



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 05:23 am BST

PDB ID : 4V97  
Title : Crystal structure of the bacterial ribosome ram mutation G299A.  
Authors : Fagan, C.E.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.  
Deposited on : 2012-04-06  
Resolution : 3.52 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11



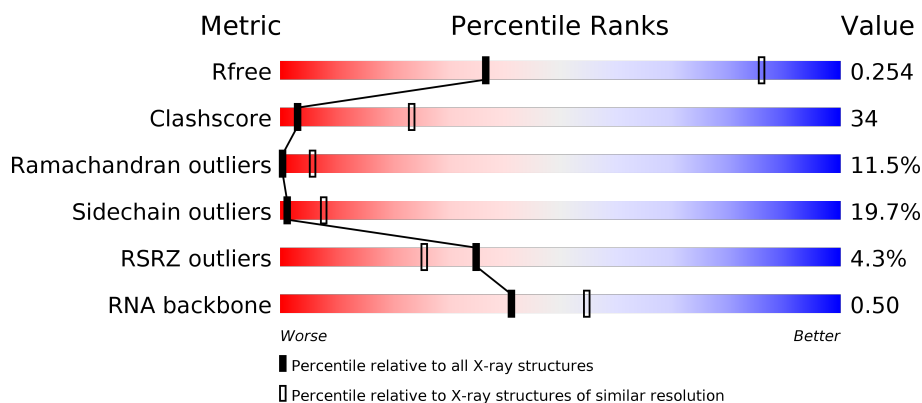
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.52 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)
RNA backbone	3102	1003 (4.02-3.00)


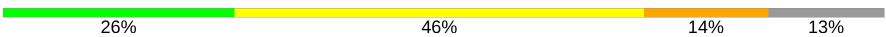
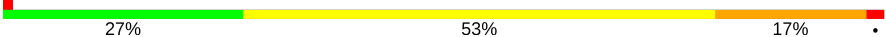

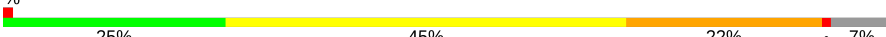
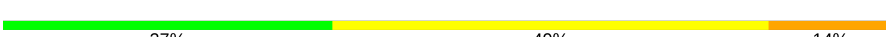
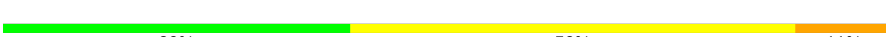
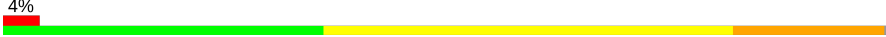
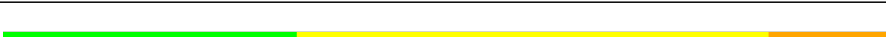

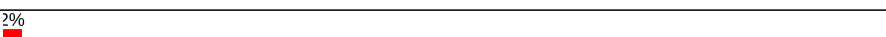




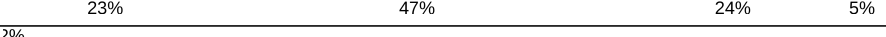
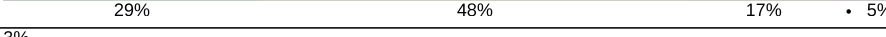
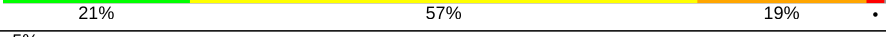
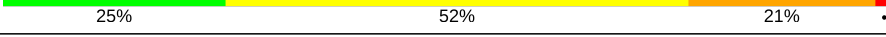

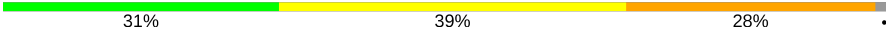
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

Mol	Chain	Length	Quality of chain
1	AA	1522	 3% 49% 35% 15%
1	CA	1522	 4% 49% 33% 16%
2	AB	256	 2% 21% 50% 19% 8%
2	CB	256	 4% 18% 50% 22% 8%

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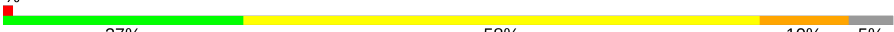
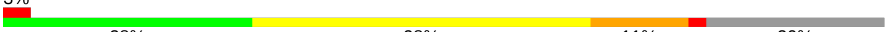
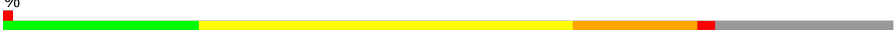







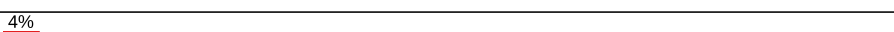

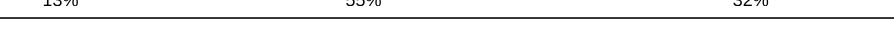

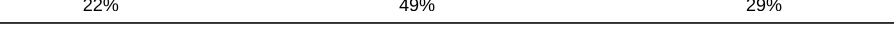






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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	CV	77	
23	AW	76	
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	24	
24	CX	24	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	

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Mol	Chain	Length	Quality of chain
27	BC	229	
27	DC	229	
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	

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Mol	Chain	Length	Quality of chain
39	DS	112	
40	BT	146	
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	71	
51	D4	71	

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Mol	Chain	Length	Quality of chain
52	B5	60	
52	D5	60	
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	
56	B9	37	
56	D9	37	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	7002	-	-	-	X
57	MG	AA	7027	-	-	-	X
57	MG	AA	7046	-	-	-	X
57	MG	AA	7055	-	-	-	X
57	MG	AA	7069	-	-	-	X
57	MG	AA	7071	-	-	-	X
57	MG	AA	7074	-	-	-	X
57	MG	AA	7076	-	-	-	X
57	MG	AA	7080	-	-	-	X
57	MG	AA	7086	-	-	-	X
57	MG	AA	7097	-	-	-	X
57	MG	BA	3021	-	-	-	X
57	MG	BA	3026	-	-	-	X
57	MG	BA	3028	-	-	-	X
57	MG	BA	3052	-	-	-	X
57	MG	BA	3063	-	-	-	X
57	MG	BA	3074	-	-	-	X
57	MG	BA	3095	-	-	-	X
57	MG	BA	3107	-	-	-	X
57	MG	BA	3110	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3117	-	-	-	X
57	MG	BA	3120	-	-	-	X
57	MG	BA	3126	-	-	-	X
57	MG	BA	3155	-	-	-	X
57	MG	BA	3164	-	-	-	X
57	MG	BA	3173	-	-	-	X
57	MG	BA	3196	-	-	-	X
57	MG	BA	3203	-	-	-	X
57	MG	BA	3216	-	-	-	X
57	MG	BA	3227	-	-	-	X
57	MG	BA	3242	-	-	-	X
57	MG	BA	3245	-	-	-	X
57	MG	BA	3246	-	-	-	X
57	MG	BA	3248	-	-	-	X
57	MG	BA	3262	-	-	-	X
57	MG	BA	3271	-	-	-	X
57	MG	BA	3277	-	-	-	X
57	MG	BA	3278	-	-	-	X
57	MG	BA	3290	-	-	-	X
57	MG	BA	3297	-	-	-	X
57	MG	BA	3306	-	-	-	X
57	MG	BA	3315	-	-	-	X
57	MG	BA	3317	-	-	-	X
57	MG	BA	3318	-	-	-	X
57	MG	BA	3320	-	-	-	X
57	MG	BB	203	-	-	-	X
57	MG	CA	1609	-	-	-	X
57	MG	CA	1610	-	-	-	X
57	MG	CA	1639	-	-	-	X
57	MG	CA	1651	-	-	-	X
57	MG	CA	1674	-	-	-	X
57	MG	CA	1691	-	-	-	X
57	MG	CA	1694	-	-	-	X
57	MG	CA	1704	-	-	-	X
57	MG	CA	1708	-	-	-	X
57	MG	CA	1713	-	-	-	X
57	MG	CA	1714	-	-	-	X
57	MG	CA	1716	-	-	-	X
57	MG	CA	1739	-	-	-	X
57	MG	D1	101	-	-	-	X
57	MG	DA	9329	-	-	-	X
57	MG	DA	9399	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	9429	-	-	-	X
57	MG	DA	9432	-	-	-	X
57	MG	DA	9434	-	-	-	X
57	MG	DA	9440	-	-	-	X
57	MG	DA	9441	-	-	-	X
57	MG	DA	9450	-	-	-	X
57	MG	DA	9458	-	-	-	X
57	MG	DA	9550	-	-	-	X
57	MG	DA	9552	-	-	-	X
57	MG	DA	9559	-	-	-	X
57	MG	DA	9569	-	-	-	X
57	MG	DA	9573	-	-	-	X
57	MG	DA	9595	-	-	-	X
57	MG	DA	9602	-	-	-	X
57	MG	DA	9603	-	-	-	X
57	MG	DA	9615	-	-	-	X
57	MG	DA	9620	-	-	-	X
57	MG	DA	9622	-	-	-	X
57	MG	DA	9643	-	-	-	X
57	MG	DA	9645	-	-	-	X
57	MG	DA	9655	-	-	-	X
57	MG	DA	9665	-	-	-	X
57	MG	DA	9674	-	-	-	X
57	MG	DA	9677	-	-	-	X
57	MG	DA	9685	-	-	-	X
57	MG	DA	9694	-	-	-	X
59	ZN	CN	101	-	-	X	-



## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 293977 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32328	14390	5992	10443	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32328	14390	5992	10443	1503			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	299	A	G	ENGINEERED MUTATION	GB AP008226.1
CA	299	A	G	ENGINEERED MUTATION	GB AP008226.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1010	639	197	174			
9	CI	127	Total	C	N	O	0	0	0
			1010	639	197	174			



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- 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
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- 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	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called P-SITE tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	CV	77	Total	C	N	O	P	0	0	0
			1643	732	297	537	77			

- Molecule 23 is a RNA chain called E-SITE TRNA PHE OR A-SITE tRNA Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	AY	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
23	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	CY	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	12	Total	C	N	O	P	0	0	0
			255	115	46	82	12			
24	CX	10	Total	C	N	O	P	0	0	0
			210	96	39	66	9			

- Molecule 25 is a RNA chain called 23S rRNA.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2810	Total	C	N	O	P	0	0	0
			60527	26937	11326	19455	2809			
25	DA	2824	Total	C	N	O	P	0	0	0
			60827	27071	11381	19552	2823			

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
26	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BC	191	Total	C	N	O		0	0	1
			1142	691	221	230				
27	DC	191	Total	C	N	O		0	0	1
			1142	691	221	230				

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
28	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
29	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
31	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
32	DH	168	Total	C	N	O	S	0	0	0
			1290	820	240	229	1			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
33	DI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
34	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L14.

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



- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
36	DP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	117	Total	C	N	O		0	0	0
			960	599	202	159				
38	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				
39	DS	111	Total	C	N	O		0	0	0
			882	556	176	150				

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
40	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L20.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
41	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
42	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
43	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BX	93	Total	C	N	O		0	0	1
			726	471	132	123				
44	DX	93	Total	C	N	O		0	0	1
			726	471	132	123				

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
45	DY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

*Continued on next page...*



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
47	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
48	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
49	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
50	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
51	D4	40	Total	C	N	O	S	0	0	1
			298	189	50	54	5			



- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
52	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			
53	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
54	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
55	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
56	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	BA	323	Total Mg 323 323	0	0
57	CA	141	Total Mg 141 141	0	0
57	DQ	1	Total Mg 1 1	0	0
57	DF	1	Total Mg 1 1	0	0
57	CV	5	Total Mg 5 5	0	0
57	D2	1	Total Mg 1 1	0	0
57	BE	3	Total Mg 3 3	0	0
57	DU	3	Total Mg 3 3	0	0
57	BP	1	Total Mg 1 1	0	0
57	AX	1	Total Mg 1 1	0	0
57	CY	1	Total Mg 1 1	0	0
57	DD	3	Total Mg 3 3	0	0
57	B5	1	Total Mg 1 1	0	0
57	BB	5	Total Mg 5 5	0	0
57	AE	1	Total Mg 1 1	0	0
57	BF	1	Total Mg 1 1	0	0
57	AV	5	Total Mg 5 5	0	0
57	D8	1	Total Mg 1 1	0	0
57	AA	110	Total Mg 110 110	0	0
57	CX	1	Total Mg 1 1	0	0
57	BU	1	Total Mg 1 1	0	0
57	BN	1	Total Mg 1 1	0	0

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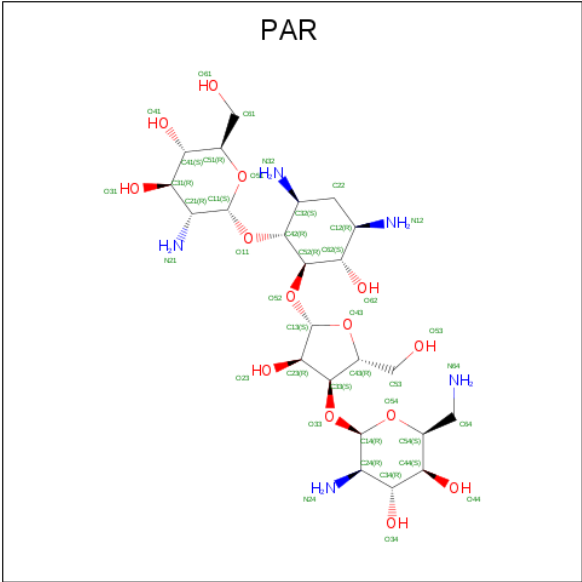


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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	D0	2	Total 2	Mg 2	0	0
57	DE	2	Total 2	Mg 2	0	0
57	DX	1	Total 1	Mg 1	0	0
57	DA	397	Total 397	Mg 397	0	0
57	DW	1	Total 1	Mg 1	0	0
57	B7	1	Total 1	Mg 1	0	0
57	BO	1	Total 1	Mg 1	0	0
57	D1	2	Total 2	Mg 2	0	0
57	DP	3	Total 3	Mg 3	0	0
57	CW	1	Total 1	Mg 1	0	0
57	D5	2	Total 2	Mg 2	0	0
57	BD	2	Total 2	Mg 2	0	0
57	CE	2	Total 2	Mg 2	0	0
57	DB	5	Total 5	Mg 5	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	AA	1	Total	C	N	O	0	0
			42	23	5	14		
58	CA	1	Total	C	N	O	0	0
			42	23	5	14		

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

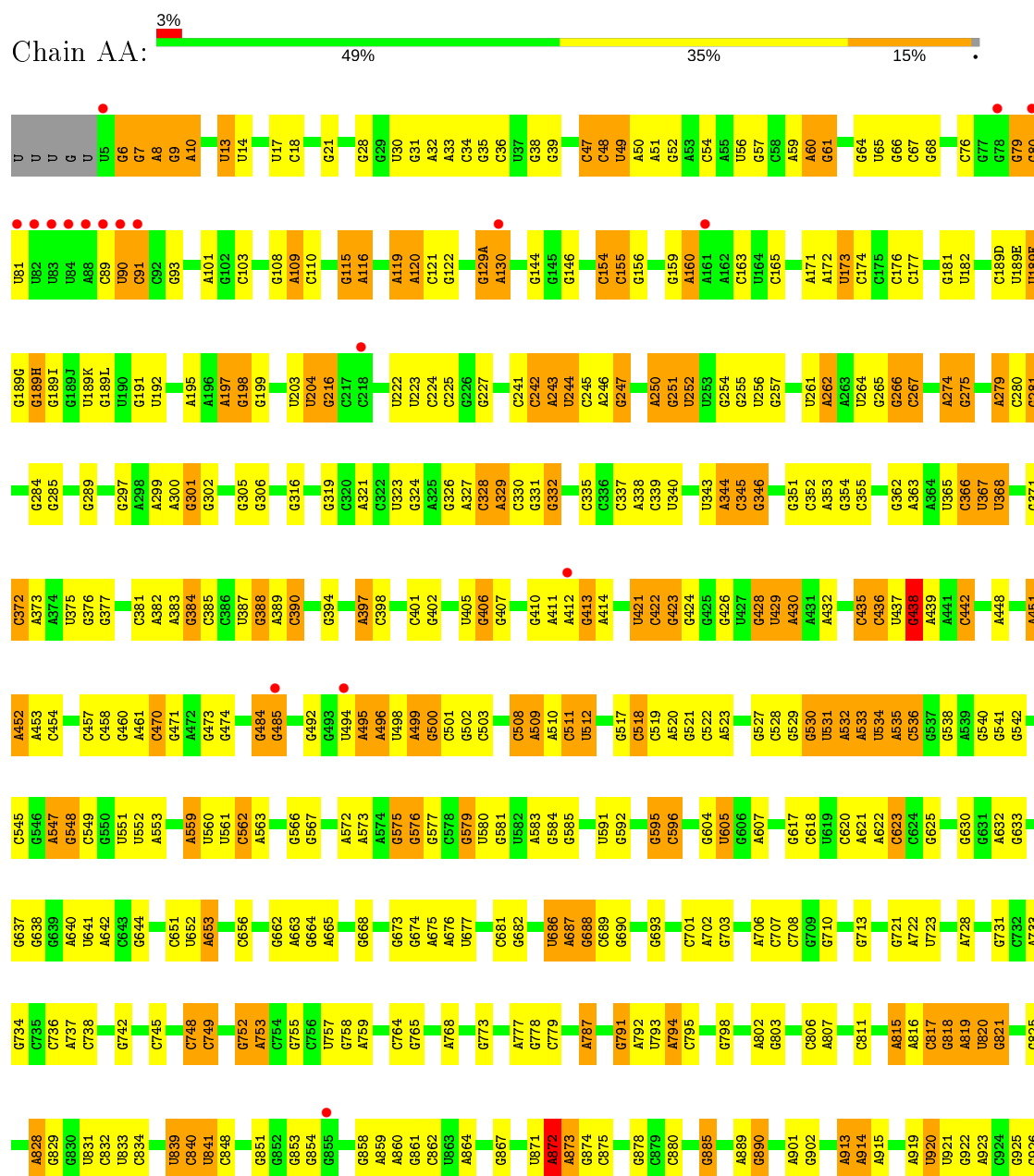
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CN	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		



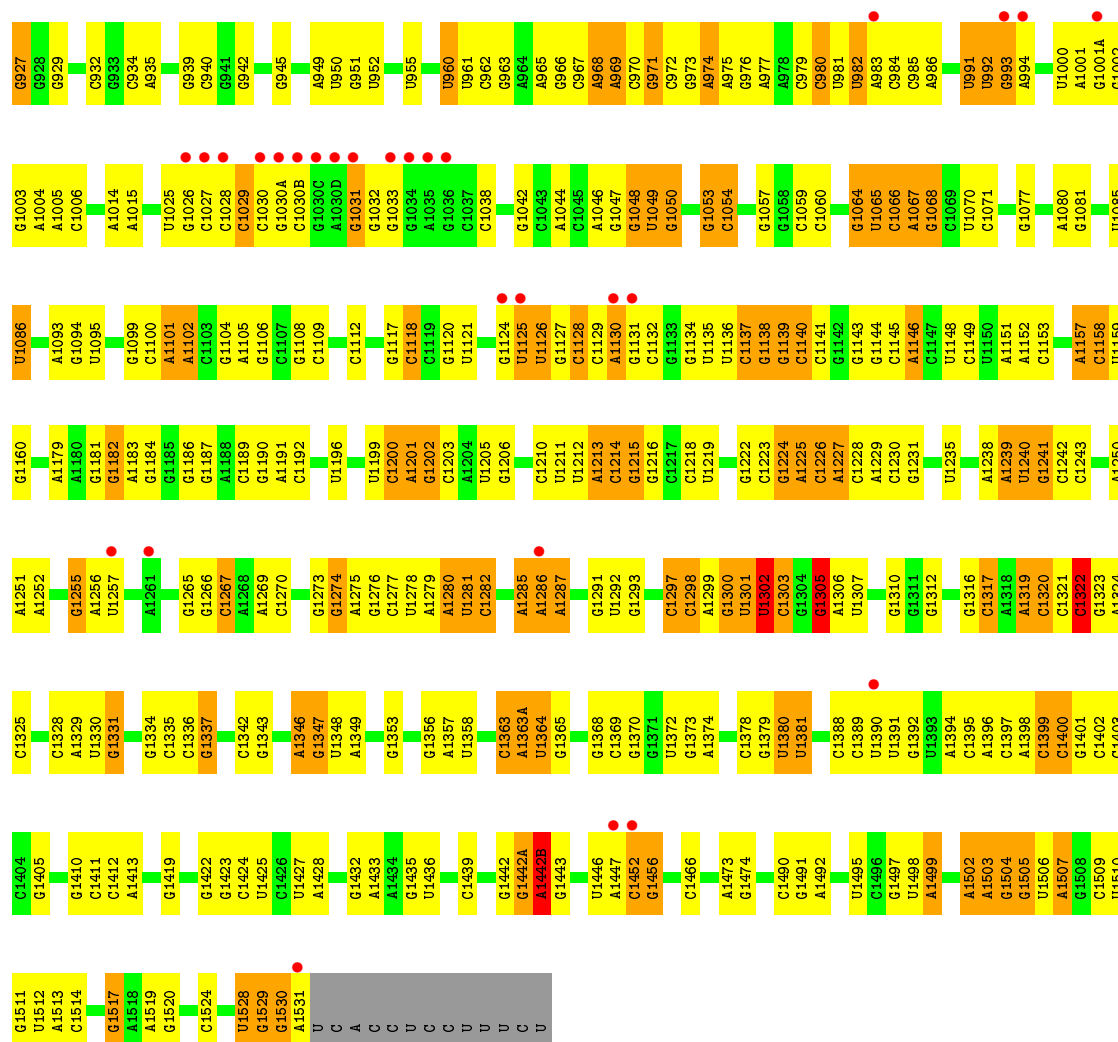
### 3 Residue-property plots [i](#)

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

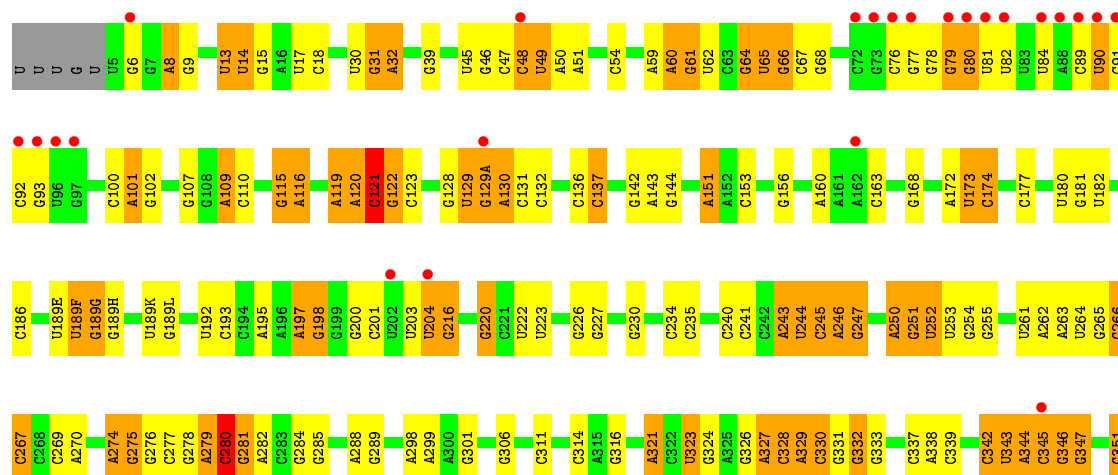
#### • Molecule 1: 16S rRNA







● Molecule 1: 16S rRNA

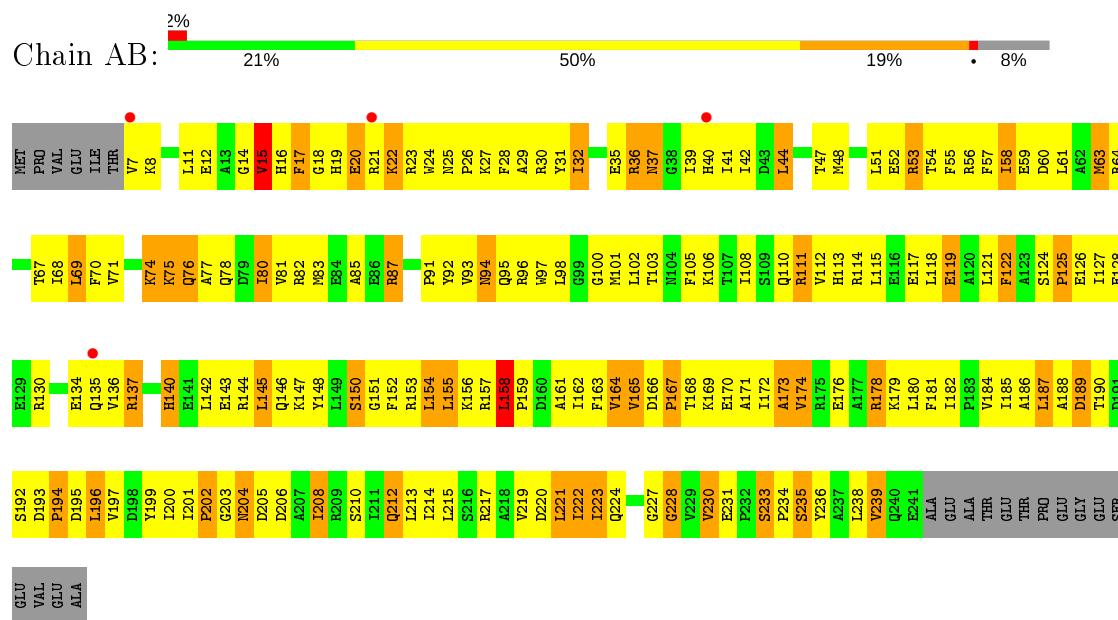




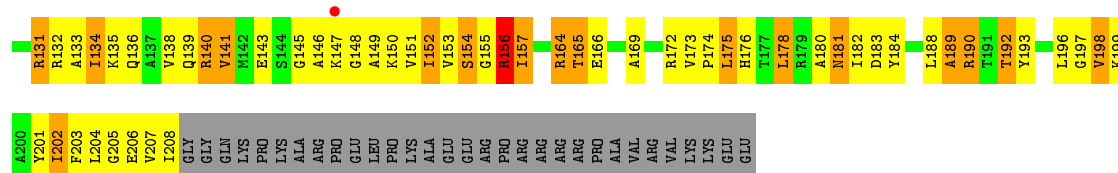




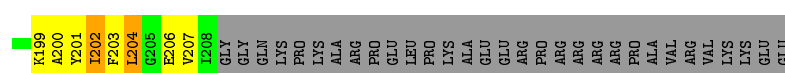
- Molecule 2: 30S ribosomal protein S2



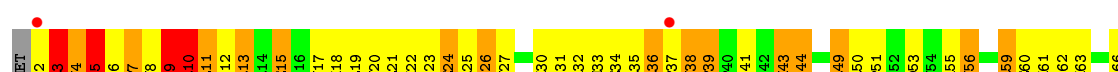




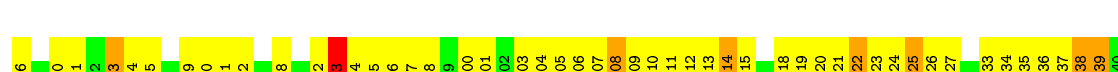
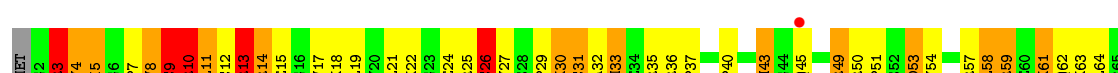
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4



