15	-0.67	114,114,114,114	0
56	MG	BA	3006	1/1	0.10	-0.71	101,101,101,101	0
56	MG	BA	3039	1/1	0.15	-0.73	96,96,96,96	0
56	MG	CA	1639	1/1	0.11	-0.76	94,94,94,94	0
56	MG	DA	3089	1/1	0.09	-1.01	97,97,97,97	0
56	MG	BA	3073	1/1	0.14	-1.01	101,101,101,101	0
56	MG	DA	3046	1/1	0.15	-1.10	86,86,86,86	0
56	MG	DA	3027	1/1	0.15	-1.10	79,79,79,79	0
56	MG	DA	3041	1/1	0.12	-1.29	81,81,81,81	0
56	MG	DA	3033	1/1	0.14	-1.33	91,91,91,91	0
56	MG	DA	3132	1/1	0.14	-1.51	96,96,96,96	0
56	MG	BA	3086	1/1	0.11	-2.05	109,109,109,109	0
56	MG	DA	3191	1/1	0.14	-2.35	80,80,80,80	0
56	MG	AA	1604	1/1	0.12	-2.37	102,102,102,102	0
56	MG	BA	3042	1/1	0.09	-2.44	97,97,97,97	0
56	MG	CA	1619	1/1	0.14	-2.50	93,93,93,93	0
56	MG	BA	3080	1/1	0.15	-2.98	73,73,73,73	0
56	MG	BA	3128	1/1	0.12	-3.05	94,94,94,94	0
56	MG	BA	3048	1/1	0.09	-3.13	93,93,93,93	0
56	MG	BA	3010	1/1	0.12	-3.40	85,85,85,85	0
56	MG	DA	3063	1/1	0.09	-3.42	69,69,69,69	0
56	MG	DA	3086	1/1	0.10	-3.81	97,97,97,97	0
56	MG	AA	1611	1/1	0.07	-4.45	104,104,104,104	0
56	MG	CA	1604	1/1	0.11	-5.14	86,86,86,86	0
56	MG	DA	3126	1/1	0.15	-5.16	60,60,60,60	0
56	MG	DA	3002	1/1	0.08	-5.67	86,86,86,86	0
56	MG	BA	3067	1/1	0.10	-6.43	89,89,89,89	0
56	MG	CA	1649	1/1	1.19	-	107,107,107,107	0
56	MG	CA	1657	1/1	1.33	-	119,119,119,119	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.