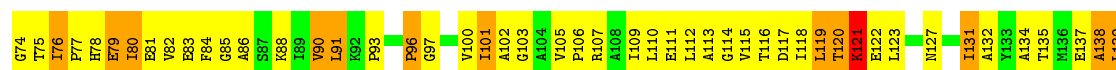
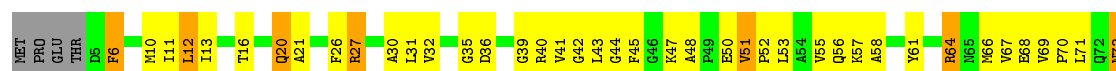
• Molecule 4: 30S ribosomal protein S4



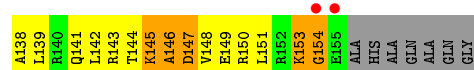
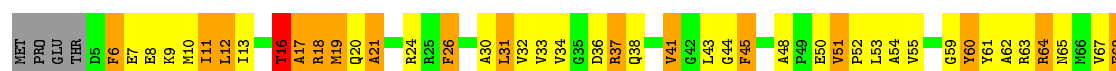




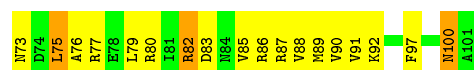
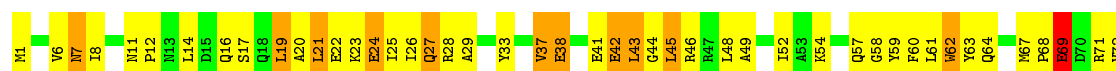
• Molecule 5: 30S ribosomal protein S5



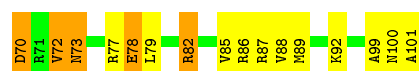
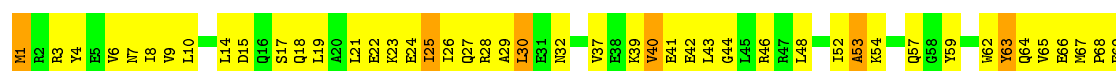
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

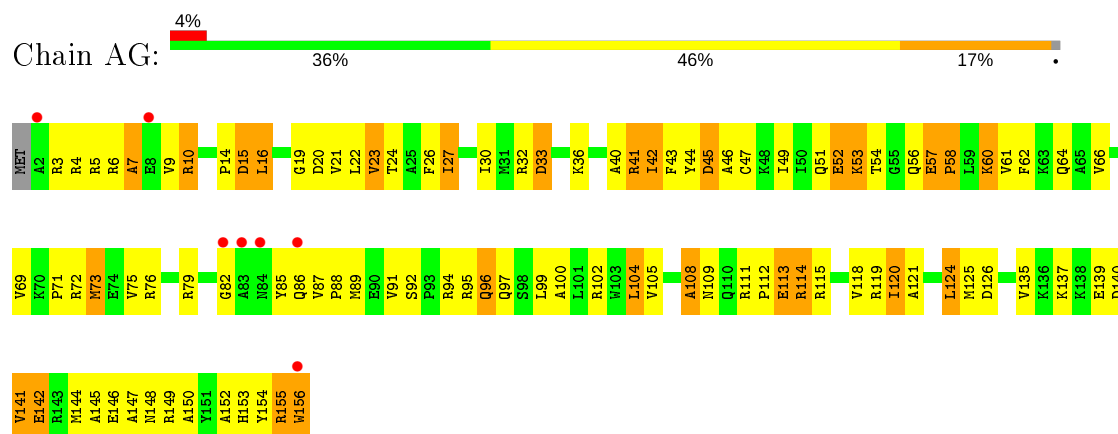


• Molecule 6: 30S ribosomal protein S6

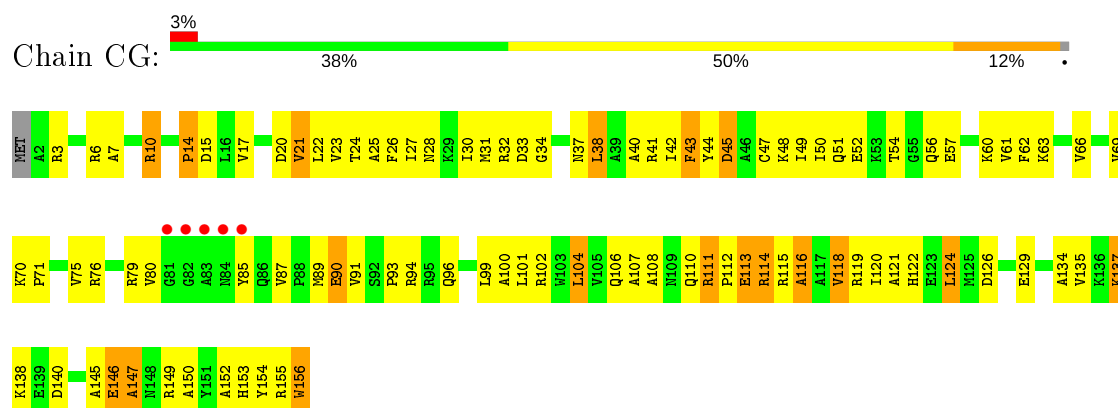




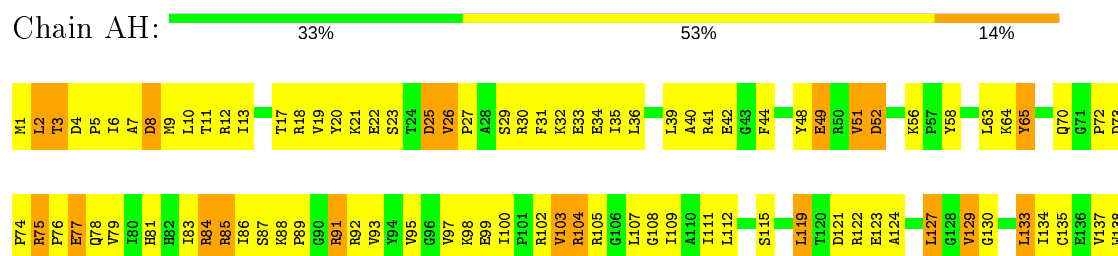
- Molecule 7: 30S ribosomal protein S7



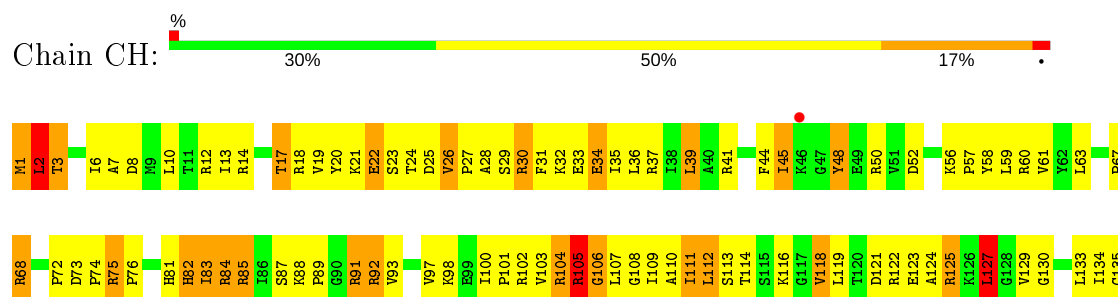
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8





E436  
V137  
W138

• Molecule 9: 30S ribosomal protein S9

Chain AI: 2% 28% 53% 14% . .

MET E2 Q3 Y4 Y5 Y6 Y7 Y8 Y9 K10 K11 K12 K13 K14 K15 K16 K17 K18 K19 K20 K21 K25 K26 K27 K28 K29 K30 K31 K32 K33 K34 K35 K36 K37 K38 K39 K40 K41 K42 K43 K44 K45 K46 K47 K48 K49 K50 K51 K52 K53 K54 K55 K56 K57 K58 K59 K60 K61 K62

I63 I64 I65 K70 K71 K72 K73 K74 K75 K76 K77 K78 K79 K80 K81 K82 K83 K84 K85 K86 K87 K88 K89 K90 K91 K92 K93 K94 K95 K96 K97 K98 K99 K100 K101 K102 K103 K104 K105 K106 K107 K108 K109 K110 K111 K112 K113 K114 K115 K116 K117 K118 K119 K120 K121 K122 K123 K124 K125 K126 K127 K128

• Molecule 9: 30S ribosomal protein S9

Chain CI: 2% 21% 55% 21% . .

MET E2 Q3 Y4 Y5 Y6 Y7 Y8 Y9 K10 K11 K12 K13 K14 K15 K16 K17 K18 K19 K20 K21 K25 K26 K27 K28 K29 K30 K31 K32 K33 K34 K35 K36 K37 K38 K39 K40 K41 K42 K43 K44 K45 K46 K47 K48 K49 K50 K51 K52 K53 K54 K55 K56 K57 K58 K59 K60 K61 K62 K63 K64 K65

G68 G69 G70 G71 G72 G73 G74 G75 G76 G77 G78 G79 G80 G81 G82 G83 G84 G85 G86 G87 G88 G89 G90 G91 G92 G93 G94 G95 G96 G97 G98 G99 G100 G101 G102 G103 G104 G105 G106 G107 G108 G109 G110 G111 G112 G113 G114 G115 G116 G117 G118 G119 G120 G121 G122 G123 G124 G125 G126 G127 G128

• Molecule 10: 30S ribosomal protein S10

Chain AJ: 4% 19% 52% 23% 6%

MET P40 K3 K4 K5 K6 K7 K8 K9 H13 H14 H15 H16 H17 H18 H19 H20 H21 H22 H23 H24 H25 H26 H27 H28 H29 H30 H31 H32 H33 H34 H35 H36 H37 H38 H39 H40 H41 H42 H43 H44 H45 H46 H47 H48 H49 H50 H51 H52 H53 H54 H55 H56 H57 H58 H59 H60 H61 H62 H63 H64 H65

R66 R67 R68 R69 R70 R71 R72 R73 R74 R75 R76 R77 R78 R79 R80 R81 R82 R83 R84 R85 R86 R87 R88 R89 R90 R91 R92 R93 R94 R95 R96 R97 R98 R99 R100 R101 R102 R103 R104 R105 R106 R107 R108 R109 R110 R111 R112 R113 R114 R115 R116 R117 R118 R119 R120 R121 R122 R123 R124 R125 R126 R127 R128

• Molecule 10: 30S ribosomal protein S10

Chain CJ: 5% 19% 50% 21% . 6%

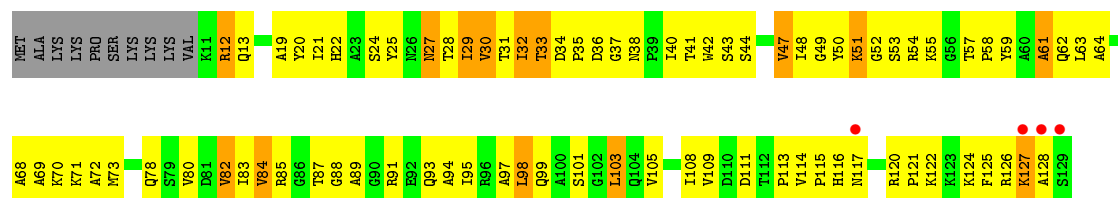
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E64 E65 E66 E67 E68 E69 E70 E71 E72 E73 E74 E75 E76 E77 E78 E79 E80 E81 E82 E83 E84 E85 E86 E87 E88 E89 E90 E91 E92 E93 E94 E95 E96 E97 E98 E99 E100 E101 E102 E103 E104 E105 E106 E107 E108 E109 E110 E111 E112 E113 E114 E115 E116 E117 E118 E119 E120 E121 E122 E123 E124 E125 E126 E127 E128

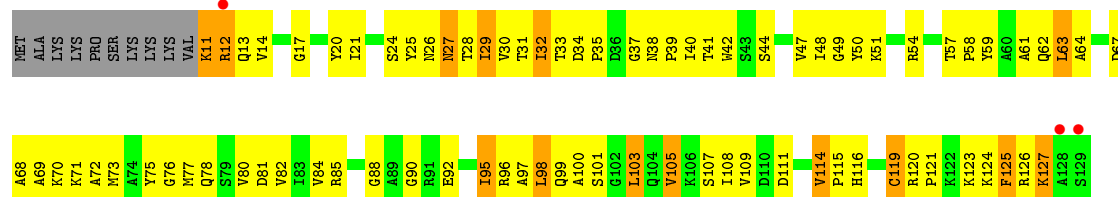
• Molecule 11: 30S ribosomal protein S11

Chain AK: 3% 29% 53% 11% 8%

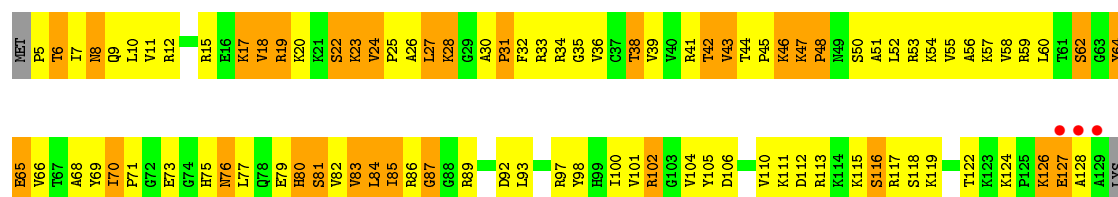




• Molecule 11: 30S ribosomal protein S11

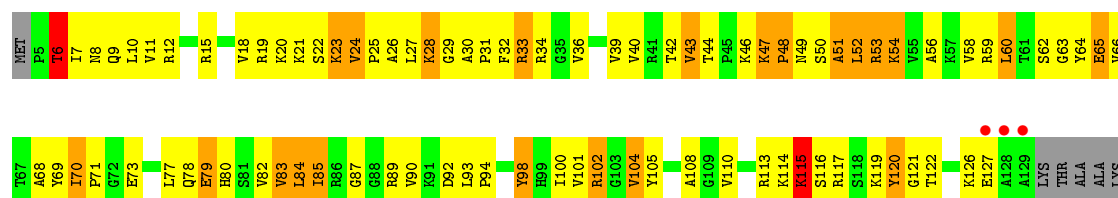


• Molecule 12: 30S ribosomal protein S12



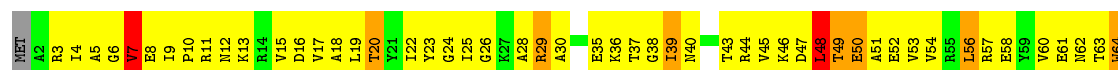
THR  
ALA  
LYS

• Molecule 12: 30S ribosomal protein S12

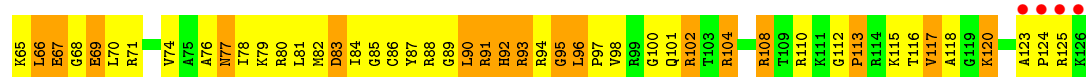


LYS

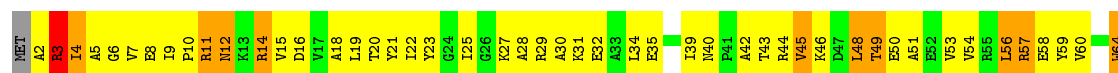
• Molecule 13: 30S ribosomal protein S13



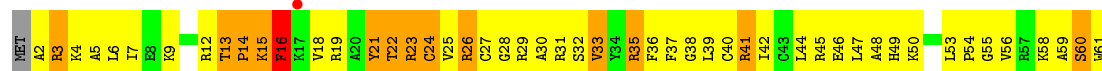
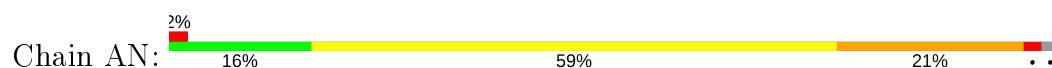




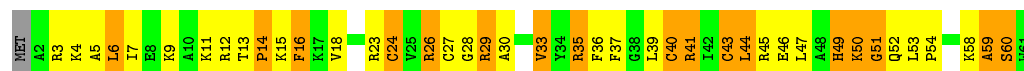
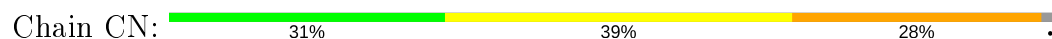
- Molecule 13: 30S ribosomal protein S13



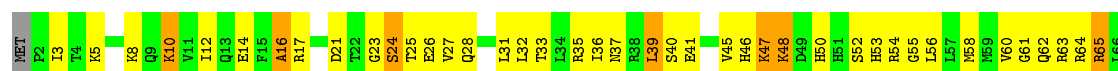
- Molecule 14: 30S ribosomal protein S14 type Z



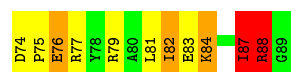
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15

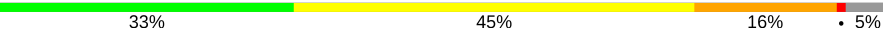


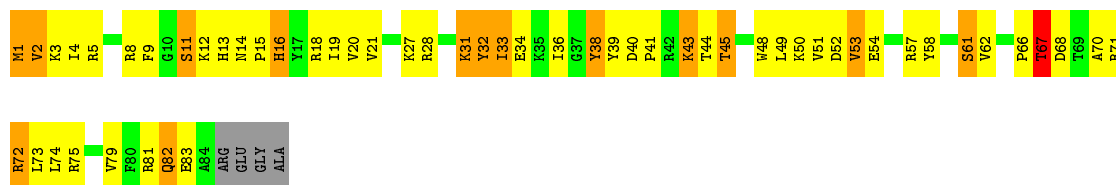
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

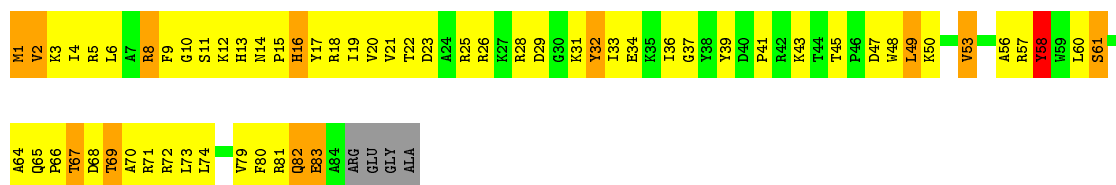


Chain AP:  33% 45% 16% • 5%



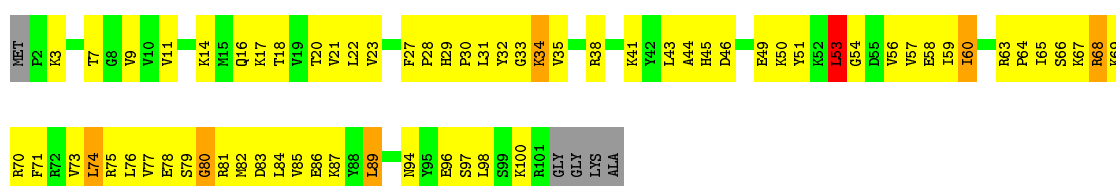
- Molecule 16: 30S ribosomal protein S16

Chain CP:  25% 56% 14% • 5%



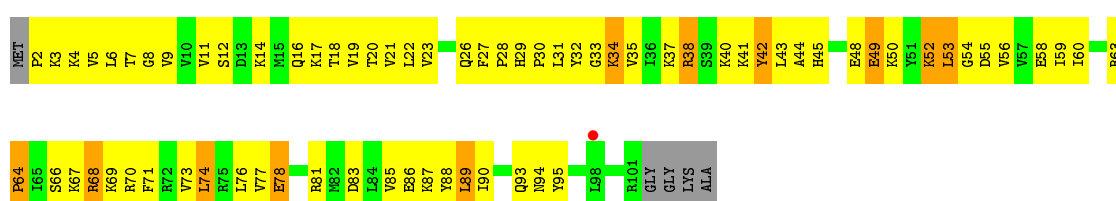
- Molecule 17: 30S ribosomal protein S17

Chain AQ:  31% 57% 6% • 5%

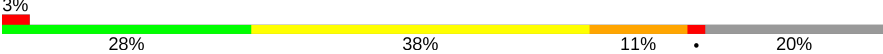


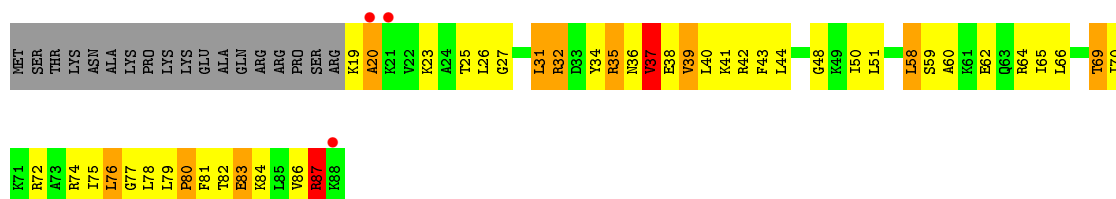
- Molecule 17: 30S ribosomal protein S17

Chain CQ:  27% 58% 10% 5%



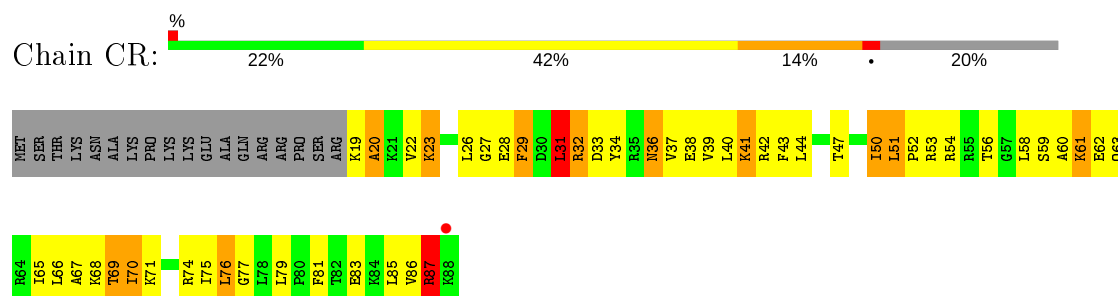
- Molecule 18: 30S ribosomal protein S18

Chain AR:  3% 28% 38% 11% • 20%

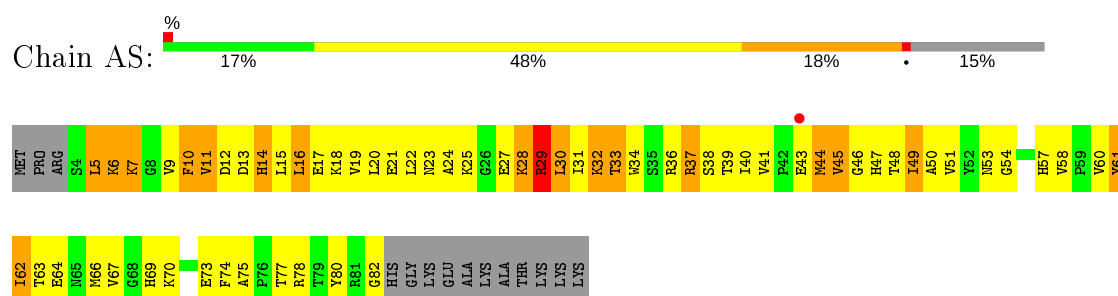




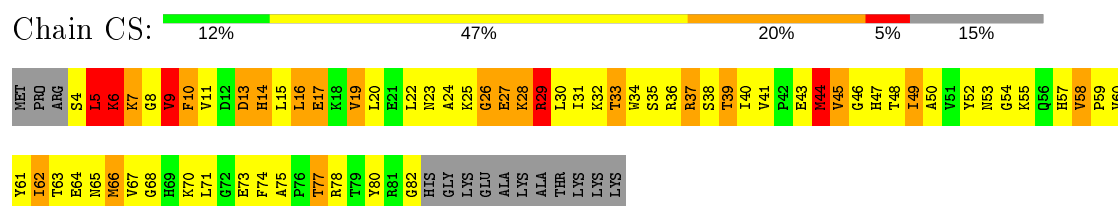
- Molecule 18: 30S ribosomal protein S18



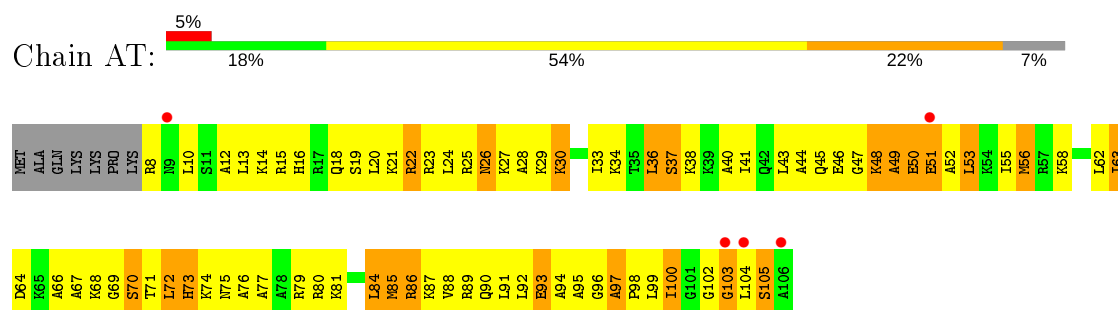
- Molecule 19: 30S ribosomal protein S19



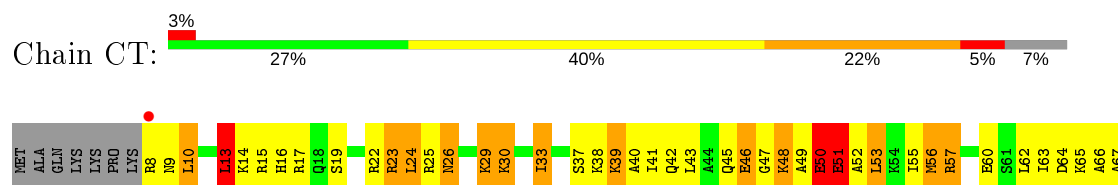
- Molecule 19: 30S ribosomal protein S19



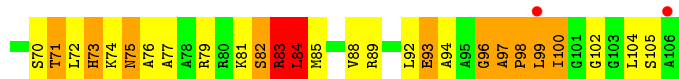
- Molecule 20: 30S ribosomal protein S20



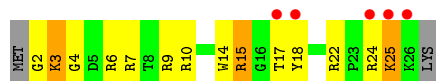
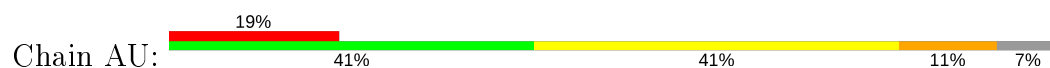
- Molecule 20: 30S ribosomal protein S20







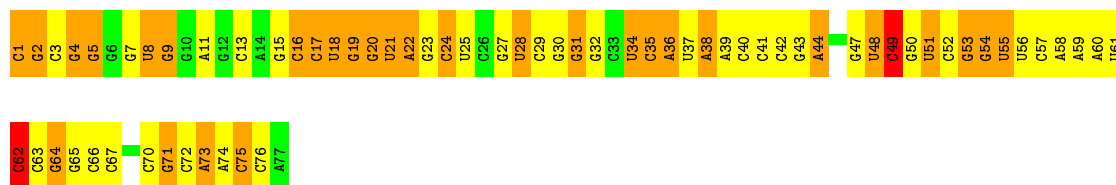
- Molecule 21: 30S ribosomal protein Thx



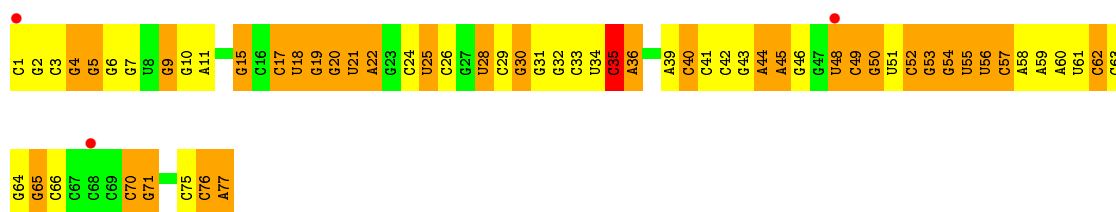
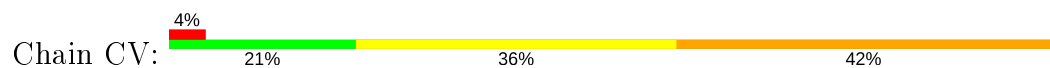
- Molecule 21: 30S ribosomal protein Thx



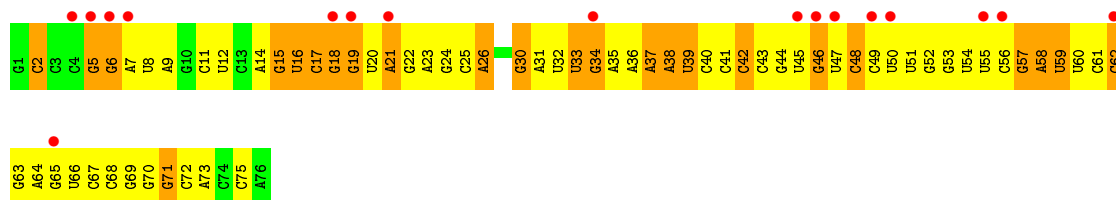
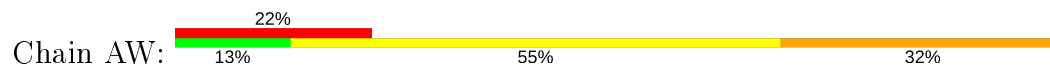
- Molecule 22: P-SITE tRNA fMet



- Molecule 22: P-SITE tRNA fMet



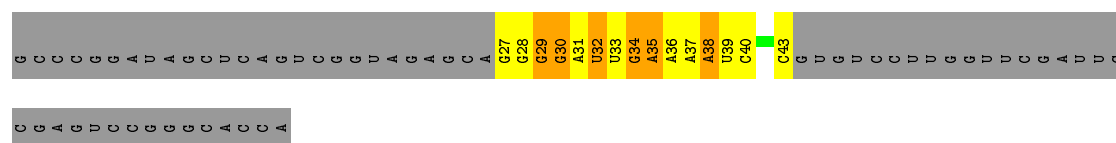
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe



- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe

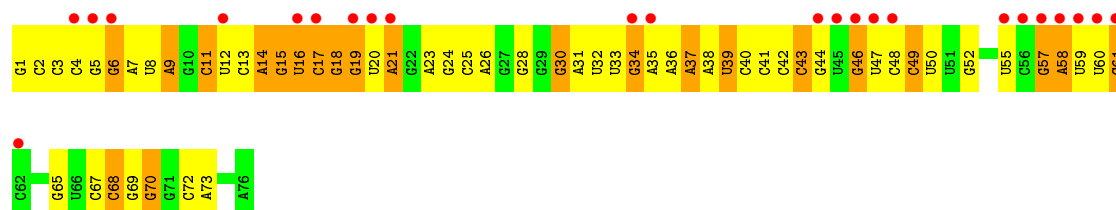


Chain AY: 



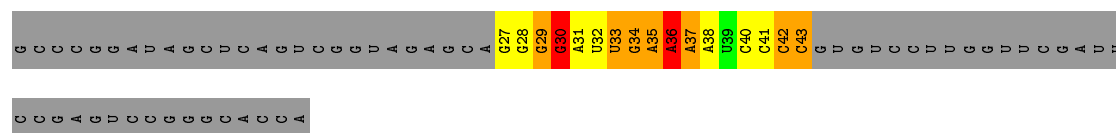
- Molecule 23: E-SITE tRNA PHE OR A-SITE tRNA Phe

Chain CW: 




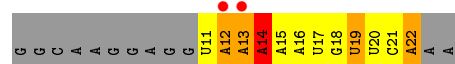
- Molecule 23: E-SITE tRNA PHE OR A-SITE tRNA Phe

Chain CY: 




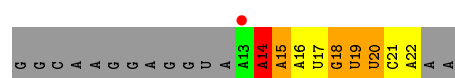
- Molecule 24: mRNA

Chain AX: 



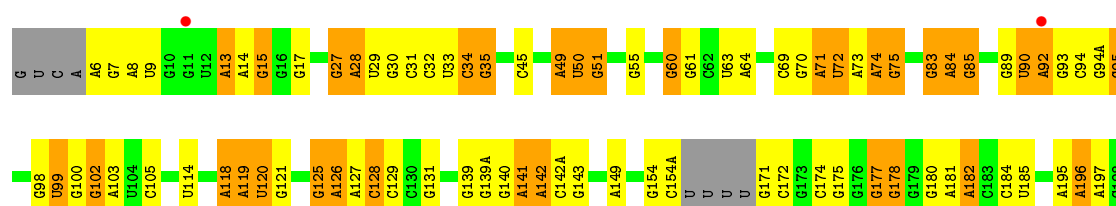
- Molecule 24: mRNA

Chain CX: 



- Molecule 25: 23S rRNA

Chain BA: 



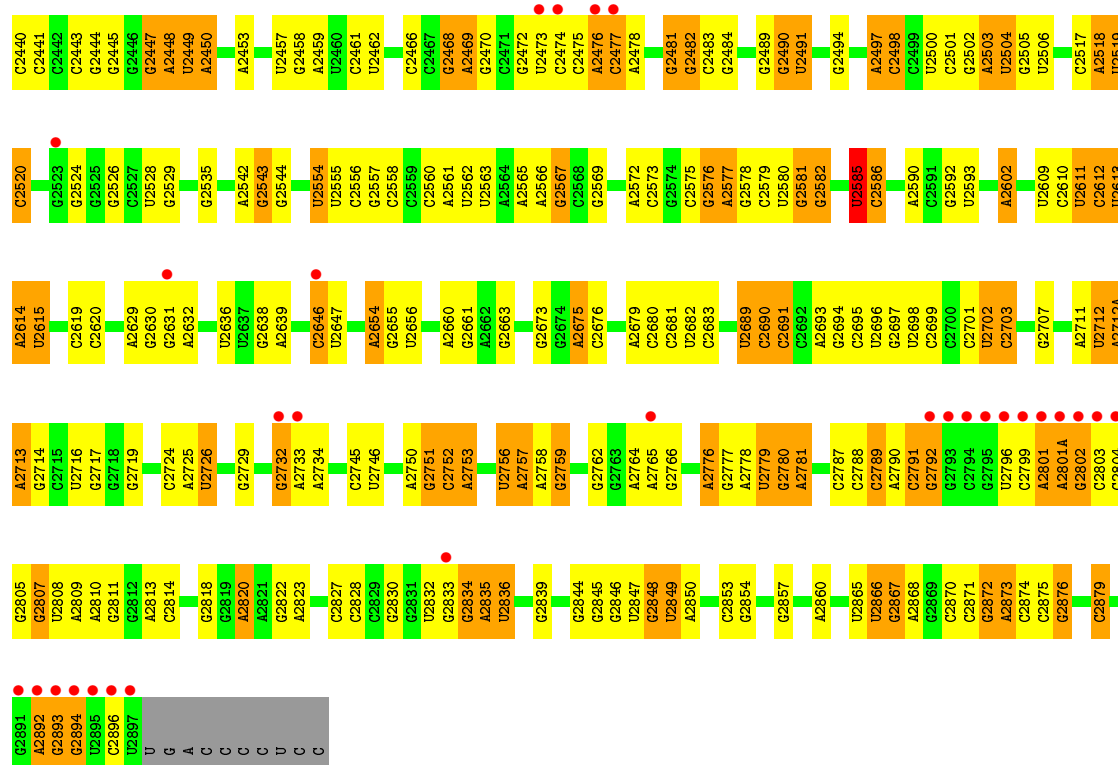






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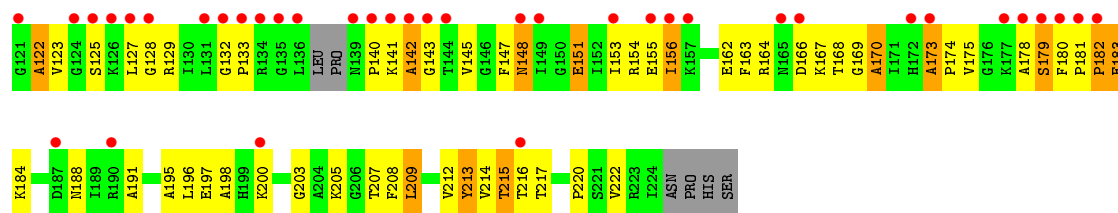
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C	G2842	C2583	G2668	G2407	G2407	U2301	C2204	C2149	A2050	A1951	G1852	
C	C2843	C2584	A2669	G2407	G2407	U2302	C2205	C2150	A2051	A1952	G1853	
C	A2844	C2585	C2670	G2407	G2407	U2303	C2206	C2151	A2052	A1953	G1854	
C	G2845	C2586	G2671	G2407	G2407	U2304	C2207	C2152	A2053	A1954	G1855	
C	C2846	C2587	A2672	G2407	G2407	U2305	C2208	C2153	A2054	A1955	G1856	
C	A2847	C2588	C2673	G2407	G2407	U2306	C2209	C2154	A2055	A1956	G1857	
C	G2848	C2589	G2674	G2407	G2407	U2307	C2210	C2155	A2056	A1957	G1858	
C	C2849	C2590	A2675	G2407	G2407	U2308	C2211	C2156	A2057	A1958	G1859	
C	A2850	C2591	C2676	G2407	G2407	U2309	C2212	C2157	A2058	A1959	G1860	
C	G2851	C2592	G2677	G2407	G2407	U2310	C2213	C2158	A2059	A1960	G1861	
C	C2852	C2593	A2678	G2407	G2407	U2311	C2214	C2159	A2060	A1961	G1862	
C	A2853	C2594	C2679	G2407	G2407	U2312	C2215	C2160	A2061	A1962	G1863	
C	G2854	C2595	G2680	G2407	G2407	U2313	C2216	C2161	A2062	A1963	G1864	
C	C2855	C2596	A2681	G2407	G2407	U2314	C2217	C2162	A2063	A1964	G1865	
C	A2856	C2597	C2682	G2407	G2407	U2315	C2218	C2163	A2064	A1965	G1866	
C	G2857	C2598	G2683	G2407	G2407	U2316	C2219	C2164	A2065	A1966	G1867	
C	C2858	C2599	A2684	G2407	G2407	U2317	C2220	C2165	A2066	A1967	G1868	
C	A2859	C2600	C2685	G2407	G2407	U2318	C2221	C2166	A2067	A1968	G1869	
C	G2860	C2601	G2686	G2407	G2407	U2319	C2222	C2167	A2068	A1969	G1870	
C	C2861	C2602	A2687	G2407	G2407	U2320	C2223	C2168	A2069	A1970	G1871	
C	A2862	C2603	C2688	G2407	G2407	U2321	C2224	C2169	A2070	A1971	G1872	
C	G2863	C2604	G2689	G2407	G2407	U2322	C2225	C2170	A2071	A1972	G1873	
C	C2864	C2605	A2689	G2407	G2407	U2323	C2226	C2171	A2072	A1973	G1874	
C	A2865	C2606	C2690	G2407	G2407	U2324	C2227	C2172	A2073	A1974	G1875	
C	G2866	C2607	G2691	G2407	G2407	U2325	C2228	C2173	A2074	A1975	G1876	



Category	Group 1 (Yellow)	Group 2 (Green)	Group 3 (Orange)	Group 4 (Light Green)	Group 5 (Grey)
U1	1	1	1	1	1
U2	1	1	1	1	1
U3	1	1	1	1	1
U8	1	1	1	1	1
U9	1	1	1	1	1
U12	1	1	1	1	1
U13	1	1	1	1	1
U14	1	1	1	1	1
U15	1	1	1	1	1
U22	1	1	1	1	1
U25	1	1	1	1	1
U26	1	1	1	1	1
U27	1	1	1	1	1
U30	1	1	1	1	1
U31	1	1	1	1	1
U34	1	1	1	1	1
U35	1	1	1	1	1
U40	1	1	1	1	1
U41	1	1	1	1	1
U42	1	1	1	1	1
U43	1	1	1	1	1
U44	1	1	1	1	1
U45	1	1	1	1	1
U46	1	1	1	1	1
U47	1	1	1	1	1
U48	1	1	1	1	1
U49	1	1	1	1	1
U50	1	1	1	1	1
U51	1	1	1	1	1
U52	1	1	1	1	1
U53	1	1	1	1	1
U56	1	1	1	1	1
U57	1	1	1	1	1
U60	1	1	1	1	1
U61	1	1	1	1	1
U66	1	1	1	1	1
U67	1	1	1	1	1
U70	1	1	1	1	1
U73	1	1	1	1	1
U79	1	1	1	1	1
U80	1	1	1	1	1
U88	1	1	1	1	1
U89	1	1	1	1	1
U90	1	1	1	1	1
U91	1	1	1	1	1
G92	1	0	0	0	0
U108	1	1	0	0	0
G109	1	0	0	0	0
G110	1	0	0	0	0
G114	1	1	0	0	0
G115	1	1	0	0	0
G116	1	1	0	0	0
G117	1	1	0	0	0
G118	1	1	0	0	0
G119	1	1	0	0	0
A	0	0	0	0	1
U	0	0	0	0	1
U	0	0	0	0	1

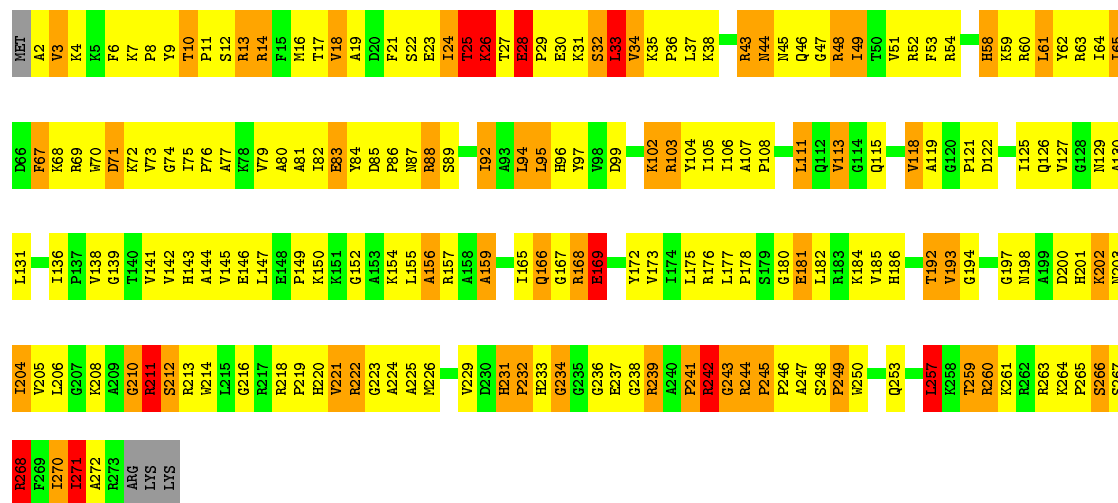
[illegible][illegible]





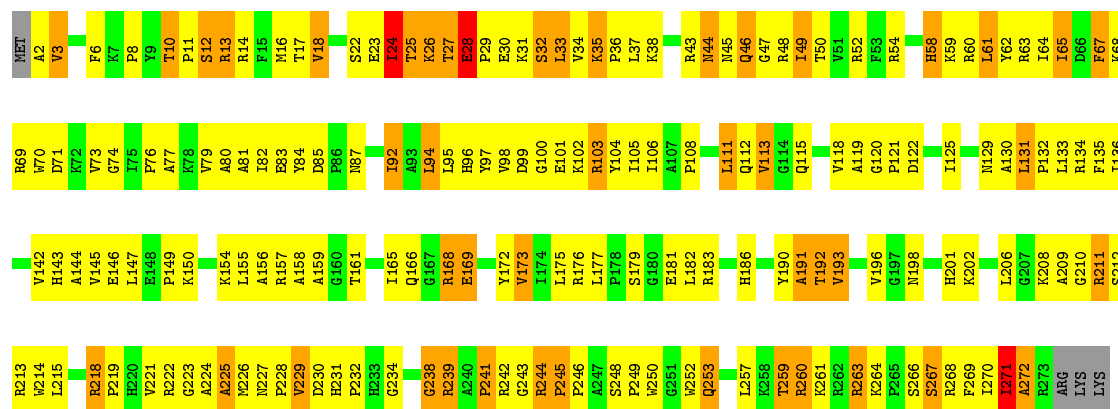
• Molecule 28: 50S RIBOSOMAL PROTEIN L2

Chain BD: 27% 49% 19%



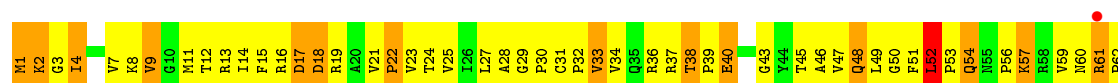
• Molecule 28: 50S RIBOSOMAL PROTEIN L2

Chain DD: 32% 49% 16%

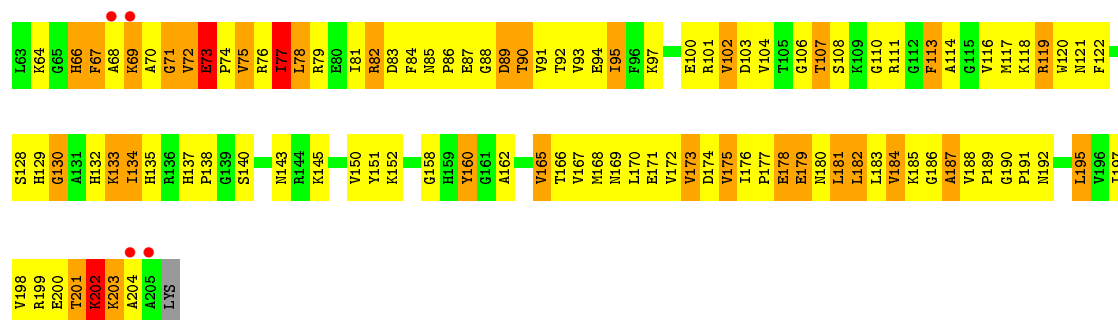


• Molecule 29: 50S RIBOSOMAL PROTEIN L3

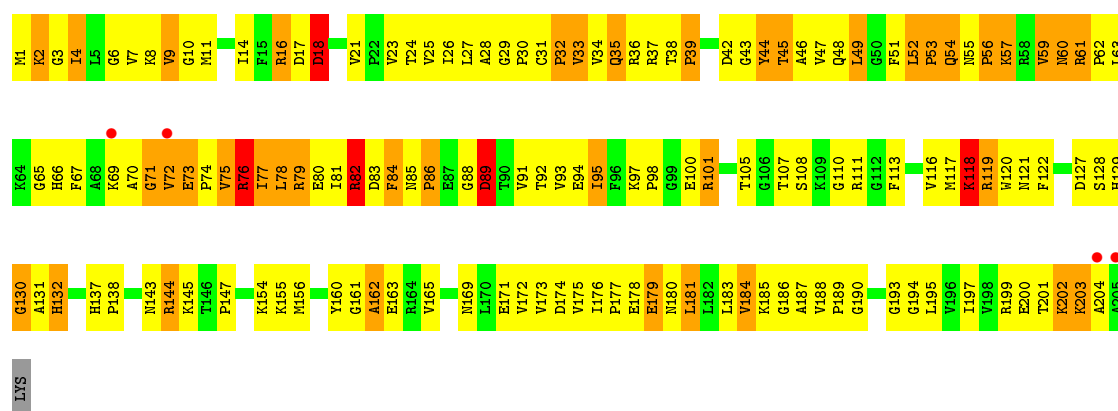
Chain BE: 2% 24% 52% 22%



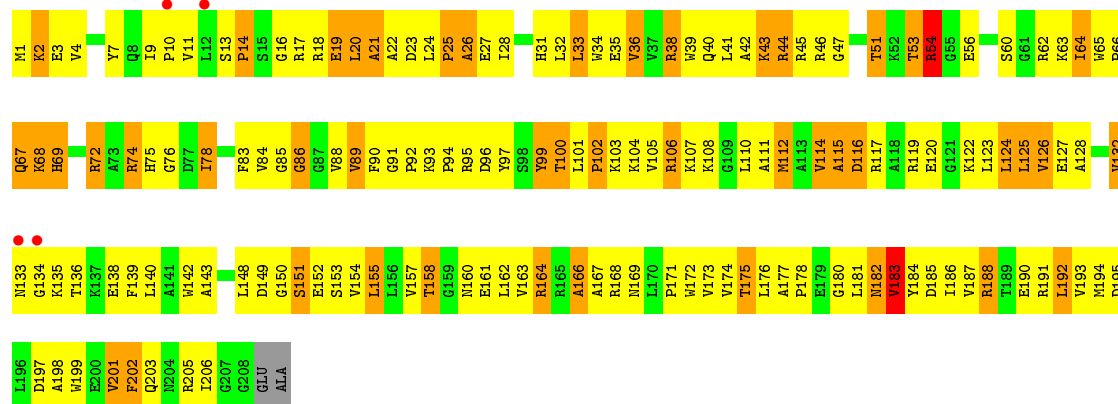




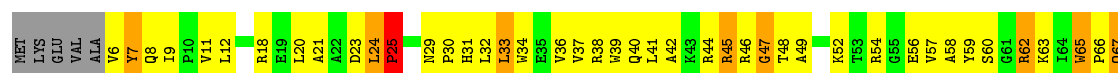
• Molecule 29: 50S RIBOSOMAL PROTEIN L3



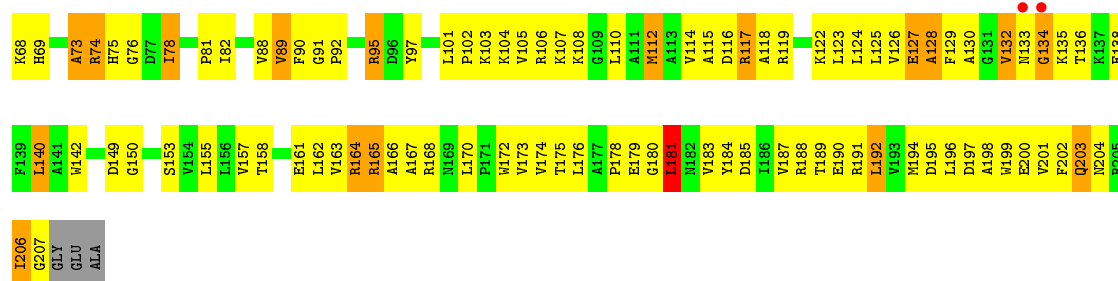
• Molecule 30: 50S RIBOSOMAL PROTEIN L4



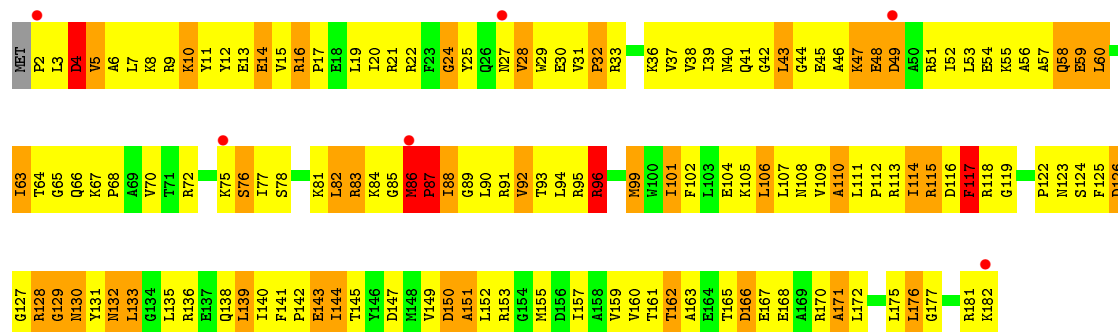
• Molecule 30: 50S RIBOSOMAL PROTEIN L4



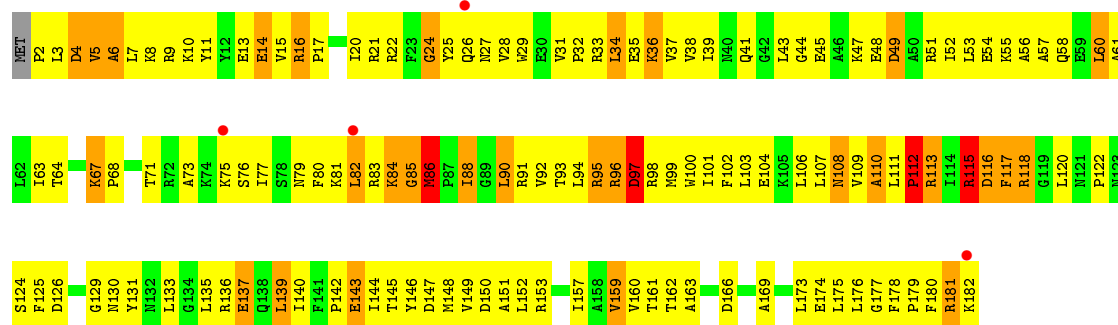




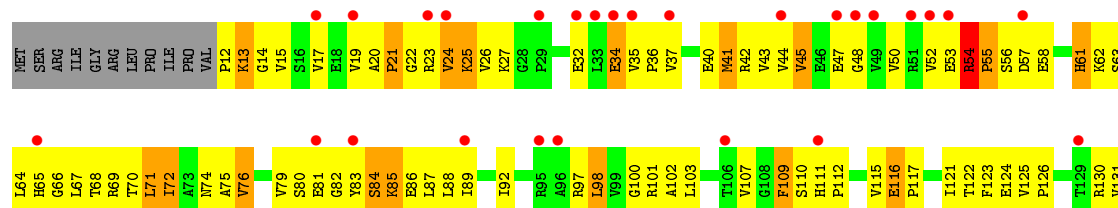
• Molecule 31: 50S RIBOSOMAL PROTEIN L5



• Molecule 31: 50S RIBOSOMAL PROTEIN L5



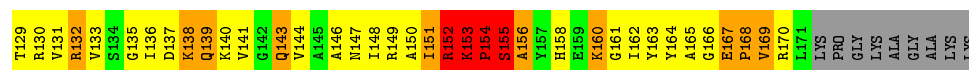
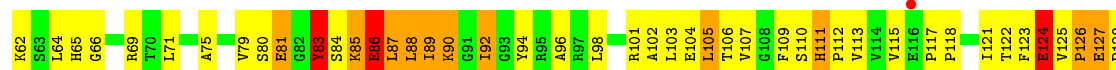
• Molecule 32: 50S RIBOSOMAL PROTEIN L6



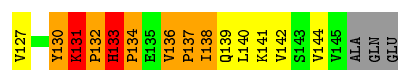
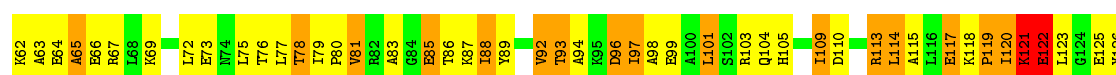
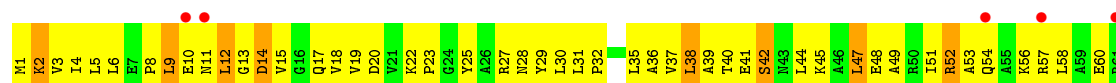




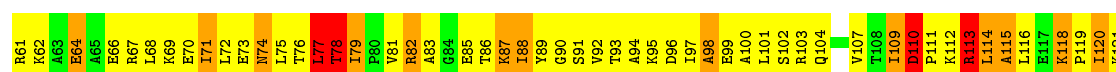
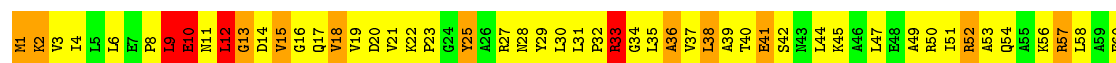
• Molecule 32: 50S RIBOSOMAL PROTEIN L6



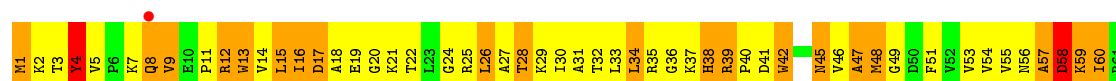
• Molecule 33: 50S RIBOSOMAL PROTEIN L9



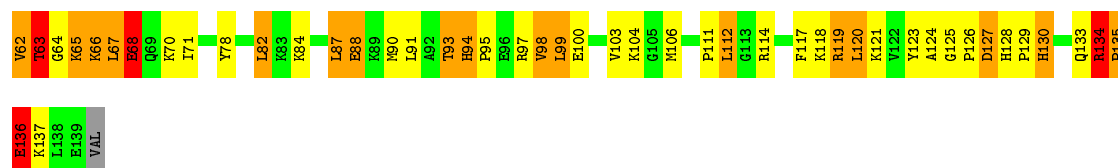
• Molecule 33: 50S RIBOSOMAL PROTEIN L9



• Molecule 34: 50S RIBOSOMAL PROTEIN L13







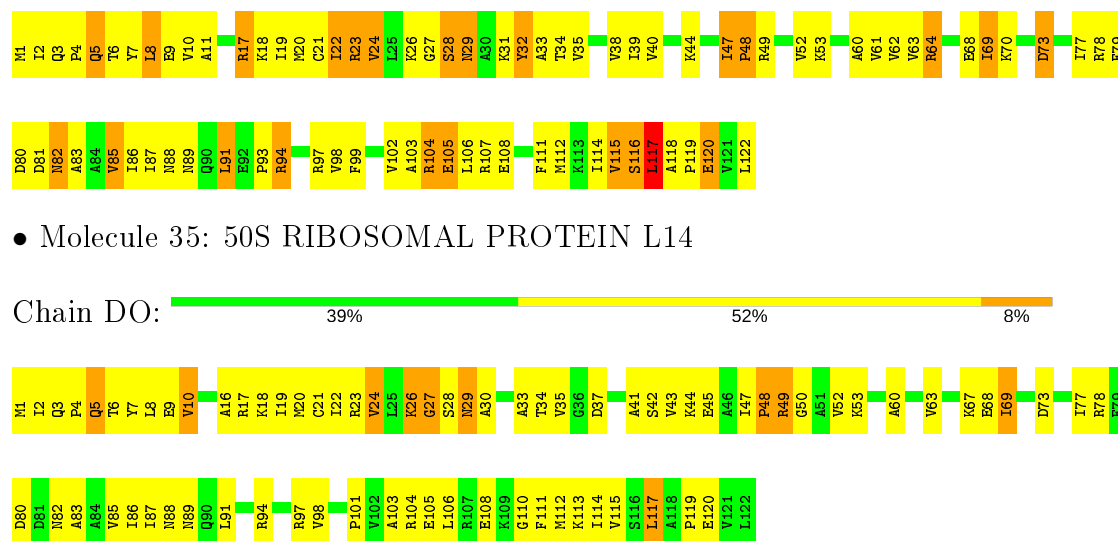
• Molecule 34: 50S RIBOSOMAL PROTEIN L13

Chain DN: 29% 51% 19% ..



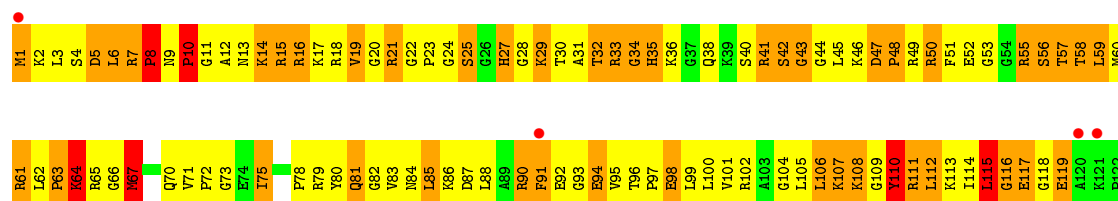
• Molecule 35: 50S RIBOSOMAL PROTEIN L14

Chain BO: 34% 47% 19% .



• Molecule 36: 50S RIBOSOMAL PROTEIN L15

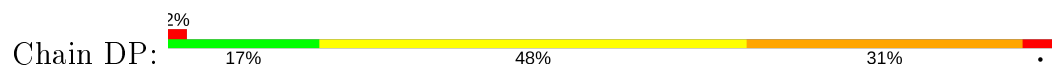
Chain BP: 3% 15% 49% 32% 5%



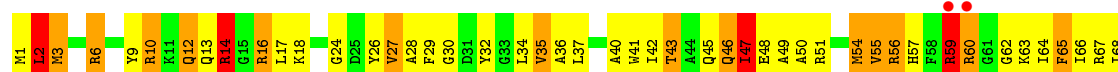




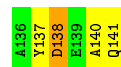
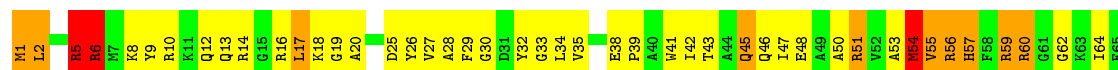
• Molecule 36: 50S RIBOSOMAL PROTEIN L15



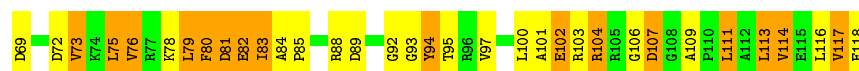
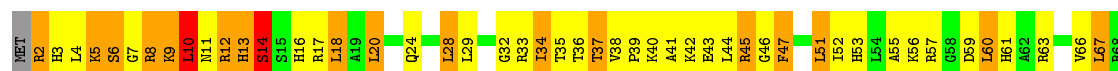
• Molecule 37: 50S RIBOSOMAL PROTEIN L16



• Molecule 37: 50S RIBOSOMAL PROTEIN L16



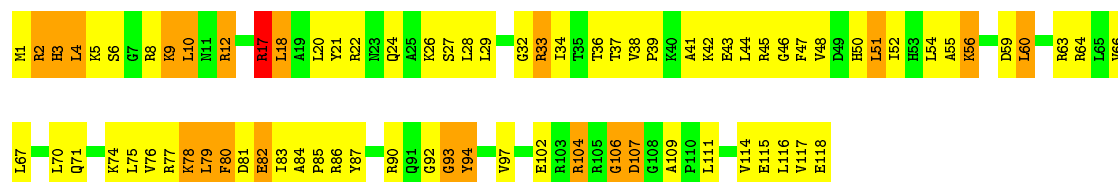
• Molecule 38: 50S RIBOSOMAL PROTEIN L17






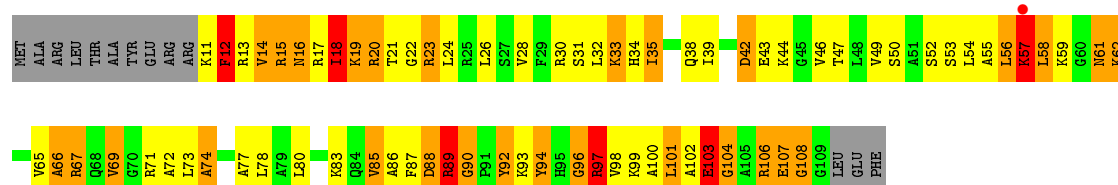
- Molecule 38: 50S RIBOSOMAL PROTEIN L17

Chain DR: 



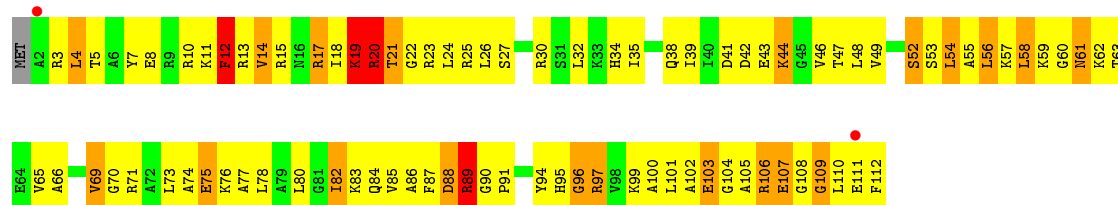
- Molecule 39: 50S RIBOSOMAL PROTEIN L18

Chain BS: 




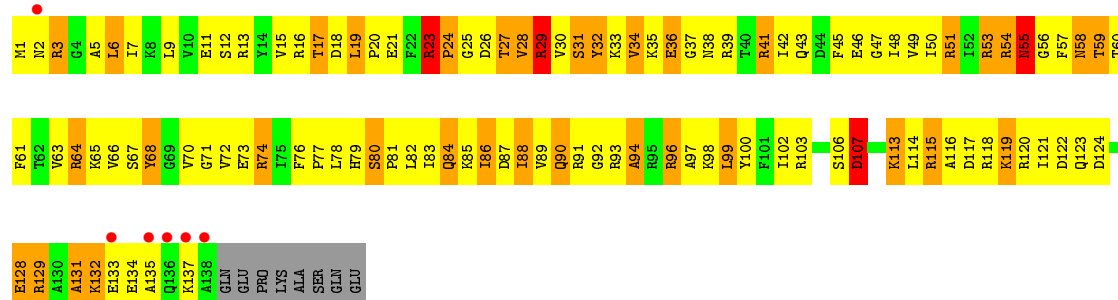
- Molecule 39: 50S RIBOSOMAL PROTEIN L18

Chain DS: 




- Molecule 40: 50S RIBOSOMAL PROTEIN L19

Chain BT: 

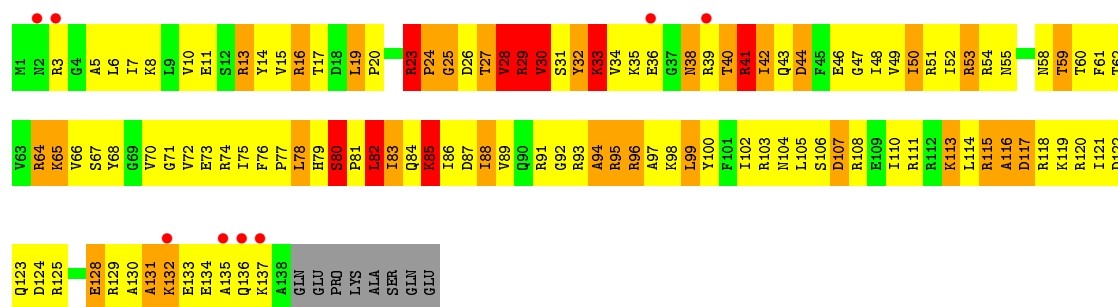


- Molecule 40: 50S RIBOSOMAL PROTEIN L19

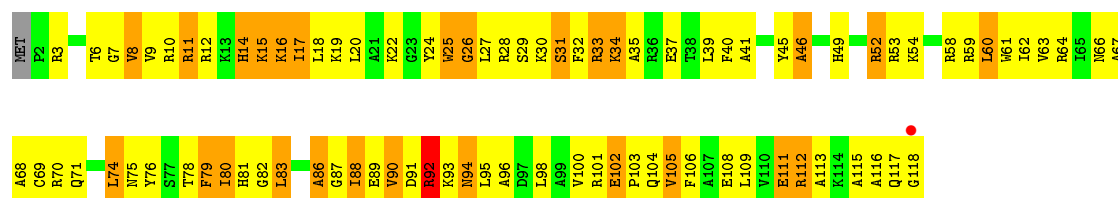
Chain DT: 



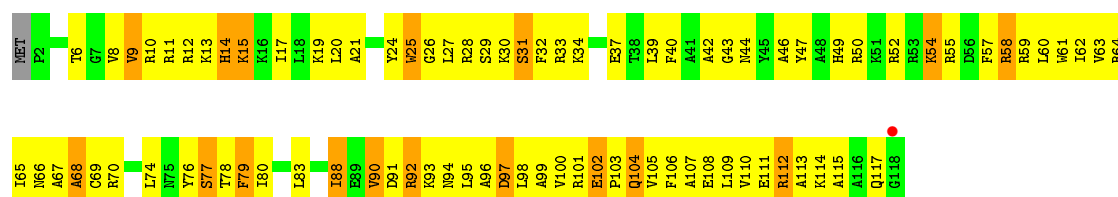




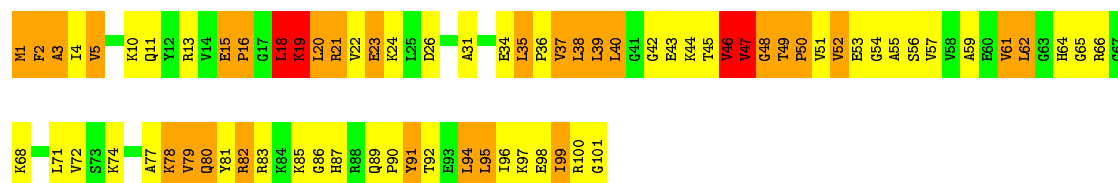
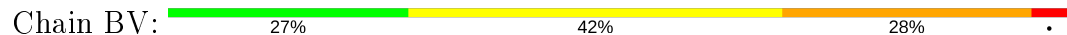
• Molecule 41: 50S RIBOSOMAL PROTEIN L20



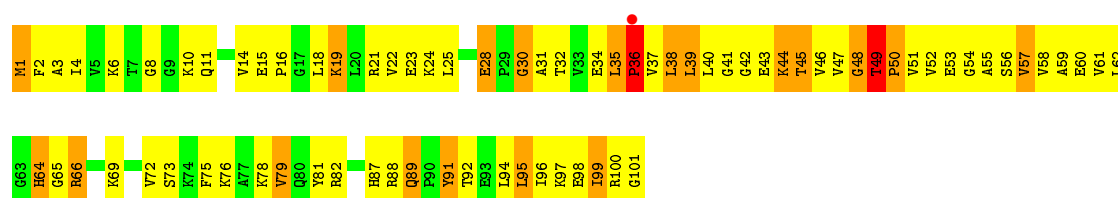
• Molecule 41: 50S RIBOSOMAL PROTEIN L20



• Molecule 42: 50S RIBOSOMAL PROTEIN L21

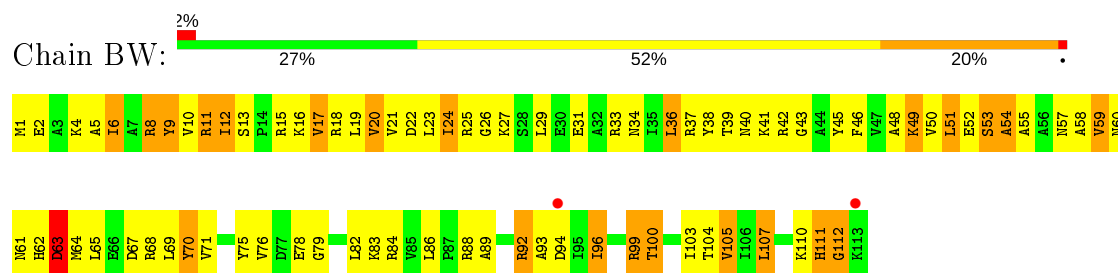


• Molecule 42: 50S RIBOSOMAL PROTEIN L21

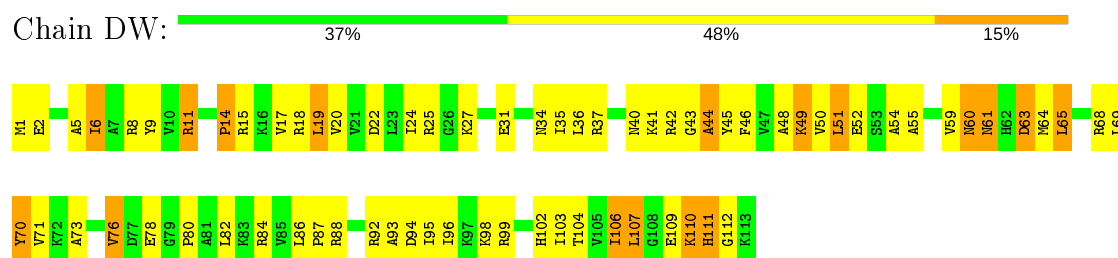




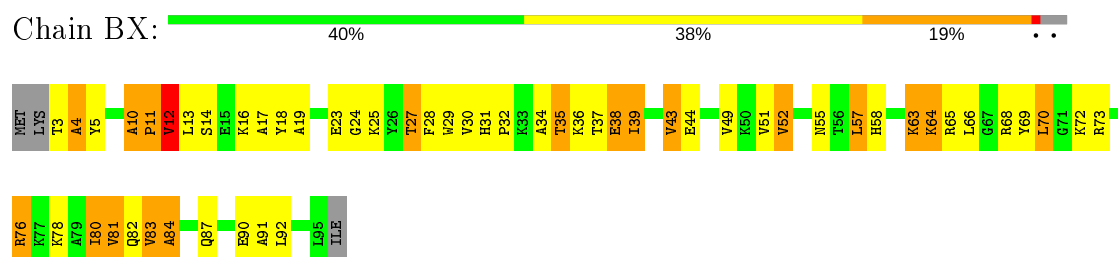
- Molecule 43: 50S RIBOSOMAL PROTEIN L22



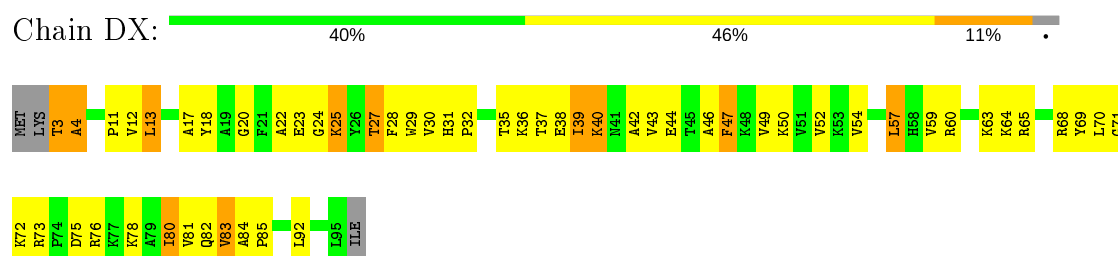
- Molecule 43: 50S RIBOSOMAL PROTEIN L22



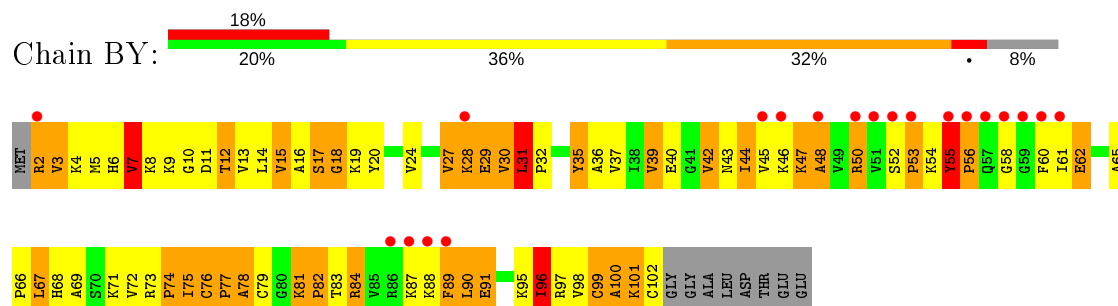
- Molecule 44: 50S RIBOSOMAL PROTEIN L23



- Molecule 44: 50S RIBOSOMAL PROTEIN L23




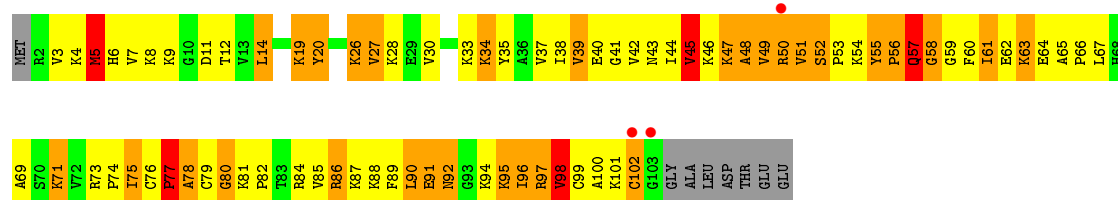
- Molecule 45: 50S RIBOSOMAL PROTEIN L24





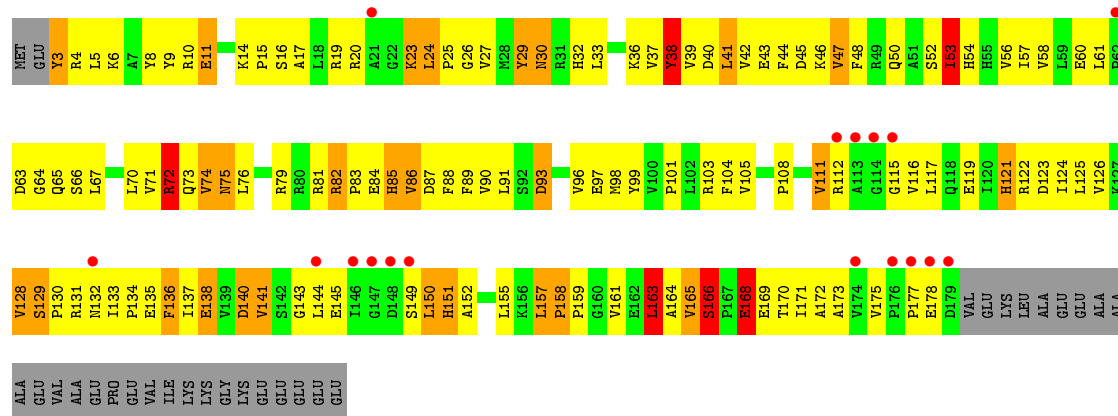
- Molecule 45: 50S RIBOSOMAL PROTEIN L24

Chain DY: 




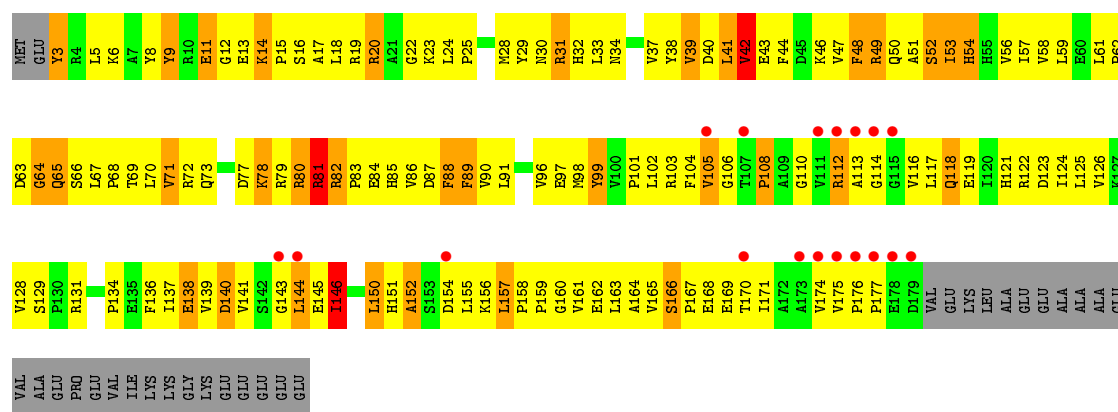
- Molecule 46: 50S RIBOSOMAL PROTEIN L25

Chain BZ: 



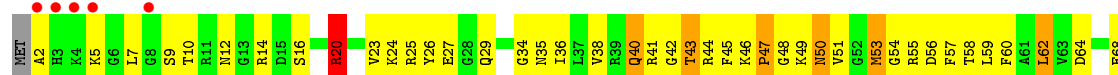
- Molecule 46: 50S RIBOSOMAL PROTEIN L25

Chain DZ: 

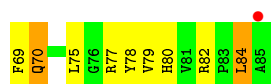


- Molecule 47: 50S RIBOSOMAL PROTEIN L27

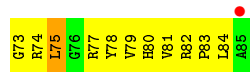
Chain B0: 







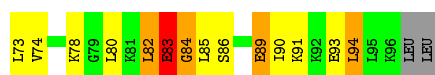
• Molecule 47: 50S RIBOSOMAL PROTEIN L27



• Molecule 48: 50S RIBOSOMAL PROTEIN L28



• Molecule 48: 50S RIBOSOMAL PROTEIN L28



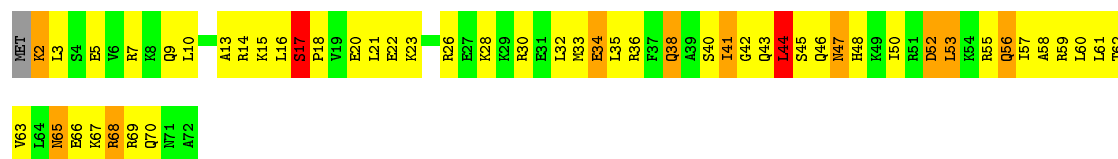
• Molecule 49: 50S RIBOSOMAL PROTEIN L29



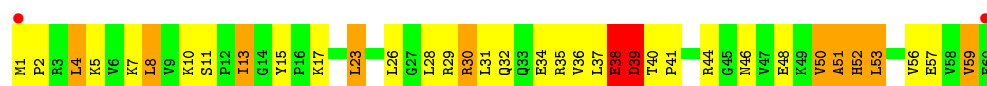
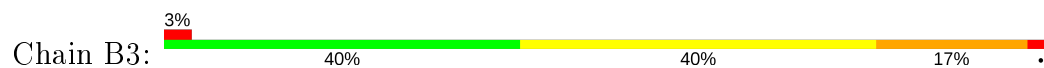
• Molecule 49: 50S RIBOSOMAL PROTEIN L29



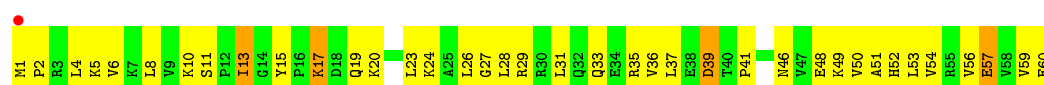




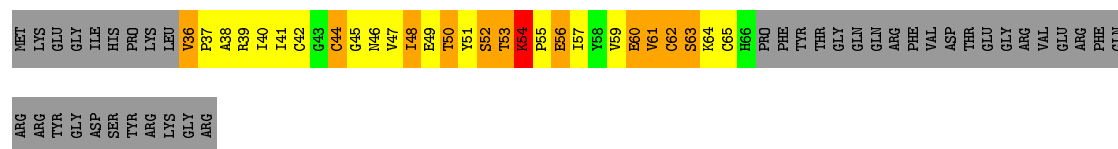
• Molecule 50: 50S RIBOSOMAL PROTEIN L30



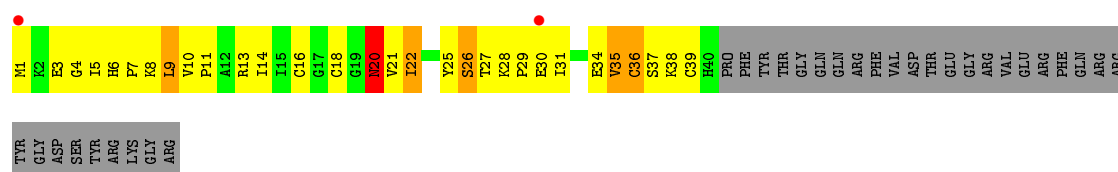
• Molecule 50: 50S RIBOSOMAL PROTEIN L30



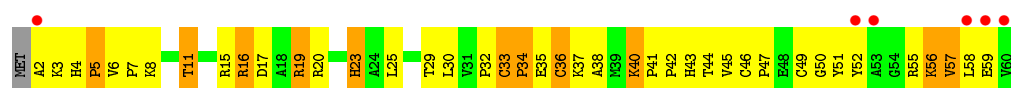
• Molecule 51: 50S RIBOSOMAL PROTEIN L31



• Molecule 51: 50S RIBOSOMAL PROTEIN L31



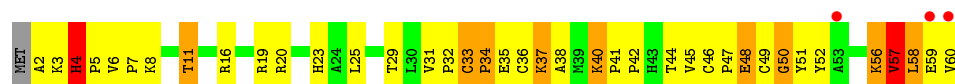
• Molecule 52: 50S RIBOSOMAL PROTEIN L32



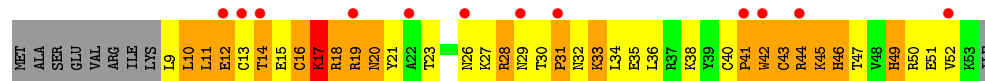
• Molecule 52: 50S RIBOSOMAL PROTEIN L32



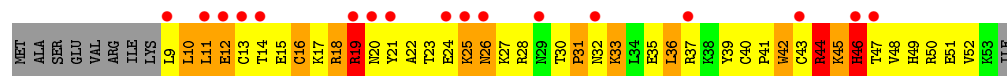




• Molecule 53: 50S RIBOSOMAL PROTEIN L33



• Molecule 53: 50S RIBOSOMAL PROTEIN L33



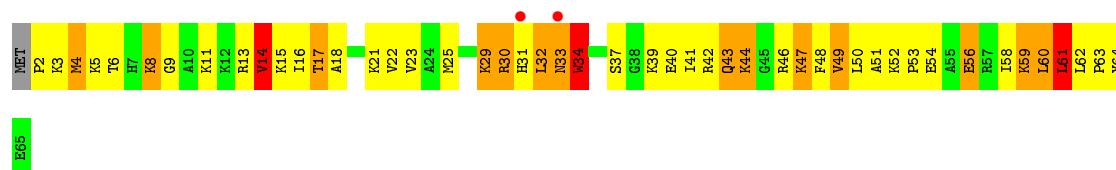
• Molecule 54: 50S RIBOSOMAL PROTEIN L34



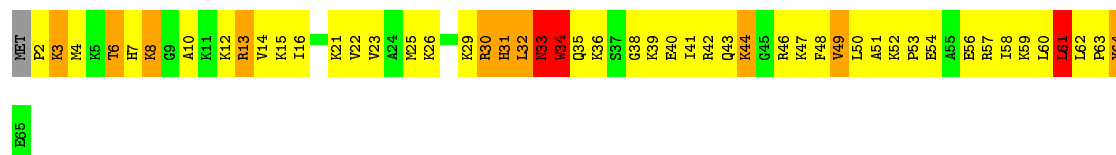
• Molecule 54: 50S RIBOSOMAL PROTEIN L34



• Molecule 55: 50S RIBOSOMAL PROTEIN L35

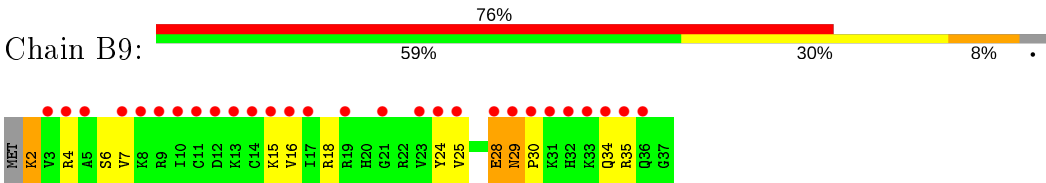


• Molecule 55: 50S RIBOSOMAL PROTEIN L35

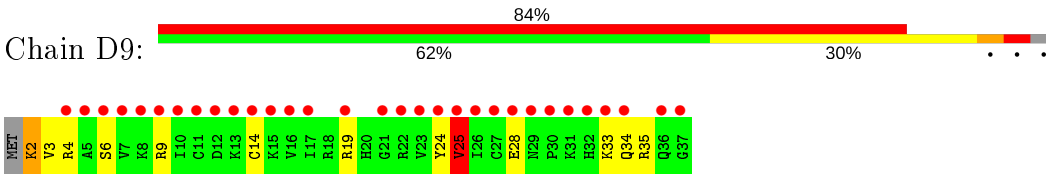




● Molecule 56: 50S RIBOSOMAL PROTEIN L36



● Molecule 56: 50S RIBOSOMAL PROTEIN L36





## 4 Data and refinement statistics

Property	Value
Space group	P 21 21 21
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.46 Å   447.34 Å   622.30 Å 90.00°   90.00°   90.00°
Resolution (Å)	35.07 – 3.52 35.07 – 3.52
% Data completeness (in resolution range)	99.9 (35.07-3.52) 99.9 (35.07-3.52)
$R_{merge}$	0.44
$R_{sym}$	0.46
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 3.47 Å)
Refinement program	PHENIX (phenix.refine: 1.7_641), PHENIX (phenix.refine: 1.8_1069)
R, $R_{free}$	0.210   ,   0.249 0.214   ,   0.254
$R_{free}$ test set	32826 reflections (4.56%)
Wilson B-factor (Å <sup>2</sup> )	91.1
Anisotropy	0.109
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 80.8
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$
Estimated twinning fraction	No twinning to report.
$F_o, F_c$ correlation	0.91
Total number of atoms	293977
Average B, all atoms (Å <sup>2</sup> )	79.0

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.28	0/36189	0.82	11/56484 (0.0%)
1	CA	0.29	0/36189	0.82	14/56484 (0.0%)
2	AB	0.59	0/1936	0.68	0/2611
2	CB	0.67	0/1936	0.77	0/2611
3	AC	0.70	0/1637	0.76	0/2207
3	CC	0.73	0/1637	0.82	0/2207
4	AD	0.69	0/1733	0.80	0/2318
4	CD	0.77	1/1733 (0.1%)	0.85	0/2318
5	AE	0.71	0/1163	0.88	0/1566
5	CE	0.74	0/1163	0.84	0/1566
6	AF	0.73	0/856	0.89	0/1154
6	CF	0.79	0/856	0.82	0/1154
7	AG	0.72	0/1276	0.79	0/1709
7	CG	0.71	0/1276	0.77	0/1709
8	AH	0.69	1/1136 (0.1%)	0.78	0/1527
8	CH	0.73	0/1136	0.80	1/1527 (0.1%)
9	AI	0.71	0/1029	0.80	0/1379
9	CI	0.70	0/1029	0.81	1/1379 (0.1%)
10	AJ	0.70	0/808	0.79	0/1087
10	CJ	0.65	0/808	0.77	0/1087
11	AK	0.67	0/900	0.81	0/1213
11	CK	0.70	0/900	0.82	0/1213
12	AL	0.86	0/987	0.95	0/1322
12	CL	0.92	1/987 (0.1%)	1.01	0/1322
13	AM	0.67	0/999	0.82	0/1338
13	CM	0.48	1/1008 (0.1%)	0.75	1/1347 (0.1%)
14	AN	0.73	0/501	0.83	1/664 (0.2%)
14	CN	0.77	0/501	0.95	0/664
15	AO	0.72	0/745	0.79	0/992
15	CO	0.71	0/745	0.81	0/992
16	AP	0.72	0/717	0.86	0/965
16	CP	0.79	0/717	0.84	0/965



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.69	0/837	0.79	0/1119
17	CQ	0.73	0/837	0.81	0/1119
18	AR	0.69	0/579	0.83	0/768
18	CR	0.76	0/579	0.98	0/768
19	AS	0.66	0/643	0.76	0/867
19	CS	0.80	1/643 (0.2%)	0.86	0/867
20	AT	0.73	0/765	0.77	0/1007
20	CT	0.61	0/765	0.63	0/1007
21	AU	0.73	0/213	0.83	0/279
21	CU	0.75	0/213	0.78	0/279
22	AV	1.13	5/1836 (0.3%)	1.33	13/2859 (0.5%)
22	CV	1.02	0/1835	1.20	13/2859 (0.5%)
23	AW	0.93	3/1809 (0.2%)	1.07	4/2819 (0.1%)
23	AY	1.07	1/408 (0.2%)	1.39	4/634 (0.6%)
23	CW	0.90	0/1809	1.01	0/2819
23	CY	1.15	0/408	1.42	4/634 (0.6%)
24	AX	1.10	1/285 (0.4%)	0.91	2/441 (0.5%)
24	CX	0.96	0/235	1.27	3/364 (0.8%)
25	BA	0.34	1/67788 (0.0%)	0.87	42/105819 (0.0%)
25	DA	0.35	0/68124	0.88	36/106343 (0.0%)
26	BB	0.26	0/2853	0.78	0/4451
26	DB	0.28	0/2853	0.80	0/4451
27	BC	0.65	1/1145 (0.1%)	0.67	0/1556
27	DC	0.24	0/1145	0.46	0/1556
28	BD	0.85	0/2155	0.95	1/2907 (0.0%)
28	DD	0.54	0/2155	0.74	0/2907
29	BE	0.75	0/1597	0.89	0/2155
29	DE	0.49	1/1597 (0.1%)	0.72	0/2155
30	BF	0.80	0/1659	0.87	1/2246 (0.0%)
30	DF	0.49	0/1620	0.76	1/2194 (0.0%)
31	BG	0.70	0/1499	0.78	1/2016 (0.0%)
31	DG	0.42	1/1499 (0.1%)	0.68	1/2016 (0.0%)
32	BH	0.63	0/1246	0.69	0/1684
32	DH	0.40	0/1315	0.79	1/1780 (0.1%)
33	BI	0.67	0/1146	0.81	0/1551
33	DI	0.36	0/1151	0.74	1/1558 (0.1%)
34	BN	0.76	0/1132	0.83	0/1527
34	DN	0.43	0/1132	0.69	0/1527
35	BO	0.76	0/943	0.87	0/1269
35	DO	0.46	0/943	0.68	0/1269
36	BP	0.40	1/1162 (0.1%)	0.78	2/1544 (0.1%)
36	DP	0.39	0/1162	0.76	1/1544 (0.1%)
37	BQ	0.75	0/1143	0.87	0/1527



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	DQ	0.48	0/1143	0.65	0/1527
38	BR	0.80	0/974	0.90	1/1302 (0.1%)
38	DR	0.57	1/982 (0.1%)	0.79	2/1312 (0.2%)
39	BS	0.77	0/779	0.90	0/1038
39	DS	0.40	0/892	0.81	1/1187 (0.1%)
40	BT	0.71	0/1156	0.90	1/1544 (0.1%)
40	DT	0.56	1/1156 (0.1%)	0.84	6/1544 (0.4%)
41	BU	0.81	0/982	0.91	1/1306 (0.1%)
41	DU	0.51	0/975	0.75	0/1297
42	BV	0.72	0/790	0.90	1/1057 (0.1%)
42	DV	0.53	1/790 (0.1%)	0.82	0/1057
43	BW	0.81	0/907	0.89	1/1216 (0.1%)
43	DW	0.48	0/907	0.69	1/1216 (0.1%)
44	BX	0.75	0/740	0.89	1/995 (0.1%)
44	DX	0.52	0/740	0.68	0/995
45	BY	0.74	0/789	0.95	2/1053 (0.2%)
45	DY	0.55	2/798 (0.3%)	0.78	0/1064
46	BZ	0.72	0/1436	0.74	1/1951 (0.1%)
46	DZ	0.35	0/1436	0.57	0/1951
47	B0	0.79	1/671 (0.1%)	0.84	0/892
47	D0	0.44	0/671	0.64	0/892
48	B1	0.87	0/739	0.94	0/983
48	D1	0.48	0/739	0.73	0/983
49	B2	0.72	0/600	0.83	0/793
49	D2	0.54	0/600	0.71	0/793
50	B3	0.73	0/473	0.83	0/636
50	D3	0.43	0/473	0.71	0/636
51	B4	0.72	0/229	0.76	0/311
51	D4	0.40	0/303	0.70	0/409
52	B5	0.82	1/473 (0.2%)	0.83	0/639
52	D5	0.44	0/473	0.65	0/639
53	B6	0.67	0/388	0.92	0/520
53	D6	0.30	0/388	0.58	0/520
54	B7	0.88	0/427	0.99	0/563
54	D7	0.54	0/427	0.75	1/563 (0.2%)
55	B8	0.76	0/516	0.91	0/681
55	D8	0.51	0/516	0.82	0/681
56	B9	0.64	0/302	0.59	0/397
56	D9	0.26	0/302	0.46	0/397
All	All	0.48	27/318178 (0.0%)	0.85	180/475682 (0.0%)

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
28	BD	0	1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1453	U	O3'-P	29.98	1.97	1.61
24	AX	14	A	O3'-P	-13.06	1.45	1.61
38	DR	12	ARG	C-N	11.33	1.60	1.34
40	DT	28	VAL	C-N	10.90	1.59	1.34
22	AV	1	C	OP3-P	-9.31	1.50	1.61

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1453	U	P-O3'-C3'	-10.66	106.91	119.70
38	DR	12	ARG	O-C-N	9.52	137.93	122.70
36	BP	1	MET	CG-SD-CE	9.44	115.30	100.20
40	DT	28	VAL	O-C-N	8.73	136.67	122.70
40	DT	28	VAL	CA-C-N	-7.49	100.72	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	BD	222	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32328	0	16317	795	0
1	CA	32328	0	16317	871	1
2	AB	1901	0	1951	245	0
2	CB	1901	0	1951	232	0
3	AC	1613	0	1677	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CC	1613	0	1677	148	0
4	AD	1703	0	1765	191	0
4	CD	1703	0	1764	174	0
5	AE	1147	0	1207	148	0
5	CE	1147	0	1207	159	0
6	AF	843	0	857	87	0
6	CF	843	0	857	63	0
7	AG	1257	0	1296	123	0
7	CG	1257	0	1296	102	0
8	AH	1116	0	1177	111	0
8	CH	1116	0	1177	111	0
9	AI	1010	0	1037	133	0
9	CI	1010	0	1037	144	0
10	AJ	795	0	840	127	0
10	CJ	795	0	840	135	0
11	AK	885	0	904	97	0
11	CK	885	0	904	109	0
12	AL	971	0	1057	126	0
12	CL	971	0	1057	123	0
13	AM	988	0	1059	151	0
13	CM	997	0	1072	164	0
14	AN	492	0	529	87	0
14	CN	492	0	531	69	0
15	AO	734	0	771	61	0
15	CO	734	0	771	51	0
16	AP	701	0	720	62	0
16	CP	701	0	720	101	0
17	AQ	824	0	891	68	0
17	CQ	824	0	891	85	0
18	AR	574	0	644	62	0
18	CR	574	0	644	68	0
19	AS	630	0	652	117	0
19	CS	630	0	652	106	0
20	AT	763	0	861	132	0
20	CT	763	0	861	166	0
21	AU	209	0	221	12	0
21	CU	209	0	221	22	0
22	AV	1644	0	836	110	0
22	CV	1643	0	836	143	0
23	AW	1619	0	822	122	0
23	AY	365	0	185	29	0
23	CW	1619	0	822	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	CY	365	0	185	37	0
24	AX	255	0	129	49	0
24	CX	210	0	109	23	0
25	BA	60527	0	30515	1623	1
25	DA	60827	0	30663	1373	0
26	BB	2551	0	1295	57	1
26	DB	2551	0	1295	55	0
27	BC	1142	0	865	78	0
27	DC	1142	0	865	70	0
28	BD	2105	0	2182	310	0
28	DD	2105	0	2182	277	0
29	BE	1564	0	1629	216	0
29	DE	1564	0	1629	206	0
30	BF	1624	0	1677	246	0
30	DF	1585	0	1632	188	0
31	BG	1474	0	1535	264	0
31	DG	1474	0	1535	209	0
32	BH	1223	0	1282	136	1
32	DH	1290	0	1364	238	0
33	BI	1131	0	1218	152	0
33	DI	1136	0	1223	229	0
34	BN	1105	0	1180	188	0
34	DN	1105	0	1180	140	0
35	BO	933	0	996	117	0
35	DO	933	0	996	90	0
36	BP	1145	0	1228	279	0
36	DP	1145	0	1228	283	3
37	BQ	1122	0	1179	129	0
37	DQ	1122	0	1179	123	0
38	BR	960	0	1021	146	0
38	DR	968	0	1033	109	0
39	BS	771	0	832	127	0
39	DS	882	0	943	149	0
40	BT	1142	0	1202	240	0
40	DT	1142	0	1202	269	0
41	BU	964	0	1022	160	0
41	DU	958	0	1014	198	0
42	BV	779	0	852	135	0
42	DV	779	0	852	150	3
43	BW	896	0	953	104	0
43	DW	896	0	953	89	0
44	BX	726	0	778	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DX	726	0	778	67	0
45	BY	776	0	870	172	0
45	DY	785	0	878	176	0
46	BZ	1404	0	1432	148	0
46	DZ	1404	0	1432	214	0
47	B0	662	0	688	60	0
47	D0	662	0	688	60	0
48	B1	732	0	808	78	0
48	D1	732	0	808	66	0
49	B2	598	0	653	64	0
49	D2	598	0	653	53	0
50	B3	468	0	523	40	3
50	D3	468	0	523	50	0
51	B4	226	0	229	39	0
51	D4	298	0	312	43	0
52	B5	459	0	480	50	0
52	D5	459	0	480	53	3
53	B6	381	0	391	51	0
53	D6	381	0	391	99	0
54	B7	419	0	467	35	0
54	D7	419	0	467	33	0
55	B8	508	0	576	115	0
55	D8	508	0	576	85	0
56	B9	299	0	326	13	0
56	D9	299	0	326	14	0
57	AA	110	0	0	0	0
57	AE	1	0	0	0	0
57	AV	5	0	0	0	0
57	AX	1	0	0	0	0
57	B5	1	0	0	0	0
57	B7	1	0	0	0	0
57	BA	323	0	0	0	0
57	BB	5	0	0	0	0
57	BD	2	0	0	0	0
57	BE	3	0	0	0	0
57	BF	1	0	0	0	0
57	BN	1	0	0	0	0
57	BO	1	0	0	0	0
57	BP	1	0	0	0	0
57	BU	1	0	0	0	0
57	CA	141	0	0	0	0
57	CE	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	CV	5	0	0	0	0
57	CW	1	0	0	0	0
57	CX	1	0	0	0	0
57	CY	1	0	0	0	0
57	D0	2	0	0	0	0
57	D1	2	0	0	0	0
57	D2	1	0	0	0	0
57	D5	2	0	0	0	0
57	D8	1	0	0	0	0
57	DA	397	0	0	0	0
57	DB	5	0	0	0	0
57	DD	3	0	0	0	0
57	DE	2	0	0	0	0
57	DF	1	0	0	0	0
57	DP	3	0	0	0	0
57	DQ	1	0	0	0	0
57	DU	3	0	0	0	0
57	DW	1	0	0	0	0
57	DX	1	0	0	0	0
58	AA	42	0	45	3	0
58	CA	42	0	45	2	0
59	AD	1	0	0	0	0
59	AN	1	0	0	1	0
59	CD	1	0	0	0	0
59	CN	1	0	0	3	0
All	All	293977	0	199058	16442	8

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

The worst 5 of 16442 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:BS:34:HIS:CE1	39:BS:54:LEU:HB2	1.32	1.58
42:DV:1:MET:SD	42:DV:1:MET:CG	2.01	1.47
40:BT:28:VAL:CG1	40:BT:46:GLU:HA	1.42	1.44
1:CA:748:C:H1'	1:CA:749:C:C5	1.53	1.44
34:BN:62:VAL:HG22	34:BN:66:LYS:CD	1.49	1.42

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:B3:1:MET:N	36:DP:122:PRO:CG[3_455]	1.46	0.74
50:B3:1:MET:N	36:DP:122:PRO:CD[3_455]	1.64	0.56
42:DV:50:PRO:CG	52:D5:58:LEU:O[4_445]	1.80	0.40
42:DV:48:GLY:O	52:D5:58:LEU:CD1[4_445]	1.84	0.36
25:BA:1593:G:O2'	26:BB:54:G:OP1[1_655]	2.09	0.11

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	159 (68%)	53 (23%)	21 (9%)	1	9
2	CB	233/256 (91%)	158 (68%)	45 (19%)	30 (13%)	0	4
3	AC	205/239 (86%)	129 (63%)	54 (26%)	22 (11%)	0	6
3	CC	205/239 (86%)	135 (66%)	52 (25%)	18 (9%)	1	9
4	AD	206/209 (99%)	142 (69%)	43 (21%)	21 (10%)	0	7
4	CD	206/209 (99%)	141 (68%)	47 (23%)	18 (9%)	1	9
5	AE	149/162 (92%)	117 (78%)	20 (13%)	12 (8%)	1	10
5	CE	149/162 (92%)	113 (76%)	22 (15%)	14 (9%)	0	8
6	AF	99/101 (98%)	63 (64%)	29 (29%)	7 (7%)	1	13
6	CF	99/101 (98%)	80 (81%)	14 (14%)	5 (5%)	2	20
7	AG	153/156 (98%)	116 (76%)	26 (17%)	11 (7%)	1	13
7	CG	153/156 (98%)	117 (76%)	29 (19%)	7 (5%)	2	22
8	AH	136/138 (99%)	96 (71%)	35 (26%)	5 (4%)	3	28
8	CH	136/138 (99%)	102 (75%)	28 (21%)	6 (4%)	2	23
9	AI	125/128 (98%)	84 (67%)	32 (26%)	9 (7%)	1	13
9	CI	125/128 (98%)	87 (70%)	23 (18%)	15 (12%)	0	5
10	AJ	97/105 (92%)	59 (61%)	31 (32%)	7 (7%)	1	13
10	CJ	97/105 (92%)	60 (62%)	25 (26%)	12 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	117/129 (91%)	92 (79%)	19 (16%)	6 (5%)	2	20
11	CK	117/129 (91%)	92 (79%)	23 (20%)	2 (2%)	9	44
12	AL	123/132 (93%)	78 (63%)	25 (20%)	20 (16%)	0	3
12	CL	123/132 (93%)	91 (74%)	20 (16%)	12 (10%)	0	8
13	AM	123/126 (98%)	82 (67%)	23 (19%)	18 (15%)	0	3
13	CM	123/126 (98%)	78 (63%)	22 (18%)	23 (19%)	0	1
14	AN	58/61 (95%)	40 (69%)	11 (19%)	7 (12%)	0	5
14	CN	58/61 (95%)	37 (64%)	14 (24%)	7 (12%)	0	5
15	AO	86/89 (97%)	65 (76%)	20 (23%)	1 (1%)	13	51
15	CO	86/89 (97%)	55 (64%)	25 (29%)	6 (7%)	1	14
16	AP	82/88 (93%)	53 (65%)	25 (30%)	4 (5%)	2	21
16	CP	82/88 (93%)	66 (80%)	13 (16%)	3 (4%)	3	28
17	AQ	98/105 (93%)	79 (81%)	13 (13%)	6 (6%)	1	16
17	CQ	98/105 (93%)	77 (79%)	15 (15%)	6 (6%)	1	16
18	AR	68/88 (77%)	49 (72%)	12 (18%)	7 (10%)	0	7
18	CR	68/88 (77%)	49 (72%)	11 (16%)	8 (12%)	0	5
19	AS	77/93 (83%)	56 (73%)	15 (20%)	6 (8%)	1	11
19	CS	77/93 (83%)	47 (61%)	17 (22%)	13 (17%)	0	2
20	AT	97/106 (92%)	68 (70%)	22 (23%)	7 (7%)	1	13
20	CT	97/106 (92%)	67 (69%)	18 (19%)	12 (12%)	0	5
21	AU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2
21	CU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	1	9
27	BC	183/229 (80%)	85 (46%)	52 (28%)	46 (25%)	0	0
27	DC	183/229 (80%)	87 (48%)	45 (25%)	51 (28%)	0	0
28	BD	270/276 (98%)	200 (74%)	38 (14%)	32 (12%)	0	5
28	DD	270/276 (98%)	202 (75%)	44 (16%)	24 (9%)	1	9
29	BE	203/206 (98%)	145 (71%)	36 (18%)	22 (11%)	0	6
29	DE	203/206 (98%)	134 (66%)	36 (18%)	33 (16%)	0	3
30	BF	206/210 (98%)	142 (69%)	44 (21%)	20 (10%)	0	8
30	DF	200/210 (95%)	160 (80%)	29 (14%)	11 (6%)	2	19
31	BG	179/182 (98%)	121 (68%)	36 (20%)	22 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	DG	179/182 (98%)	124 (69%)	30 (17%)	25 (14%)	0	4
32	BH	158/180 (88%)	96 (61%)	37 (23%)	25 (16%)	0	3
32	DH	166/180 (92%)	96 (58%)	42 (25%)	28 (17%)	0	2
33	BI	143/148 (97%)	101 (71%)	26 (18%)	16 (11%)	0	6
33	DI	144/148 (97%)	78 (54%)	39 (27%)	27 (19%)	0	1
34	BN	137/140 (98%)	91 (66%)	24 (18%)	22 (16%)	0	3
34	DN	137/140 (98%)	86 (63%)	39 (28%)	12 (9%)	1	9
35	BO	120/122 (98%)	95 (79%)	17 (14%)	8 (7%)	1	15
35	DO	120/122 (98%)	97 (81%)	18 (15%)	5 (4%)	3	24
36	BP	148/150 (99%)	86 (58%)	26 (18%)	36 (24%)	0	0
36	DP	148/150 (99%)	86 (58%)	23 (16%)	39 (26%)	0	0
37	BQ	139/141 (99%)	104 (75%)	24 (17%)	11 (8%)	1	11
37	DQ	139/141 (99%)	109 (78%)	18 (13%)	12 (9%)	1	9
38	BR	115/118 (98%)	78 (68%)	25 (22%)	12 (10%)	0	7
38	DR	116/118 (98%)	86 (74%)	20 (17%)	10 (9%)	1	9
39	BS	97/112 (87%)	53 (55%)	16 (16%)	28 (29%)	0	0
39	DS	109/112 (97%)	71 (65%)	21 (19%)	17 (16%)	0	3
40	BT	136/146 (93%)	90 (66%)	28 (21%)	18 (13%)	0	4
40	DT	136/146 (93%)	95 (70%)	19 (14%)	22 (16%)	0	3
41	BU	115/118 (98%)	73 (64%)	30 (26%)	12 (10%)	0	7
41	DU	115/118 (98%)	75 (65%)	30 (26%)	10 (9%)	1	9
42	BV	99/101 (98%)	75 (76%)	9 (9%)	15 (15%)	0	3
42	DV	99/101 (98%)	80 (81%)	9 (9%)	10 (10%)	0	7
43	BW	111/113 (98%)	81 (73%)	22 (20%)	8 (7%)	1	13
43	DW	111/113 (98%)	82 (74%)	19 (17%)	10 (9%)	1	9
44	BX	91/96 (95%)	69 (76%)	16 (18%)	6 (7%)	1	15
44	DX	91/96 (95%)	76 (84%)	11 (12%)	4 (4%)	2	23
45	BY	99/110 (90%)	50 (50%)	22 (22%)	27 (27%)	0	0
45	DY	100/110 (91%)	64 (64%)	11 (11%)	25 (25%)	0	0
46	BZ	175/206 (85%)	114 (65%)	40 (23%)	21 (12%)	0	5
46	DZ	175/206 (85%)	101 (58%)	46 (26%)	28 (16%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	B0	82/85 (96%)	64 (78%)	13 (16%)	5 (6%)	1	16
47	D0	82/85 (96%)	67 (82%)	8 (10%)	7 (8%)	1	10
48	B1	92/98 (94%)	68 (74%)	13 (14%)	11 (12%)	0	5
48	D1	92/98 (94%)	69 (75%)	12 (13%)	11 (12%)	0	5
49	B2	69/72 (96%)	49 (71%)	15 (22%)	5 (7%)	1	13
49	D2	69/72 (96%)	57 (83%)	5 (7%)	7 (10%)	0	7
50	B3	58/60 (97%)	48 (83%)	3 (5%)	7 (12%)	0	5
50	D3	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	1	9
51	B4	29/71 (41%)	17 (59%)	8 (28%)	4 (14%)	0	4
51	D4	38/71 (54%)	21 (55%)	12 (32%)	5 (13%)	0	4
52	B5	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	1	9
52	D5	57/60 (95%)	46 (81%)	5 (9%)	6 (10%)	0	7
53	B6	43/54 (80%)	17 (40%)	14 (33%)	12 (28%)	0	0
53	D6	43/54 (80%)	18 (42%)	15 (35%)	10 (23%)	0	0
54	B7	47/49 (96%)	38 (81%)	5 (11%)	4 (8%)	1	10
54	D7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	7	39
55	B8	62/65 (95%)	42 (68%)	14 (23%)	6 (10%)	0	8
55	D8	62/65 (95%)	41 (66%)	14 (23%)	7 (11%)	0	6
56	B9	34/37 (92%)	23 (68%)	10 (29%)	1 (3%)	4	33
56	D9	34/37 (92%)	27 (79%)	6 (18%)	1 (3%)	4	33
All	All	11730/12586 (93%)	8097 (69%)	2283 (20%)	1350 (12%)	0	6

5 of 1350 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	195	ASP
2	AB	238	LEU
3	AC	18	TRP
3	AC	20	SER

### 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	202/220 (92%)	161 (80%)	41 (20%)	1	7
2	CB	202/220 (92%)	155 (77%)	47 (23%)	1	4
3	AC	160/188 (85%)	127 (79%)	33 (21%)	1	7
3	CC	160/188 (85%)	130 (81%)	30 (19%)	1	8
4	AD	180/181 (99%)	149 (83%)	31 (17%)	2	12
4	CD	180/181 (99%)	151 (84%)	29 (16%)	2	15
5	AE	115/123 (94%)	97 (84%)	18 (16%)	2	16
5	CE	115/123 (94%)	87 (76%)	28 (24%)	0	4
6	AF	90/90 (100%)	76 (84%)	14 (16%)	2	17
6	CF	90/90 (100%)	79 (88%)	11 (12%)	5	24
7	AG	126/127 (99%)	103 (82%)	23 (18%)	1	9
7	CG	126/127 (99%)	106 (84%)	20 (16%)	2	15
8	AH	119/119 (100%)	101 (85%)	18 (15%)	3	18
8	CH	119/119 (100%)	87 (73%)	32 (27%)	0	3
9	AI	98/99 (99%)	77 (79%)	21 (21%)	1	6
9	CI	98/99 (99%)	72 (74%)	26 (26%)	0	3
10	AJ	88/92 (96%)	66 (75%)	22 (25%)	0	4
10	CJ	88/92 (96%)	66 (75%)	22 (25%)	0	4
11	AK	90/99 (91%)	74 (82%)	16 (18%)	2	10
11	CK	90/99 (91%)	72 (80%)	18 (20%)	1	7
12	AL	104/109 (95%)	85 (82%)	19 (18%)	1	9
12	CL	104/109 (95%)	84 (81%)	20 (19%)	1	8
13	AM	99/101 (98%)	82 (83%)	17 (17%)	2	12
13	CM	100/101 (99%)	83 (83%)	17 (17%)	2	12
14	AN	49/50 (98%)	37 (76%)	12 (24%)	0	4
14	CN	49/50 (98%)	38 (78%)	11 (22%)	1	5
15	AO	79/80 (99%)	64 (81%)	15 (19%)	1	8
15	CO	79/80 (99%)	66 (84%)	13 (16%)	2	14
16	AP	72/74 (97%)	58 (81%)	14 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	CP	72/74 (97%)	58 (81%)	14 (19%)	1	8
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	10	40
17	CQ	94/97 (97%)	82 (87%)	12 (13%)	4	23
18	AR	61/77 (79%)	51 (84%)	10 (16%)	2	14
18	CR	61/77 (79%)	50 (82%)	11 (18%)	1	10
19	AS	69/80 (86%)	51 (74%)	18 (26%)	0	3
19	CS	69/80 (86%)	49 (71%)	20 (29%)	0	3
20	AT	76/82 (93%)	56 (74%)	20 (26%)	0	3
20	CT	76/82 (93%)	53 (70%)	23 (30%)	0	2
21	AU	19/22 (86%)	18 (95%)	1 (5%)	22	56
21	CU	19/22 (86%)	14 (74%)	5 (26%)	0	3
27	BC	61/181 (34%)	49 (80%)	12 (20%)	1	8
27	DC	61/181 (34%)	53 (87%)	8 (13%)	4	22
28	BD	213/218 (98%)	164 (77%)	49 (23%)	1	5
28	DD	213/218 (98%)	178 (84%)	35 (16%)	2	14
29	BE	165/166 (99%)	125 (76%)	40 (24%)	0	4
29	DE	165/166 (99%)	141 (86%)	24 (14%)	3	19
30	BF	165/166 (99%)	127 (77%)	38 (23%)	1	5
30	DF	161/166 (97%)	136 (84%)	25 (16%)	2	17
31	BG	155/156 (99%)	118 (76%)	37 (24%)	0	4
31	DG	155/156 (99%)	135 (87%)	20 (13%)	4	22
32	BH	132/148 (89%)	114 (86%)	18 (14%)	3	21
32	DH	140/148 (95%)	114 (81%)	26 (19%)	1	9
33	BI	122/124 (98%)	95 (78%)	27 (22%)	1	5
33	DI	122/124 (98%)	92 (75%)	30 (25%)	0	4
34	BN	117/119 (98%)	88 (75%)	29 (25%)	0	4
34	DN	117/119 (98%)	96 (82%)	21 (18%)	2	10
35	BO	100/100 (100%)	77 (77%)	23 (23%)	1	5
35	DO	100/100 (100%)	90 (90%)	10 (10%)	7	33
36	BP	116/116 (100%)	86 (74%)	30 (26%)	0	3
36	DP	116/116 (100%)	89 (77%)	27 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	BQ	111/111 (100%)	81 (73%)	30 (27%)	0	3
37	DQ	111/111 (100%)	92 (83%)	19 (17%)	2	12
38	BR	100/101 (99%)	68 (68%)	32 (32%)	0	2
38	DR	101/101 (100%)	86 (85%)	15 (15%)	3	18
39	BS	77/88 (88%)	56 (73%)	21 (27%)	0	3
39	DS	87/88 (99%)	75 (86%)	12 (14%)	3	21
40	BT	120/127 (94%)	90 (75%)	30 (25%)	0	4
40	DT	120/127 (94%)	91 (76%)	29 (24%)	0	4
41	BU	93/94 (99%)	70 (75%)	23 (25%)	0	4
41	DU	92/94 (98%)	80 (87%)	12 (13%)	4	22
42	BV	82/82 (100%)	55 (67%)	27 (33%)	0	2
42	DV	82/82 (100%)	64 (78%)	18 (22%)	1	5
43	BW	91/92 (99%)	69 (76%)	22 (24%)	0	4
43	DW	91/92 (99%)	83 (91%)	8 (9%)	10	39
44	BX	74/78 (95%)	58 (78%)	16 (22%)	1	6
44	DX	74/78 (95%)	61 (82%)	13 (18%)	2	11
45	BY	84/91 (92%)	67 (80%)	17 (20%)	1	7
45	DY	85/91 (93%)	66 (78%)	19 (22%)	1	5
46	BZ	155/179 (87%)	124 (80%)	31 (20%)	1	7
46	DZ	155/179 (87%)	136 (88%)	19 (12%)	4	24
47	B0	66/67 (98%)	57 (86%)	9 (14%)	3	21
47	D0	66/67 (98%)	57 (86%)	9 (14%)	3	21
48	B1	78/83 (94%)	61 (78%)	17 (22%)	1	5
48	D1	78/83 (94%)	61 (78%)	17 (22%)	1	5
49	B2	66/67 (98%)	53 (80%)	13 (20%)	1	8
49	D2	66/67 (98%)	53 (80%)	13 (20%)	1	8
50	B3	51/52 (98%)	40 (78%)	11 (22%)	1	6
50	D3	51/52 (98%)	49 (96%)	2 (4%)	32	65
51	B4	27/63 (43%)	17 (63%)	10 (37%)	0	1
51	D4	35/63 (56%)	31 (89%)	4 (11%)	5	28
52	B5	51/52 (98%)	42 (82%)	9 (18%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	D5	51/52 (98%)	43 (84%)	8 (16%)	2	16
53	B6	43/52 (83%)	31 (72%)	12 (28%)	0	3
53	D6	43/52 (83%)	33 (77%)	10 (23%)	1	4
54	B7	41/42 (98%)	35 (85%)	6 (15%)	3	19
54	D7	41/42 (98%)	37 (90%)	4 (10%)	8	34
55	B8	53/55 (96%)	38 (72%)	15 (28%)	0	3
55	D8	53/55 (96%)	41 (77%)	12 (23%)	1	5
56	B9	33/34 (97%)	29 (88%)	4 (12%)	5	25
56	D9	33/34 (97%)	29 (88%)	4 (12%)	5	25
All	All	9688/10428 (93%)	7777 (80%)	1911 (20%)	1	8

5 of 1911 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	BX	43	VAL
2	CB	196	LEU
42	DV	91	TYR
45	BY	89	PHE
50	B3	53	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
2	CB	204	ASN
12	CL	9	GLN
48	D1	45	ASN
5	CE	78	HIS
9	CI	38	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	366 (24%)	109 (7%)
1	CA	1503/1522 (98%)	359 (23%)	115 (7%)
22	AV	76/77 (98%)	26 (34%)	3 (3%)
22	CV	76/77 (98%)	30 (39%)	4 (5%)
23	AW	75/76 (98%)	22 (29%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	AY	16/76 (21%)	5 (31%)	0
23	CW	75/76 (98%)	26 (34%)	0
23	CY	16/76 (21%)	8 (50%)	0
24	AX	11/24 (45%)	4 (36%)	0
24	CX	9/24 (37%)	4 (44%)	1 (11%)
25	BA	2804/2915 (96%)	803 (28%)	260 (9%)
25	DA	2818/2915 (96%)	804 (28%)	264 (9%)
26	BB	118/122 (96%)	25 (21%)	5 (4%)
26	DB	118/122 (96%)	24 (20%)	7 (5%)
All	All	9218/9624 (95%)	2506 (27%)	768 (8%)

5 of 2506 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	10	A
1	AA	13	U

5 of 768 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2602	A
1	CA	575	G
25	DA	2238	G
25	BA	2750	A
1	CA	129(A)	G

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1039 ligands modelled in this entry, 1037 are monoatomic - leaving 2 for Mogul analysis.



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	PAR	CA	1741	-	45,45,45	1.55	8 (17%)	64,67,67	1.18	5 (7%)
58	PAR	AA	7111	-	45,45,45	1.54	9 (20%)	64,67,67	1.18	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	CA	1741	-	-	3/18/94/94	0/4/4/4
58	PAR	AA	7111	-	-	3/18/94/94	0/4/4/4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	CA	1741	PAR	C64-C54	3.95	1.57	1.52
58	AA	7111	PAR	O54-C14	3.93	1.51	1.41
58	CA	1741	PAR	O54-C14	3.91	1.51	1.41
58	AA	7111	PAR	C64-C54	3.90	1.57	1.52
58	CA	1741	PAR	C31-C21	3.20	1.57	1.53

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AA	7111	PAR	O33-C14-C24	3.35	113.99	108.22
58	CA	1741	PAR	O33-C14-C24	3.31	113.91	108.22
58	CA	1741	PAR	C14-O54-C54	3.22	120.01	113.69
58	AA	7111	PAR	C14-O54-C54	3.22	120.01	113.69
58	AA	7111	PAR	O54-C54-C64	3.22	112.00	106.01

There are no chirality outliers.

5 of 6 torsion outliers are listed below:



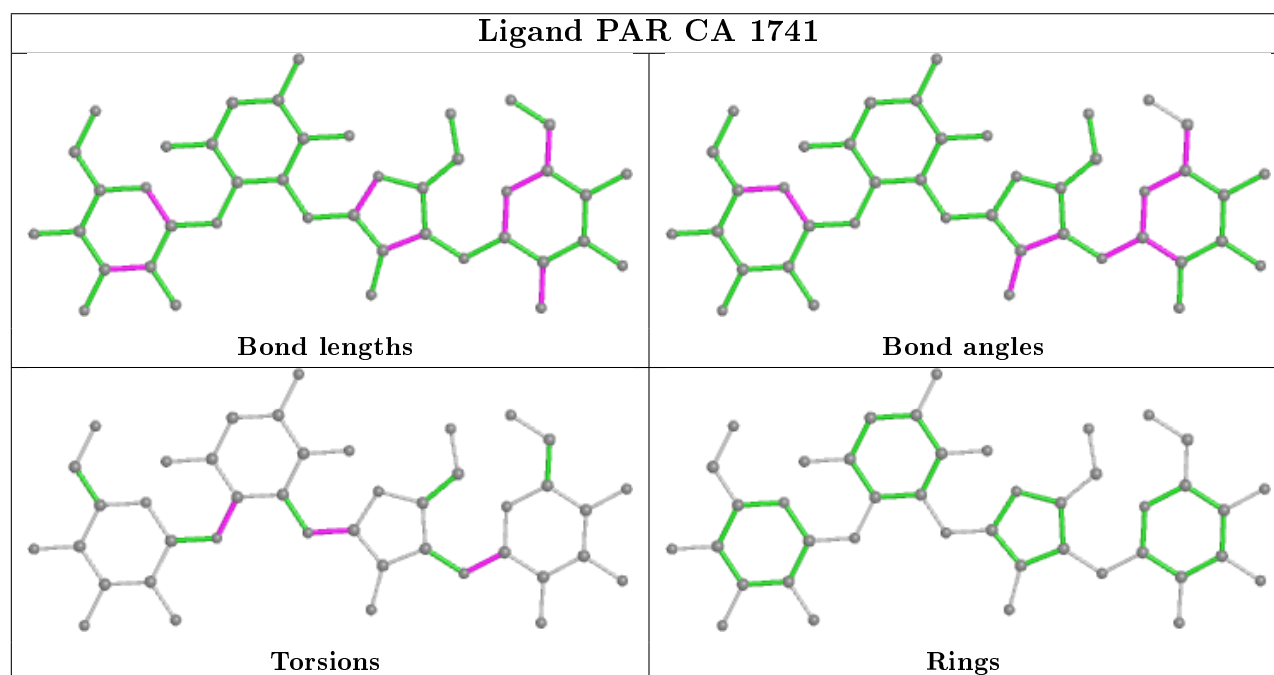
Mol	Chain	Res	Type	Atoms
58	CA	1741	PAR	C24-C14-O33-C33
58	AA	7111	PAR	C24-C14-O33-C33
58	CA	1741	PAR	C52-C42-O11-C11
58	AA	7111	PAR	C52-C42-O11-C11
58	CA	1741	PAR	C23-C13-O52-C52

There are no ring outliers.

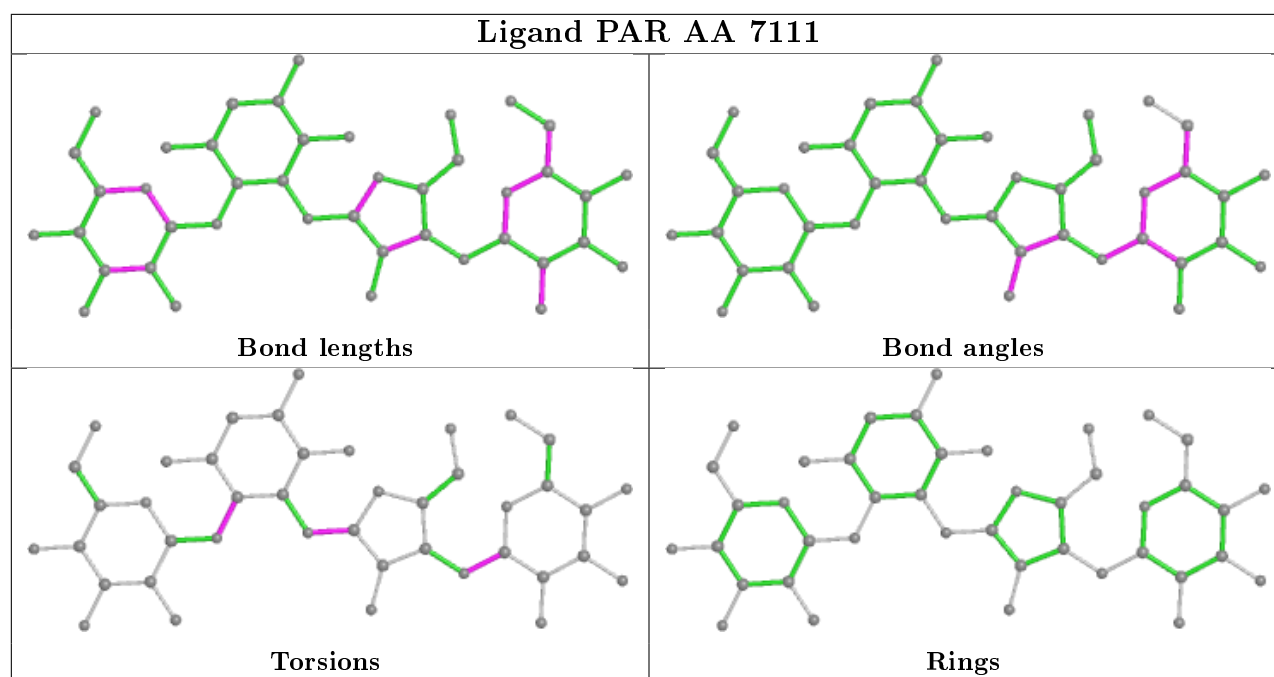
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	CA	1741	PAR	2	0
58	AA	7111	PAR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1453:U	O3'	1455:G	P	1.97



## 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	1504/1522 (98%)	0.18	46 (3%) 49 36	31, 78, 168, 331	0
1	CA	1504/1522 (98%)	0.21	58 (3%) 39 29	24, 68, 165, 363	0
2	AB	235/256 (91%)	-0.08	4 (1%) 70 57	67, 121, 201, 279	0
2	CB	235/256 (91%)	-0.10	9 (3%) 40 30	44, 109, 202, 287	0
3	AC	207/239 (86%)	-0.13	1 (0%) 91 84	44, 104, 173, 240	0
3	CC	207/239 (86%)	-0.21	1 (0%) 91 84	38, 90, 151, 227	0
4	AD	208/209 (99%)	-0.29	3 (1%) 75 62	37, 89, 153, 217	0
4	CD	208/209 (99%)	-0.31	1 (0%) 91 84	30, 77, 129, 209	0
5	AE	151/162 (93%)	-0.24	2 (1%) 77 65	44, 87, 151, 240	0
5	CE	151/162 (93%)	-0.24	2 (1%) 77 65	22, 71, 131, 266	0
6	AF	101/101 (100%)	-0.20	0 100 100	29, 74, 120, 178	0
6	CF	101/101 (100%)	-0.30	0 100 100	25, 68, 134, 192	0
7	AG	155/156 (99%)	-0.15	7 (4%) 33 24	50, 93, 149, 256	0
7	CG	155/156 (99%)	-0.14	5 (3%) 47 36	32, 87, 151, 269	0
8	AH	138/138 (100%)	-0.28	0 100 100	41, 85, 129, 183	0
8	CH	138/138 (100%)	-0.34	1 (0%) 87 79	38, 75, 123, 181	0
9	AI	127/128 (99%)	0.02	3 (2%) 59 45	55, 113, 161, 319	0
9	CI	127/128 (99%)	-0.06	3 (2%) 59 45	45, 97, 170, 245	0
10	AJ	99/105 (94%)	0.29	4 (4%) 38 28	58, 124, 197, 302	0
10	CJ	99/105 (94%)	0.26	5 (5%) 28 20	38, 115, 191, 204	0
11	AK	119/129 (92%)	-0.12	4 (3%) 45 34	41, 77, 147, 249	0
11	CK	119/129 (92%)	-0.06	3 (2%) 57 43	29, 73, 139, 188	0
12	AL	125/132 (94%)	-0.15	3 (2%) 59 45	31, 64, 129, 300	0
12	CL	125/132 (94%)	-0.29	3 (2%) 59 45	9, 47, 127, 252	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	125/126 (99%)	0.03	4 (3%) 47 36	29, 94, 148, 314	0
13	CM	125/126 (99%)	0.08	6 (4%) 30 23	39, 87, 174, 274	0
14	AN	60/61 (98%)	-0.06	1 (1%) 70 57	53, 92, 138, 207	0
14	CN	60/61 (98%)	-0.12	0 100 100	34, 71, 111, 194	0
15	AO	88/89 (98%)	-0.28	0 100 100	35, 80, 132, 142	0
15	CO	88/89 (98%)	-0.33	0 100 100	23, 69, 122, 147	0
16	AP	84/88 (95%)	-0.43	0 100 100	48, 74, 122, 182	0
16	CP	84/88 (95%)	-0.30	0 100 100	44, 76, 139, 200	0
17	AQ	100/105 (95%)	-0.22	0 100 100	50, 91, 141, 174	0
17	CQ	100/105 (95%)	-0.18	1 (1%) 82 71	38, 87, 144, 192	0
18	AR	70/88 (79%)	-0.21	3 (4%) 35 26	35, 77, 126, 183	0
18	CR	70/88 (79%)	-0.35	1 (1%) 75 62	36, 70, 122, 205	0
19	AS	79/93 (84%)	0.13	1 (1%) 77 65	46, 104, 202, 268	0
19	CS	79/93 (84%)	0.08	0 100 100	27, 82, 153, 206	0
20	AT	99/106 (93%)	0.06	5 (5%) 28 20	42, 90, 173, 211	0
20	CT	99/106 (93%)	0.13	3 (3%) 50 37	40, 97, 192, 295	0
21	AU	25/27 (92%)	0.72	5 (20%) 1 1	36, 92, 165, 229	0
21	CU	25/27 (92%)	-0.03	0 100 100	50, 78, 107, 150	0
22	AV	77/77 (100%)	0.10	0 100 100	45, 82, 163, 276	0
22	CV	77/77 (100%)	0.19	3 (3%) 39 29	32, 72, 133, 253	0
23	AW	76/76 (100%)	1.27	17 (22%) 0 0	48, 175, 249, 317	0
23	AY	17/76 (22%)	0.41	0 100 100	64, 94, 167, 176	0
23	CW	76/76 (100%)	1.63	24 (31%) 0 0	34, 184, 271, 295	0
23	CY	17/76 (22%)	0.69	0 100 100	44, 75, 149, 186	0
24	AX	12/24 (50%)	0.73	2 (16%) 1 1	49, 74, 217, 234	0
24	CX	10/24 (41%)	0.55	1 (10%) 7 6	42, 58, 144, 213	0
25	BA	2810/2915 (96%)	0.18	115 (4%) 37 27	17, 58, 187, 375	0
25	DA	2824/2915 (96%)	0.11	106 (3%) 40 30	6, 42, 178, 370	0
26	BB	119/122 (97%)	0.17	1 (0%) 86 75	59, 94, 132, 182	0
26	DB	119/122 (97%)	0.12	2 (1%) 70 57	38, 68, 113, 174	0
27	BC	191/229 (83%)	1.88	74 (38%) 0 0	89, 200, 319, 378	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	DC	191/229 (83%)	2.28	93 (48%) 0 0	64, 208, 290, 334	0
28	BD	272/276 (98%)	-0.40	0 100 100	9, 45, 89, 166	0
28	DD	272/276 (98%)	-0.49	0 100 100	3, 33, 80, 197	0
29	BE	205/206 (99%)	-0.23	5 (2%) 59 45	17, 66, 128, 289	0
29	DE	205/206 (99%)	-0.23	4 (1%) 65 52	11, 55, 160, 338	0
30	BF	208/210 (99%)	-0.36	4 (1%) 66 53	14, 64, 164, 286	0
30	DF	202/210 (96%)	-0.32	2 (0%) 82 71	5, 51, 127, 208	0
31	BG	181/182 (99%)	-0.18	6 (3%) 46 35	40, 95, 175, 268	0
31	DG	181/182 (99%)	-0.18	4 (2%) 62 48	25, 76, 143, 219	0
32	BH	160/180 (88%)	0.89	31 (19%) 1 1	85, 179, 331, 429	0
32	DH	168/180 (93%)	0.02	1 (0%) 89 81	29, 81, 155, 234	0
33	BI	145/148 (97%)	-0.13	5 (3%) 45 34	33, 96, 156, 185	0
33	DI	146/148 (98%)	-0.07	1 (0%) 87 79	15, 104, 166, 207	0
34	BN	139/140 (99%)	-0.30	1 (0%) 87 79	36, 79, 147, 305	0
34	DN	139/140 (99%)	-0.34	0 100 100	7, 61, 137, 185	0
35	BO	122/122 (100%)	-0.50	0 100 100	32, 65, 97, 124	0
35	DO	122/122 (100%)	-0.61	0 100 100	10, 41, 84, 112	0
36	BP	150/150 (100%)	0.30	5 (3%) 46 35	27, 87, 179, 250	0
36	DP	150/150 (100%)	0.07	3 (2%) 65 52	23, 71, 151, 264	0
37	BQ	141/141 (100%)	-0.24	3 (2%) 63 50	36, 74, 126, 421	0
37	DQ	141/141 (100%)	-0.40	0 100 100	12, 52, 108, 281	0
38	BR	117/118 (99%)	-0.42	0 100 100	21, 57, 107, 148	0
38	DR	118/118 (100%)	-0.47	0 100 100	15, 50, 92, 126	0
39	BS	99/112 (88%)	-0.17	1 (1%) 82 71	38, 100, 171, 347	0
39	DS	111/112 (99%)	-0.13	2 (1%) 68 55	33, 73, 147, 197	0
40	BT	138/146 (94%)	-0.04	6 (4%) 35 26	29, 80, 225, 351	0
40	DT	138/146 (94%)	-0.05	8 (5%) 23 17	20, 71, 212, 304	0
41	BU	117/118 (99%)	-0.40	1 (0%) 84 73	29, 64, 131, 281	0
41	DU	117/118 (99%)	-0.51	1 (0%) 84 73	17, 52, 114, 180	0
42	BV	101/101 (100%)	-0.28	0 100 100	23, 90, 149, 344	0
42	DV	101/101 (100%)	-0.12	1 (0%) 82 71	9, 70, 131, 303	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BW	113/113 (100%)	-0.23	2 (1%) 68 55	19, 49, 113, 319	0
43	DW	113/113 (100%)	-0.32	0 100 100	14, 42, 128, 204	0
44	BX	93/96 (96%)	-0.34	0 100 100	30, 63, 99, 149	0
44	DX	93/96 (96%)	-0.33	0 100 100	12, 42, 87, 144	0
45	BY	101/110 (91%)	0.88	20 (19%) 1 1	42, 92, 253, 363	0
45	DY	102/110 (92%)	0.06	3 (2%) 51 38	28, 82, 182, 226	0
46	BZ	177/206 (85%)	0.41	17 (9%) 8 6	45, 125, 202, 316	0
46	DZ	177/206 (85%)	0.54	18 (10%) 6 6	29, 116, 254, 322	0
47	B0	84/85 (98%)	-0.03	6 (7%) 16 13	31, 69, 170, 242	0
47	D0	84/85 (98%)	-0.08	7 (8%) 11 10	18, 52, 136, 286	0
48	B1	94/98 (95%)	-0.18	1 (1%) 80 69	17, 53, 113, 219	0
48	D1	94/98 (95%)	-0.31	0 100 100	7, 44, 122, 237	0
49	B2	71/72 (98%)	-0.24	2 (2%) 53 40	35, 77, 128, 195	0
49	D2	71/72 (98%)	-0.23	0 100 100	14, 54, 137, 267	0
50	B3	60/60 (100%)	-0.03	2 (3%) 46 35	35, 75, 125, 382	0
50	D3	60/60 (100%)	-0.25	1 (1%) 70 57	20, 65, 142, 236	0
51	B4	31/71 (43%)	-0.16	0 100 100	67, 121, 152, 204	0
51	D4	40/71 (56%)	0.07	2 (5%) 28 21	55, 116, 173, 266	0
52	B5	59/60 (98%)	0.15	6 (10%) 6 6	17, 72, 180, 340	0
52	D5	59/60 (98%)	0.16	3 (5%) 28 20	12, 63, 214, 299	0
53	B6	45/54 (83%)	1.21	12 (26%) 0 0	44, 138, 207, 343	0
53	D6	45/54 (83%)	1.82	17 (37%) 0 0	59, 139, 235, 285	0
54	B7	49/49 (100%)	-0.41	0 100 100	11, 41, 123, 149	0
54	D7	49/49 (100%)	-0.59	0 100 100	1, 23, 101, 204	0
55	B8	64/65 (98%)	-0.05	2 (3%) 49 36	20, 60, 129, 325	0
55	D8	64/65 (98%)	-0.38	0 100 100	12, 51, 115, 172	0
56	B9	36/37 (97%)	3.56	28 (77%) 0 0	120, 197, 269, 389	0
56	D9	36/37 (97%)	3.45	31 (86%) 0 0	115, 172, 217, 282	0
All	All	21184/22210 (95%)	0.06	911 (4%) 35 26	1, 71, 192, 429	0

The worst 5 of 911 RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
25	DA	2802	G	15.7
25	BA	2802	G	13.6
1	AA	81	U	13.5
1	AA	89	C	12.6
23	CW	20	U	12.5

## 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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	BA	3315	1/1	0.16	0.44	84,84,84,84	0
57	MG	DA	9655	1/1	0.37	0.92	35,35,35,35	0
57	MG	DA	9350	1/1	0.44	0.18	48,48,48,48	1
57	MG	BA	3149	1/1	0.47	0.34	27,27,27,27	0
57	MG	BA	3036	1/1	0.47	0.19	78,78,78,78	1
57	MG	BA	3037	1/1	0.49	0.27	83,83,83,83	0
57	MG	BA	3126	1/1	0.49	0.61	44,44,44,44	0
57	MG	CA	1687	1/1	0.52	0.36	47,47,47,47	0
57	MG	BA	3122	1/1	0.55	0.30	13,13,13,13	0
57	MG	DA	9661	1/1	0.57	0.38	57,57,57,57	0
57	MG	AA	7086	1/1	0.57	1.00	30,30,30,30	0
57	MG	BA	3271	1/1	0.57	0.73	52,52,52,52	0
57	MG	DA	9626	1/1	0.57	0.19	8,8,8,8	1
57	MG	CA	1639	1/1	0.58	0.69	55,55,55,55	0
57	MG	BA	3227	1/1	0.58	0.72	40,40,40,40	0
57	MG	DA	9429	1/1	0.60	0.97	51,51,51,51	0
57	MG	BB	205	1/1	0.61	0.11	19,19,19,19	1
57	MG	CA	1699	1/1	0.61	0.40	45,45,45,45	1
57	MG	CA	1702	1/1	0.61	0.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3273	1/1	0.63	0.26	71,71,71,71	0
57	MG	BA	3063	1/1	0.63	0.47	55,55,55,55	0
57	MG	BA	3248	1/1	0.63	0.70	49,49,49,49	0
57	MG	CA	1651	1/1	0.64	0.44	39,39,39,39	0
57	MG	BA	3277	1/1	0.64	0.56	2,2,2,2	1
57	MG	AA	7002	1/1	0.64	0.48	35,35,35,35	0
57	MG	BA	3216	1/1	0.65	0.50	48,48,48,48	0
57	MG	CA	1683	1/1	0.65	0.26	29,29,29,29	0
57	MG	DA	9685	1/1	0.65	0.64	22,22,22,22	0
57	MG	BA	3306	1/1	0.66	0.47	48,48,48,48	0
57	MG	BB	203	1/1	0.66	0.69	16,16,16,16	1
57	MG	CA	1609	1/1	0.66	0.42	30,30,30,30	0
57	MG	CA	1621	1/1	0.66	0.38	52,52,52,52	0
57	MG	D1	101	1/1	0.66	0.60	55,55,55,55	0
57	MG	AA	7076	1/1	0.66	0.57	60,60,60,60	0
57	MG	DA	9687	1/1	0.67	0.29	12,12,12,12	0
57	MG	CA	1704	1/1	0.67	0.99	28,28,28,28	0
57	MG	DA	9440	1/1	0.67	0.49	25,25,25,25	0
57	MG	BA	3203	1/1	0.68	0.45	37,37,37,37	0
57	MG	CA	1723	1/1	0.68	0.34	15,15,15,15	0
57	MG	CA	1658	1/1	0.68	0.34	44,44,44,44	0
57	MG	BA	3120	1/1	0.68	0.64	24,24,24,24	0
57	MG	AA	7055	1/1	0.68	0.46	29,29,29,29	0
57	MG	DA	9595	1/1	0.68	0.58	49,49,49,49	0
57	MG	BA	3028	1/1	0.68	0.54	44,44,44,44	0
57	MG	BA	3039	1/1	0.69	0.39	30,30,30,30	0
57	MG	BA	3313	1/1	0.69	0.26	42,42,42,42	0
57	MG	DA	9657	1/1	0.69	0.32	29,29,29,29	0
57	MG	AA	7046	1/1	0.70	0.43	35,35,35,35	0
57	MG	CA	1731	1/1	0.70	0.15	30,30,30,30	0
57	MG	AA	7071	1/1	0.70	0.52	38,38,38,38	0
57	MG	DA	9434	1/1	0.70	0.45	4,4,4,4	0
57	MG	DA	9622	1/1	0.70	0.55	36,36,36,36	0
57	MG	BA	3076	1/1	0.70	0.22	18,18,18,18	0
57	MG	BA	3052	1/1	0.70	0.46	40,40,40,40	0
57	MG	CA	1708	1/1	0.70	0.67	34,34,34,34	0
57	MG	DA	9665	1/1	0.70	0.99	9,9,9,9	0
57	MG	DA	9624	1/1	0.70	0.23	18,18,18,18	1
57	MG	DA	9559	1/1	0.71	0.55	58,58,58,58	0
57	MG	BA	3074	1/1	0.71	0.62	34,34,34,34	0
57	MG	DA	9395	1/1	0.71	0.24	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	1691	1/1	0.71	0.69	91,91,91,91	0
57	MG	BA	3245	1/1	0.71	0.72	45,45,45,45	0
57	MG	BA	3278	1/1	0.71	0.40	22,22,22,22	0
57	MG	DA	9416	1/1	0.71	0.33	38,38,38,38	0
57	MG	DA	9405	1/1	0.71	0.29	5,5,5,5	0
57	MG	BA	3262	1/1	0.72	0.64	39,39,39,39	0
57	MG	CA	1674	1/1	0.72	0.40	89,89,89,89	0
57	MG	DA	9329	1/1	0.72	0.50	21,21,21,21	0
57	MG	CA	1716	1/1	0.72	0.46	26,26,26,26	0
57	MG	AA	7080	1/1	0.72	0.43	8,8,8,8	1
57	MG	DA	9388	1/1	0.72	0.18	28,28,28,28	0
57	MG	AA	7097	1/1	0.72	0.46	20,20,20,20	0
57	MG	CA	1637	1/1	0.72	0.34	57,57,57,57	0
57	MG	DA	9569	1/1	0.73	0.82	54,54,54,54	0
57	MG	DA	9674	1/1	0.73	0.81	17,17,17,17	0
57	MG	BA	3110	1/1	0.73	0.59	23,23,23,23	1
57	MG	BA	3173	1/1	0.73	0.62	27,27,27,27	0
57	MG	CA	1713	1/1	0.73	0.54	31,31,31,31	0
57	MG	DA	9550	1/1	0.73	0.44	55,55,55,55	0
57	MG	AA	7010	1/1	0.73	0.26	30,30,30,30	0
57	MG	BA	3242	1/1	0.73	0.59	44,44,44,44	0
57	MG	BA	3119	1/1	0.73	0.32	42,42,42,42	0
57	MG	CA	1612	1/1	0.73	0.30	31,31,31,31	0
57	MG	CA	1714	1/1	0.74	0.45	53,53,53,53	0
57	MG	DA	9467	1/1	0.74	0.39	53,53,53,53	1
57	MG	DA	9694	1/1	0.74	0.85	25,25,25,25	0
57	MG	BA	3318	1/1	0.74	0.41	37,37,37,37	0
57	MG	DA	9432	1/1	0.74	0.63	38,38,38,38	0
57	MG	BA	3246	1/1	0.74	0.66	33,33,33,33	0
57	MG	DA	9658	1/1	0.74	0.19	36,36,36,36	0
57	MG	DA	9648	1/1	0.75	0.30	34,34,34,34	0
57	MG	CA	1739	1/1	0.75	0.67	36,36,36,36	0
57	MG	AA	7074	1/1	0.75	0.76	26,26,26,26	0
57	MG	BP	201	1/1	0.75	0.20	166,166,166,166	0
57	MG	AA	7092	1/1	0.75	0.13	37,37,37,37	0
57	MG	DA	9399	1/1	0.75	0.78	52,52,52,52	0
57	MG	BA	3196	1/1	0.75	0.76	30,30,30,30	0
57	MG	CA	1672	1/1	0.75	0.39	62,62,62,62	0
57	MG	DA	9412	1/1	0.75	0.34	27,27,27,27	0
57	MG	CA	1682	1/1	0.76	0.27	60,60,60,60	0
57	MG	DA	9628	1/1	0.76	0.28	35,35,35,35	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	9563	1/1	0.76	0.26	3,3,3,3	0
57	MG	DA	9573	1/1	0.76	0.40	45,45,45,45	0
57	MG	BA	3290	1/1	0.76	0.76	19,19,19,19	1
57	MG	AA	7065	1/1	0.76	0.38	23,23,23,23	0
57	MG	BA	3155	1/1	0.76	0.56	33,33,33,33	0
57	MG	DA	9643	1/1	0.76	0.72	34,34,34,34	1
57	MG	CV	103	1/1	0.77	0.33	43,43,43,43	1
57	MG	BA	3257	1/1	0.77	0.31	21,21,21,21	0
57	MG	DA	9438	1/1	0.77	0.38	21,21,21,21	0
57	MG	CA	1642	1/1	0.77	0.38	54,54,54,54	0
57	MG	DA	9677	1/1	0.77	0.50	27,27,27,27	0
57	MG	DA	9671	1/1	0.77	0.19	45,45,45,45	0
57	MG	CA	1666	1/1	0.77	0.36	66,66,66,66	0
57	MG	DA	9645	1/1	0.77	0.72	4,4,4,4	0
57	MG	DA	9602	1/1	0.77	0.52	37,37,37,37	0
57	MG	AA	7069	1/1	0.77	0.76	11,11,11,11	1
57	MG	BA	3095	1/1	0.77	1.02	35,35,35,35	0
57	MG	DA	9615	1/1	0.77	0.70	45,45,45,45	0
57	MG	BA	3026	1/1	0.77	0.50	29,29,29,29	0
57	MG	BA	3003	1/1	0.77	0.33	33,33,33,33	0
57	MG	BA	3320	1/1	0.77	0.42	54,54,54,54	0
57	MG	DA	9603	1/1	0.78	0.88	33,33,33,33	0
57	MG	CA	1728	1/1	0.78	0.35	59,59,59,59	0
57	MG	BA	3301	1/1	0.78	0.27	20,20,20,20	0
57	MG	BA	3164	1/1	0.78	0.43	39,39,39,39	0
57	MG	BA	3286	1/1	0.78	0.25	22,22,22,22	0
57	MG	CA	1722	1/1	0.78	0.34	27,27,27,27	0
57	MG	BA	3107	1/1	0.78	0.45	36,36,36,36	0
57	MG	DA	9378	1/1	0.78	0.35	29,29,29,29	0
57	MG	BA	3082	1/1	0.78	0.32	23,23,23,23	0
57	MG	DA	9570	1/1	0.79	0.31	61,61,61,61	0
57	MG	DA	9552	1/1	0.79	0.53	58,58,58,58	0
57	MG	DA	9441	1/1	0.79	0.58	31,31,31,31	1
57	MG	DA	9336	1/1	0.79	0.33	52,52,52,52	0
57	MG	CA	1694	1/1	0.79	0.72	51,51,51,51	0
57	MG	CA	1610	1/1	0.79	0.63	58,58,58,58	0
57	MG	CA	1706	1/1	0.79	0.36	32,32,32,32	0
57	MG	CA	1628	1/1	0.79	0.22	9,9,9,9	0
57	MG	BA	3297	1/1	0.79	0.93	46,46,46,46	0
57	MG	DA	9450	1/1	0.79	0.54	2,2,2,2	1
57	MG	AA	7027	1/1	0.79	0.41	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	9620	1/1	0.79	0.41	26,26,26,26	0
57	MG	DA	9600	1/1	0.79	0.34	55,55,55,55	0
57	MG	BA	3295	1/1	0.79	0.37	27,27,27,27	0
59	ZN	CN	101	1/1	0.79	0.19	171,171,171,171	0
57	MG	BA	3266	1/1	0.79	0.39	33,33,33,33	0
57	MG	BA	3117	1/1	0.79	0.67	11,11,11,11	1
57	MG	DA	9660	1/1	0.79	0.27	176,176,176,176	0
57	MG	DA	9676	1/1	0.79	0.23	13,13,13,13	0
57	MG	DA	9458	1/1	0.79	0.41	22,22,22,22	0
57	MG	BA	3317	1/1	0.79	0.73	21,21,21,21	0
57	MG	BA	3274	1/1	0.80	0.26	8,8,8,8	1
57	MG	AA	7096	1/1	0.80	0.55	31,31,31,31	0
57	MG	BA	3021	1/1	0.80	0.49	49,49,49,49	0
57	MG	BA	3108	1/1	0.80	0.25	27,27,27,27	0
57	MG	AX	101	1/1	0.80	0.28	43,43,43,43	0
57	MG	DA	9331	1/1	0.80	0.21	8,8,8,8	0
57	MG	DA	9681	1/1	0.80	0.35	13,13,13,13	0
57	MG	DA	9557	1/1	0.80	0.31	25,25,25,25	0
57	MG	AA	7082	1/1	0.80	0.28	24,24,24,24	0
57	MG	CA	1692	1/1	0.80	0.37	28,28,28,28	0
57	MG	BA	3103	1/1	0.80	0.19	31,31,31,31	0
57	MG	AA	7008	1/1	0.80	0.85	35,35,35,35	0
57	MG	DA	9419	1/1	0.80	0.95	10,10,10,10	1
57	MG	DA	9379	1/1	0.80	0.31	41,41,41,41	0
57	MG	AV	104	1/1	0.81	0.41	16,16,16,16	0
57	MG	DA	9348	1/1	0.81	0.72	47,47,47,47	0
57	MG	DA	9383	1/1	0.81	0.41	18,18,18,18	0
57	MG	AA	7031	1/1	0.81	0.20	44,44,44,44	0
57	MG	BA	3162	1/1	0.81	0.73	4,4,4,4	0
57	MG	DA	9635	1/1	0.81	0.59	24,24,24,24	0
57	MG	DB	205	1/1	0.81	0.17	6,6,6,6	1
57	MG	DA	9578	1/1	0.81	0.43	44,44,44,44	0
57	MG	BA	3322	1/1	0.81	0.35	54,54,54,54	0
57	MG	CA	1614	1/1	0.81	1.22	38,38,38,38	0
57	MG	CW	101	1/1	0.82	0.47	29,29,29,29	1
57	MG	DA	9374	1/1	0.82	0.40	28,28,28,28	0
57	MG	DA	9574	1/1	0.82	0.38	14,14,14,14	1
57	MG	DA	9421	1/1	0.82	0.36	28,28,28,28	0
57	MG	AA	7049	1/1	0.82	0.25	41,41,41,41	0
57	MG	DA	9335	1/1	0.82	0.33	21,21,21,21	0
57	MG	BA	3231	1/1	0.82	0.38	90,90,90,90	0
57	MG	DA	9579	1/1	0.82	0.67	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	7075	1/1	0.82	0.49	53,53,53,53	0
57	MG	AA	7011	1/1	0.82	0.40	43,43,43,43	0
57	MG	DA	9439	1/1	0.82	0.23	32,32,32,32	0
57	MG	BA	3264	1/1	0.82	0.65	36,36,36,36	0
57	MG	CX	101	1/1	0.82	0.23	25,25,25,25	0
57	MG	CA	1655	1/1	0.82	0.47	24,24,24,24	0
57	MG	DA	9325	1/1	0.82	0.48	32,32,32,32	0
57	MG	DA	9301	1/1	0.83	0.36	32,32,32,32	0
57	MG	DA	9688	1/1	0.83	0.40	78,78,78,78	0
57	MG	DB	202	1/1	0.83	0.23	28,28,28,28	0
57	MG	BA	3217	1/1	0.83	0.16	28,28,28,28	0
57	MG	DA	9418	1/1	0.83	0.28	61,61,61,61	0
57	MG	BA	3249	1/1	0.83	0.41	25,25,25,25	0
57	MG	DA	9693	1/1	0.83	0.97	47,47,47,47	0
57	MG	AA	7034	1/1	0.83	0.74	43,43,43,43	0
57	MG	BA	3136	1/1	0.83	0.44	46,46,46,46	1
57	MG	BA	3113	1/1	0.83	0.87	49,49,49,49	0
57	MG	BA	3321	1/1	0.83	0.35	35,35,35,35	0
57	MG	BA	3033	1/1	0.83	0.19	6,6,6,6	0
57	MG	DA	9692	1/1	0.83	0.42	30,30,30,30	0
57	MG	CA	1725	1/1	0.83	0.29	29,29,29,29	0
57	MG	AA	7014	1/1	0.83	0.96	20,20,20,20	0
57	MG	CA	1709	1/1	0.83	0.48	68,68,68,68	0
57	MG	BA	3070	1/1	0.83	0.43	34,34,34,34	0
57	MG	BA	3292	1/1	0.83	0.28	28,28,28,28	0
57	MG	DA	9431	1/1	0.83	0.30	12,12,12,12	0
57	MG	DA	9659	1/1	0.83	0.26	52,52,52,52	0
57	MG	CA	1638	1/1	0.83	0.42	24,24,24,24	0
57	MG	DA	9385	1/1	0.83	0.24	5,5,5,5	0
57	MG	DA	9572	1/1	0.83	0.42	4,4,4,4	0
57	MG	CA	1676	1/1	0.83	0.60	88,88,88,88	0
57	MG	DA	9695	1/1	0.83	0.39	63,63,63,63	0
57	MG	DA	9347	1/1	0.83	0.29	22,22,22,22	0
57	MG	DA	9461	1/1	0.83	0.34	13,13,13,13	0
57	MG	BE	301	1/1	0.83	0.24	0,0,0,0	0
57	MG	BA	3106	1/1	0.83	0.49	34,34,34,34	0
57	MG	BA	3254	1/1	0.84	0.91	54,54,54,54	0
57	MG	DA	9530	1/1	0.84	0.85	41,41,41,41	0
57	MG	DW	201	1/1	0.84	0.47	27,27,27,27	0
57	MG	BB	201	1/1	0.84	0.15	34,34,34,34	0
57	MG	BA	3282	1/1	0.84	0.47	24,24,24,24	0
57	MG	BA	3310	1/1	0.84	0.40	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3038	1/1	0.84	0.16	31,31,31,31	0
57	MG	DA	9614	1/1	0.84	0.25	12,12,12,12	0
57	MG	AE	201	1/1	0.84	0.39	45,45,45,45	0
57	MG	DA	9445	1/1	0.84	0.44	22,22,22,22	0
57	MG	BA	3134	1/1	0.84	0.48	21,21,21,21	0
57	MG	AV	102	1/1	0.84	0.43	25,25,25,25	1
57	MG	DA	9593	1/1	0.84	0.62	25,25,25,25	0
57	MG	DA	9544	1/1	0.84	0.41	10,10,10,10	0
57	MG	BA	3268	1/1	0.84	0.33	13,13,13,13	1
57	MG	AA	7105	1/1	0.84	0.74	42,42,42,42	0
57	MG	DA	9504	1/1	0.84	0.15	27,27,27,27	0
57	MG	AA	7100	1/1	0.84	0.81	21,21,21,21	0
57	MG	BA	3195	1/1	0.85	0.32	3,3,3,3	0
57	MG	DA	9667	1/1	0.85	0.36	10,10,10,10	0
57	MG	BA	3131	1/1	0.85	0.40	38,38,38,38	0
57	MG	BA	3116	1/1	0.85	0.27	38,38,38,38	0
57	MG	DA	9462	1/1	0.85	0.40	30,30,30,30	0
57	MG	CA	1681	1/1	0.85	0.86	18,18,18,18	1
57	MG	BA	3214	1/1	0.85	0.31	39,39,39,39	0
57	MG	DA	9377	1/1	0.85	0.19	19,19,19,19	0
57	MG	BA	3137	1/1	0.85	0.61	1,1,1,1	1
57	MG	DA	9640	1/1	0.85	0.40	42,42,42,42	0
57	MG	CA	1657	1/1	0.85	0.26	30,30,30,30	0
57	MG	BA	3115	1/1	0.85	0.24	33,33,33,33	0
57	MG	DA	9352	1/1	0.85	0.22	89,89,89,89	0
57	MG	AA	7083	1/1	0.85	0.55	18,18,18,18	0
57	MG	BA	3285	1/1	0.85	1.73	32,32,32,32	1
57	MG	DA	9381	1/1	0.85	0.26	12,12,12,12	0
57	MG	CA	1660	1/1	0.85	0.37	9,9,9,9	0
57	MG	BA	3221	1/1	0.85	0.69	17,17,17,17	0
57	MG	AA	7047	1/1	0.86	0.36	41,41,41,41	0
57	MG	BA	3097	1/1	0.86	0.26	43,43,43,43	0
57	MG	DX	101	1/1	0.86	0.36	6,6,6,6	0
57	MG	DA	9337	1/1	0.86	0.60	45,45,45,45	0
57	MG	BA	3319	1/1	0.86	0.29	27,27,27,27	0
57	MG	BA	3193	1/1	0.86	0.44	12,12,12,12	0
57	MG	BA	3081	1/1	0.86	0.77	24,24,24,24	1
57	MG	DA	9634	1/1	0.86	0.41	44,44,44,44	0
57	MG	CA	1673	1/1	0.86	0.25	18,18,18,18	0
57	MG	DA	9361	1/1	0.86	0.34	5,5,5,5	0
57	MG	CA	1661	1/1	0.86	0.35	50,50,50,50	0
57	MG	DA	9565	1/1	0.86	0.38	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3284	1/1	0.86	0.33	21,21,21,21	0
57	MG	BA	3220	1/1	0.86	0.77	56,56,56,56	0
57	MG	CA	1641	1/1	0.86	0.21	40,40,40,40	0
57	MG	BA	3059	1/1	0.86	0.16	0,0,0,0	0
57	MG	DA	9327	1/1	0.86	0.17	20,20,20,20	0
57	MG	AA	7067	1/1	0.86	0.45	28,28,28,28	0
57	MG	BF	301	1/1	0.86	0.22	39,39,39,39	0
57	MG	BA	3130	1/1	0.86	0.19	3,3,3,3	0
57	MG	DA	9475	1/1	0.86	0.65	26,26,26,26	0
57	MG	BA	3101	1/1	0.86	1.28	27,27,27,27	1
57	MG	BA	3294	1/1	0.86	0.50	15,15,15,15	1
57	MG	BA	3251	1/1	0.86	0.22	34,34,34,34	0
57	MG	AA	7107	1/1	0.87	0.45	24,24,24,24	0
57	MG	BA	3093	1/1	0.87	0.29	49,49,49,49	0
57	MG	DA	9380	1/1	0.87	1.55	23,23,23,23	1
57	MG	DP	202	1/1	0.87	0.25	173,173,173,173	0
57	MG	DA	9502	1/1	0.87	0.42	3,3,3,3	0
57	MG	BA	3077	1/1	0.87	0.43	21,21,21,21	0
57	MG	BA	3258	1/1	0.87	1.06	19,19,19,19	0
57	MG	AA	7108	1/1	0.87	0.42	27,27,27,27	0
57	MG	CA	1735	1/1	0.87	0.47	29,29,29,29	0
57	MG	CA	1605	1/1	0.87	0.22	32,32,32,32	0
57	MG	DA	9466	1/1	0.87	0.45	36,36,36,36	0
57	MG	AA	7045	1/1	0.87	0.75	38,38,38,38	0
57	MG	DA	9609	1/1	0.87	0.45	2,2,2,2	0
57	MG	DA	9616	1/1	0.87	0.54	54,54,54,54	0
57	MG	BA	3019	1/1	0.87	0.36	44,44,44,44	0
57	MG	DA	9302	1/1	0.87	0.18	34,34,34,34	0
57	MG	DA	9673	1/1	0.87	0.42	8,8,8,8	0
57	MG	DF	301	1/1	0.87	0.14	20,20,20,20	0
57	MG	CV	101	1/1	0.87	0.37	12,12,12,12	1
57	MG	CA	1740	1/1	0.87	0.60	48,48,48,48	0
57	MG	BA	3066	1/1	0.87	0.26	48,48,48,48	0
57	MG	CA	1675	1/1	0.87	0.42	55,55,55,55	0
57	MG	BA	3094	1/1	0.87	0.35	7,7,7,7	0
57	MG	AA	7054	1/1	0.87	0.98	29,29,29,29	0
57	MG	BA	3102	1/1	0.87	0.49	1,1,1,1	0
57	MG	BA	3298	1/1	0.87	0.80	18,18,18,18	0
57	MG	DA	9371	1/1	0.87	0.38	29,29,29,29	0
57	MG	DA	9670	1/1	0.88	0.48	11,11,11,11	0
57	MG	DA	9503	1/1	0.88	0.31	66,66,66,66	0
57	MG	BB	202	1/1	0.88	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	7084	1/1	0.88	0.12	49,49,49,49	0
57	MG	AA	7101	1/1	0.88	0.64	22,22,22,22	0
57	MG	DA	9456	1/1	0.88	0.61	19,19,19,19	0
57	MG	DA	9690	1/1	0.88	0.11	5,5,5,5	0
57	MG	DA	9444	1/1	0.88	0.50	42,42,42,42	0
57	MG	DA	9490	1/1	0.88	0.22	39,39,39,39	0
57	MG	CA	1635	1/1	0.88	0.23	4,4,4,4	0
57	MG	AA	7004	1/1	0.88	0.29	30,30,30,30	0
57	MG	BA	3031	1/1	0.88	0.23	44,44,44,44	0
57	MG	DA	9639	1/1	0.88	0.49	57,57,57,57	0
57	MG	CA	1710	1/1	0.88	0.50	19,19,19,19	0
57	MG	BA	3276	1/1	0.88	0.56	31,31,31,31	0
57	MG	BA	3150	1/1	0.88	0.30	1,1,1,1	0
57	MG	CA	1680	1/1	0.88	0.15	49,49,49,49	0
57	MG	DA	9535	1/1	0.88	0.42	14,14,14,14	0
57	MG	CA	1684	1/1	0.88	0.21	41,41,41,41	0
57	MG	CA	1601	1/1	0.88	0.38	39,39,39,39	0
57	MG	CA	1633	1/1	0.88	0.27	9,9,9,9	0
57	MG	DA	9422	1/1	0.88	0.96	56,56,56,56	0
57	MG	AA	7036	1/1	0.88	0.38	42,42,42,42	0
57	MG	BA	3267	1/1	0.88	0.39	41,41,41,41	0
57	MG	DA	9372	1/1	0.88	0.43	8,8,8,8	0
57	MG	DA	9402	1/1	0.88	0.38	25,25,25,25	0
57	MG	DA	9423	1/1	0.88	0.29	1,1,1,1	0
57	MG	DA	9686	1/1	0.88	0.20	11,11,11,11	0
57	MG	AV	103	1/1	0.88	0.26	7,7,7,7	1
57	MG	DA	9576	1/1	0.88	0.41	22,22,22,22	0
57	MG	DA	9589	1/1	0.88	0.18	32,32,32,32	0
57	MG	DA	9373	1/1	0.88	0.16	0,0,0,0	0
57	MG	CA	1738	1/1	0.88	0.42	49,49,49,49	0
57	MG	BO	201	1/1	0.88	0.42	45,45,45,45	0
57	MG	DA	9468	1/1	0.88	0.72	2,2,2,2	1
57	MG	CA	1732	1/1	0.88	0.53	27,27,27,27	0
57	MG	BA	3087	1/1	0.89	0.24	21,21,21,21	0
57	MG	DA	9443	1/1	0.89	0.24	37,37,37,37	0
57	MG	DA	9656	1/1	0.89	0.29	58,58,58,58	0
57	MG	BA	3111	1/1	0.89	0.33	35,35,35,35	0
57	MG	DA	9465	1/1	0.89	0.39	34,34,34,34	0
57	MG	DA	9526	1/1	0.89	0.50	12,12,12,12	0
57	MG	DA	9370	1/1	0.89	0.39	0,0,0,0	0
57	MG	DA	9611	1/1	0.89	0.46	8,8,8,8	0
57	MG	DA	9351	1/1	0.89	0.45	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	9376	1/1	0.89	0.27	26,26,26,26	0
57	MG	DA	9328	1/1	0.89	0.33	1,1,1,1	0
57	MG	BA	3157	1/1	0.89	0.22	6,6,6,6	0
57	MG	DA	9367	1/1	0.89	0.41	35,35,35,35	0
57	MG	CA	1717	1/1	0.89	0.29	11,11,11,11	0
57	MG	BA	3104	1/1	0.89	0.24	16,16,16,16	0
57	MG	BA	3144	1/1	0.89	0.71	41,41,41,41	0
57	MG	BA	3022	1/1	0.89	0.23	40,40,40,40	0
57	MG	DA	9568	1/1	0.89	0.37	3,3,3,3	0
57	MG	DA	9651	1/1	0.89	0.13	81,81,81,81	0
57	MG	DA	9680	1/1	0.89	0.39	24,24,24,24	0
57	MG	BA	3209	1/1	0.89	0.34	1,1,1,1	0
57	MG	CA	1671	1/1	0.89	0.23	38,38,38,38	0
57	MG	CA	1653	1/1	0.89	0.53	29,29,29,29	0
57	MG	BA	3202	1/1	0.89	0.50	7,7,7,7	0
57	MG	DA	9541	1/1	0.89	0.39	2,2,2,2	0
57	MG	AA	7090	1/1	0.89	1.01	69,69,69,69	0
58	PAR	CA	1741	42/42	0.89	0.32	55,55,55,55	0
57	MG	BE	302	1/1	0.89	0.27	74,74,74,74	0
57	MG	BA	3177	1/1	0.89	0.20	0,0,0,0	0
57	MG	DA	9460	1/1	0.89	0.25	40,40,40,40	0
57	MG	DB	203	1/1	0.89	0.91	1,1,1,1	1
57	MG	CA	1737	1/1	0.89	0.63	28,28,28,28	0
57	MG	AA	7061	1/1	0.89	0.25	19,19,19,19	0
57	MG	BA	3053	1/1	0.89	0.28	17,17,17,17	0
57	MG	AA	7012	1/1	0.89	0.78	12,12,12,12	0
57	MG	CA	1690	1/1	0.89	0.54	17,17,17,17	0
57	MG	DA	9577	1/1	0.90	0.90	102,102,102,102	0
57	MG	BA	3269	1/1	0.90	0.50	20,20,20,20	0
57	MG	BA	3308	1/1	0.90	0.40	37,37,37,37	0
57	MG	DA	9513	1/1	0.90	0.47	22,22,22,22	0
57	MG	AA	7063	1/1	0.90	0.26	31,31,31,31	0
57	MG	DA	9551	1/1	0.90	0.21	48,48,48,48	0
57	MG	DA	9425	1/1	0.90	0.41	37,37,37,37	0
57	MG	BA	3281	1/1	0.90	0.62	53,53,53,53	0
57	MG	D2	101	1/1	0.90	0.25	34,34,34,34	0
57	MG	CY	101	1/1	0.90	0.57	33,33,33,33	0
57	MG	DA	9396	1/1	0.90	0.23	26,26,26,26	0
57	MG	DA	9501	1/1	0.90	0.47	42,42,42,42	0
57	MG	AA	7023	1/1	0.90	0.26	56,56,56,56	0
57	MG	DP	203	1/1	0.90	0.24	11,11,11,11	0
57	MG	CA	1654	1/1	0.90	0.35	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	9608	1/1	0.90	0.46	19,19,19,19	0
57	MG	AA	7026	1/1	0.90	0.39	30,30,30,30	0
57	MG	BA	3187	1/1	0.90	0.61	24,24,24,24	0
57	MG	AV	105	1/1	0.90	0.34	54,54,54,54	0
57	MG	CE	202	1/1	0.90	0.38	34,34,34,34	0
57	MG	BA	3001	1/1	0.90	0.38	38,38,38,38	0
57	MG	CA	1689	1/1	0.90	0.25	15,15,15,15	0
57	MG	DA	9483	1/1	0.90	0.48	0,0,0,0	0
57	MG	AA	7088	1/1	0.90	0.13	60,60,60,60	0
57	MG	AA	7029	1/1	0.90	0.27	41,41,41,41	0
57	MG	DA	9339	1/1	0.90	0.20	13,13,13,13	0
57	MG	DA	9365	1/1	0.90	0.28	1,1,1,1	0
57	MG	CA	1646	1/1	0.90	0.42	7,7,7,7	0
57	MG	BA	3109	1/1	0.90	0.22	66,66,66,66	0
57	MG	DA	9317	1/1	0.90	0.26	18,18,18,18	0
57	MG	DA	9397	1/1	0.90	0.41	25,25,25,25	1
57	MG	BA	3158	1/1	0.90	0.37	29,29,29,29	0
57	MG	AA	7073	1/1	0.90	0.23	29,29,29,29	0
57	MG	CA	1677	1/1	0.90	0.18	22,22,22,22	0
57	MG	DA	9382	1/1	0.90	0.45	0,0,0,0	0
57	MG	CA	1663	1/1	0.90	0.66	11,11,11,11	0
57	MG	BA	3012	1/1	0.90	0.60	29,29,29,29	0
57	MG	AA	7020	1/1	0.90	0.36	33,33,33,33	0
57	MG	DA	9477	1/1	0.90	0.56	36,36,36,36	0
57	MG	CA	1688	1/1	0.90	0.15	16,16,16,16	0
57	MG	DA	9333	1/1	0.90	0.11	31,31,31,31	0
57	MG	DE	302	1/1	0.90	0.22	35,35,35,35	0
57	MG	DA	9409	1/1	0.90	0.31	4,4,4,4	0
57	MG	AA	7079	1/1	0.90	0.41	35,35,35,35	0
57	MG	DA	9679	1/1	0.90	0.31	16,16,16,16	0
57	MG	DA	9663	1/1	0.91	0.59	7,7,7,7	0
57	MG	AA	7048	1/1	0.91	0.27	27,27,27,27	0
57	MG	CA	1697	1/1	0.91	0.18	49,49,49,49	0
57	MG	BA	3323	1/1	0.91	0.48	26,26,26,26	0
57	MG	BA	3201	1/1	0.91	0.32	6,6,6,6	0
57	MG	DB	204	1/1	0.91	0.70	0,0,0,0	1
57	MG	DA	9539	1/1	0.91	0.25	35,35,35,35	0
57	MG	BA	3205	1/1	0.91	0.54	0,0,0,0	0
57	MG	DA	9420	1/1	0.91	0.52	6,6,6,6	0
57	MG	DA	9480	1/1	0.91	0.27	30,30,30,30	0
57	MG	BA	3143	1/1	0.91	0.20	7,7,7,7	0
57	MG	AA	7052	1/1	0.91	0.19	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3112	1/1	0.91	0.57	14,14,14,14	0
57	MG	BA	3006	1/1	0.91	0.33	38,38,38,38	0
57	MG	DA	9332	1/1	0.91	0.37	34,34,34,34	0
57	MG	DA	9338	1/1	0.91	0.55	58,58,58,58	0
57	MG	CA	1700	1/1	0.91	0.28	20,20,20,20	0
57	MG	DA	9585	1/1	0.91	0.18	18,18,18,18	0
57	MG	CA	1656	1/1	0.91	0.21	22,22,22,22	0
57	MG	DA	9607	1/1	0.91	0.34	49,49,49,49	0
57	MG	CA	1608	1/1	0.91	0.39	16,16,16,16	0
57	MG	DA	9453	1/1	0.91	0.44	4,4,4,4	1
57	MG	AA	7005	1/1	0.91	0.28	45,45,45,45	0
57	MG	AA	7043	1/1	0.91	0.34	16,16,16,16	0
57	MG	DA	9527	1/1	0.91	0.38	1,1,1,1	0
57	MG	DA	9605	1/1	0.91	0.20	19,19,19,19	0
57	MG	DA	9393	1/1	0.91	0.30	24,24,24,24	0
57	MG	DA	9457	1/1	0.91	0.59	13,13,13,13	0
57	MG	DA	9556	1/1	0.91	0.23	23,23,23,23	0
57	MG	BA	3226	1/1	0.91	0.65	36,36,36,36	0
57	MG	BN	201	1/1	0.91	0.30	125,125,125,125	1
57	MG	CA	1616	1/1	0.91	0.41	44,44,44,44	0
57	MG	BA	3236	1/1	0.91	0.56	17,17,17,17	0
57	MG	BA	3287	1/1	0.91	0.36	30,30,30,30	0
57	MG	BA	3154	1/1	0.91	0.43	17,17,17,17	0
57	MG	BA	3058	1/1	0.91	0.33	1,1,1,1	0
57	MG	AA	7041	1/1	0.91	0.58	20,20,20,20	0
57	MG	DA	9630	1/1	0.91	0.27	16,16,16,16	1
57	MG	CA	1736	1/1	0.91	0.31	6,6,6,6	0
57	MG	DA	9594	1/1	0.91	0.78	19,19,19,19	0
57	MG	AA	7009	1/1	0.91	0.27	18,18,18,18	0
57	MG	CA	1630	1/1	0.91	0.23	34,34,34,34	0
57	MG	DA	9319	1/1	0.91	0.81	30,30,30,30	0
57	MG	DA	9413	1/1	0.91	0.38	3,3,3,3	0
57	MG	BA	3050	1/1	0.91	0.58	4,4,4,4	0
57	MG	DA	9633	1/1	0.91	0.73	30,30,30,30	0
57	MG	BA	3171	1/1	0.91	0.45	7,7,7,7	0
57	MG	DA	9666	1/1	0.91	0.36	7,7,7,7	0
57	MG	DA	9604	1/1	0.91	0.33	21,21,21,21	0
57	MG	BA	3233	1/1	0.91	0.45	19,19,19,19	0
57	MG	BA	3141	1/1	0.91	0.26	18,18,18,18	0
57	MG	DA	9407	1/1	0.91	0.22	2,2,2,2	0
57	MG	BA	3183	1/1	0.91	0.64	56,56,56,56	0
57	MG	AA	7013	1/1	0.91	0.38	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	9464	1/1	0.91	0.14	25,25,25,25	0
57	MG	BA	3208	1/1	0.92	0.22	8,8,8,8	0
57	MG	CV	102	1/1	0.92	0.21	1,1,1,1	0
57	MG	DA	9486	1/1	0.92	0.34	21,21,21,21	0
57	MG	BA	3283	1/1	0.92	0.20	22,22,22,22	0
57	MG	BA	3256	1/1	0.92	0.15	13,13,13,13	0
57	MG	BA	3062	1/1	0.92	0.15	27,27,27,27	0
57	MG	B5	101	1/1	0.92	0.30	2,2,2,2	0
57	MG	DQ	201	1/1	0.92	0.31	36,36,36,36	0
57	MG	DA	9394	1/1	0.92	0.47	16,16,16,16	0
57	MG	DA	9303	1/1	0.92	0.31	42,42,42,42	0
57	MG	BA	3272	1/1	0.92	0.37	10,10,10,10	0
57	MG	BA	3166	1/1	0.92	0.64	40,40,40,40	0
57	MG	DA	9341	1/1	0.92	0.56	11,11,11,11	0
57	MG	BA	3168	1/1	0.92	0.71	36,36,36,36	0
57	MG	BA	3133	1/1	0.92	0.21	43,43,43,43	0
57	MG	CA	1662	1/1	0.92	0.17	29,29,29,29	0
57	MG	DA	9631	1/1	0.92	0.32	21,21,21,21	0
57	MG	BA	3263	1/1	0.92	0.64	16,16,16,16	1
57	MG	BA	3045	1/1	0.92	0.59	2,2,2,2	0
57	MG	DA	9433	1/1	0.92	0.22	13,13,13,13	0
57	MG	DA	9636	1/1	0.92	0.28	16,16,16,16	0
57	MG	CA	1727	1/1	0.92	0.34	27,27,27,27	0
57	MG	BA	3024	1/1	0.92	0.61	22,22,22,22	0
57	MG	AA	7022	1/1	0.92	0.25	32,32,32,32	0
57	MG	AA	7040	1/1	0.92	0.17	36,36,36,36	0
57	MG	AA	7053	1/1	0.92	0.49	32,32,32,32	0
57	MG	CA	1617	1/1	0.92	0.43	16,16,16,16	0
57	MG	DA	9591	1/1	0.92	0.25	52,52,52,52	0
57	MG	CA	1678	1/1	0.92	0.22	17,17,17,17	0
57	MG	DA	9469	1/1	0.92	0.58	17,17,17,17	0
57	MG	DA	9618	1/1	0.92	0.79	28,28,28,28	1
57	MG	BA	3132	1/1	0.92	0.32	51,51,51,51	0
57	MG	DA	9435	1/1	0.92	0.97	30,30,30,30	0
57	MG	DA	9691	1/1	0.92	0.41	12,12,12,12	0
57	MG	BA	3002	1/1	0.92	0.27	53,53,53,53	0
57	MG	BA	3088	1/1	0.92	0.39	43,43,43,43	0
57	MG	AA	7018	1/1	0.92	0.56	27,27,27,27	0
57	MG	BA	3186	1/1	0.92	0.36	2,2,2,2	0
57	MG	DA	9598	1/1	0.92	0.50	14,14,14,14	0
57	MG	DA	9496	1/1	0.92	0.35	26,26,26,26	0
57	MG	CA	1701	1/1	0.92	0.51	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3067	1/1	0.92	0.79	2,2,2,2	0
57	MG	BA	3199	1/1	0.92	0.48	1,1,1,1	0
57	MG	DA	9389	1/1	0.92	0.14	11,11,11,11	0
57	MG	BA	3140	1/1	0.92	0.24	40,40,40,40	0
57	MG	BA	3235	1/1	0.92	0.36	25,25,25,25	0
57	MG	DA	9489	1/1	0.92	0.41	37,37,37,37	0
57	MG	DA	9451	1/1	0.92	0.56	35,35,35,35	0
57	MG	BA	3061	1/1	0.92	0.25	32,32,32,32	0
57	MG	DA	9484	1/1	0.92	0.40	5,5,5,5	0
57	MG	CA	1643	1/1	0.92	0.58	40,40,40,40	1
57	MG	BA	3145	1/1	0.92	0.28	22,22,22,22	0
57	MG	DA	9567	1/1	0.92	0.43	31,31,31,31	0
57	MG	BA	3184	1/1	0.92	0.95	22,22,22,22	0
57	MG	AA	7050	1/1	0.92	1.07	29,29,29,29	0
57	MG	CV	104	1/1	0.92	0.28	22,22,22,22	1
57	MG	DA	9588	1/1	0.92	0.14	16,16,16,16	0
57	MG	CA	1726	1/1	0.92	0.21	38,38,38,38	0
57	MG	CA	1634	1/1	0.92	0.31	43,43,43,43	0
57	MG	BA	3123	1/1	0.92	0.20	14,14,14,14	0
57	MG	BA	3049	1/1	0.92	0.51	30,30,30,30	0
57	MG	DA	9334	1/1	0.92	0.45	27,27,27,27	0
58	PAR	AA	7111	42/42	0.92	0.26	58,58,58,58	0
57	MG	DA	9683	1/1	0.92	0.52	19,19,19,19	0
57	MG	CA	1720	1/1	0.92	0.41	2,2,2,2	0
57	MG	CA	1686	1/1	0.93	0.21	77,77,77,77	0
57	MG	BA	3057	1/1	0.93	0.54	2,2,2,2	0
57	MG	BA	3118	1/1	0.93	0.61	28,28,28,28	0
57	MG	DA	9358	1/1	0.93	0.47	5,5,5,5	0
57	MG	CA	1730	1/1	0.93	0.15	49,49,49,49	0
57	MG	DA	9629	1/1	0.93	0.15	52,52,52,52	0
57	MG	BA	3160	1/1	0.93	0.39	22,22,22,22	0
57	MG	BA	3230	1/1	0.93	0.61	22,22,22,22	0
57	MG	BA	3032	1/1	0.93	0.20	18,18,18,18	0
57	MG	DA	9561	1/1	0.93	0.28	10,10,10,10	0
57	MG	DA	9662	1/1	0.93	0.54	2,2,2,2	0
57	MG	CA	1607	1/1	0.93	0.49	32,32,32,32	0
57	MG	DA	9519	1/1	0.93	0.43	1,1,1,1	0
57	MG	AA	7098	1/1	0.93	0.34	28,28,28,28	0
57	MG	AA	7059	1/1	0.93	0.51	96,96,96,96	0
57	MG	DA	9415	1/1	0.93	0.49	0,0,0,0	0
57	MG	BA	3153	1/1	0.93	0.55	0,0,0,0	0
57	MG	BA	3029	1/1	0.93	0.15	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3098	1/1	0.93	0.29	36,36,36,36	0
57	MG	DA	9555	1/1	0.93	0.32	39,39,39,39	0
57	MG	DA	9597	1/1	0.93	0.24	12,12,12,12	0
57	MG	AA	7039	1/1	0.93	0.34	11,11,11,11	0
57	MG	BA	3017	1/1	0.93	0.55	22,22,22,22	0
57	MG	DA	9446	1/1	0.93	0.08	13,13,13,13	0
57	MG	BA	3099	1/1	0.93	0.23	30,30,30,30	0
57	MG	BA	3291	1/1	0.93	0.16	22,22,22,22	0
57	MG	BA	3075	1/1	0.93	0.70	12,12,12,12	0
57	MG	DA	9689	1/1	0.93	0.80	25,25,25,25	0
57	MG	AA	7094	1/1	0.93	0.54	8,8,8,8	0
57	MG	BA	3300	1/1	0.93	0.45	1,1,1,1	0
57	MG	AA	7051	1/1	0.93	0.44	22,22,22,22	0
57	MG	BA	3229	1/1	0.93	0.19	19,19,19,19	0
57	MG	DA	9306	1/1	0.93	0.35	4,4,4,4	0
59	ZN	AD	301	1/1	0.93	0.32	41,41,41,41	0
57	MG	BA	3232	1/1	0.93	0.18	44,44,44,44	0
57	MG	BA	3314	1/1	0.93	0.05	42,42,42,42	0
57	MG	CA	1705	1/1	0.93	0.27	15,15,15,15	0
57	MG	CA	1632	1/1	0.93	0.15	18,18,18,18	0
57	MG	BA	3174	1/1	0.93	0.14	31,31,31,31	0
57	MG	AA	7001	1/1	0.93	0.28	26,26,26,26	0
57	MG	D0	102	1/1	0.93	0.54	15,15,15,15	0
57	MG	CA	1734	1/1	0.93	0.24	22,22,22,22	0
57	MG	BA	3030	1/1	0.93	0.54	22,22,22,22	0
57	MG	DA	9470	1/1	0.93	0.27	0,0,0,0	0
57	MG	BA	3192	1/1	0.93	0.39	2,2,2,2	0
57	MG	AA	7072	1/1	0.93	0.15	23,23,23,23	0
57	MG	CA	1685	1/1	0.93	0.35	41,41,41,41	0
57	MG	AA	7093	1/1	0.93	0.34	30,30,30,30	0
57	MG	BA	3014	1/1	0.93	0.25	33,33,33,33	0
57	MG	CA	1650	1/1	0.93	0.51	34,34,34,34	0
57	MG	DA	9417	1/1	0.93	0.29	20,20,20,20	0
57	MG	DA	9320	1/1	0.93	0.25	10,10,10,10	0
57	MG	DA	9314	1/1	0.93	0.32	1,1,1,1	0
57	MG	DA	9533	1/1	0.93	0.30	0,0,0,0	0
57	MG	DA	9525	1/1	0.93	0.30	4,4,4,4	0
57	MG	DA	9512	1/1	0.93	0.43	2,2,2,2	0
57	MG	AA	7104	1/1	0.93	0.14	33,33,33,33	0
57	MG	DA	9625	1/1	0.93	0.36	26,26,26,26	0
57	MG	BA	3044	1/1	0.93	0.58	18,18,18,18	0
57	MG	CA	1695	1/1	0.93	0.36	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	9606	1/1	0.93	0.94	4,4,4,4	0
57	MG	BA	3163	1/1	0.93	0.32	28,28,28,28	0
57	MG	AA	7078	1/1	0.93	0.25	30,30,30,30	0
57	MG	DA	9482	1/1	0.93	0.21	12,12,12,12	0
57	MG	DA	9313	1/1	0.93	0.22	18,18,18,18	0
57	MG	AA	7070	1/1	0.93	0.15	61,61,61,61	0
57	MG	AA	7066	1/1	0.93	0.54	36,36,36,36	0
57	MG	BA	3135	1/1	0.93	0.58	43,43,43,43	0
57	MG	DA	9669	1/1	0.94	0.23	5,5,5,5	0
57	MG	CA	1668	1/1	0.94	0.34	56,56,56,56	0
57	MG	AA	7062	1/1	0.94	0.11	31,31,31,31	0
57	MG	DA	9583	1/1	0.94	0.18	1,1,1,1	0
57	MG	BA	3212	1/1	0.94	0.24	8,8,8,8	0
57	MG	DA	9410	1/1	0.94	0.25	4,4,4,4	0
57	MG	CA	1669	1/1	0.94	0.10	10,10,10,10	0
57	MG	CA	1721	1/1	0.94	0.20	1,1,1,1	0
57	MG	DA	9487	1/1	0.94	0.25	71,71,71,71	0
57	MG	BA	3159	1/1	0.94	0.53	9,9,9,9	0
57	MG	DA	9476	1/1	0.94	0.47	2,2,2,2	0
57	MG	CA	1670	1/1	0.94	0.36	2,2,2,2	0
57	MG	DA	9528	1/1	0.94	0.36	6,6,6,6	0
57	MG	CA	1606	1/1	0.94	0.21	8,8,8,8	0
57	MG	BA	3128	1/1	0.94	0.25	57,57,57,57	0
57	MG	BA	3225	1/1	0.94	0.28	2,2,2,2	0
57	MG	CA	1625	1/1	0.94	0.43	26,26,26,26	0
57	MG	DA	9684	1/1	0.94	0.21	8,8,8,8	0
57	MG	DA	9632	1/1	0.94	0.48	12,12,12,12	1
57	MG	DA	9549	1/1	0.94	0.74	44,44,44,44	0
57	MG	DA	9511	1/1	0.94	0.80	7,7,7,7	0
57	MG	DA	9304	1/1	0.94	0.44	27,27,27,27	0
57	MG	AA	7089	1/1	0.94	0.24	21,21,21,21	0
57	MG	BA	3304	1/1	0.94	0.43	13,13,13,13	0
57	MG	BA	3170	1/1	0.94	0.79	1,1,1,1	0
57	MG	DA	9473	1/1	0.94	0.64	0,0,0,0	0
57	MG	BA	3079	1/1	0.94	0.33	29,29,29,29	1
57	MG	DA	9514	1/1	0.94	0.82	19,19,19,19	0
57	MG	BA	3302	1/1	0.94	0.47	8,8,8,8	0
57	MG	AA	7081	1/1	0.94	0.46	44,44,44,44	0
57	MG	DA	9581	1/1	0.94	0.42	4,4,4,4	0
57	MG	AA	7102	1/1	0.94	0.49	38,38,38,38	0
57	MG	CA	1636	1/1	0.94	0.32	19,19,19,19	0
57	MG	DA	9323	1/1	0.94	0.56	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3148	1/1	0.94	0.38	16,16,16,16	0
57	MG	BA	3023	1/1	0.94	0.28	4,4,4,4	0
57	MG	BU	201	1/1	0.94	0.30	170,170,170,170	1
57	MG	DA	9532	1/1	0.94	0.44	9,9,9,9	0
57	MG	BA	3241	1/1	0.94	0.45	4,4,4,4	0
57	MG	BA	3185	1/1	0.94	0.26	14,14,14,14	0
57	MG	DA	9403	1/1	0.94	0.26	0,0,0,0	0
57	MG	DA	9471	1/1	0.94	0.55	50,50,50,50	1
57	MG	DA	9368	1/1	0.94	0.19	1,1,1,1	0
57	MG	DA	9340	1/1	0.94	0.33	1,1,1,1	0
57	MG	AA	7032	1/1	0.94	0.47	24,24,24,24	0
57	MG	BA	3042	1/1	0.94	0.67	8,8,8,8	0
57	MG	AA	7016	1/1	0.94	0.32	45,45,45,45	0
57	MG	DA	9531	1/1	0.94	0.37	1,1,1,1	0
57	MG	DA	9436	1/1	0.94	0.54	3,3,3,3	0
57	MG	DA	9442	1/1	0.94	0.54	36,36,36,36	0
57	MG	AA	7085	1/1	0.94	0.17	15,15,15,15	0
57	MG	BA	3129	1/1	0.94	0.53	1,1,1,1	0
57	MG	DA	9652	1/1	0.94	0.23	44,44,44,44	0
57	MG	B7	101	1/1	0.94	0.39	13,13,13,13	0
57	MG	BA	3213	1/1	0.94	0.41	8,8,8,8	0
57	MG	BA	3169	1/1	0.94	0.51	3,3,3,3	0
57	MG	AA	7103	1/1	0.94	0.53	13,13,13,13	0
57	MG	DA	9321	1/1	0.94	0.50	35,35,35,35	0
57	MG	BA	3253	1/1	0.94	0.60	34,34,34,34	0
57	MG	CA	1644	1/1	0.94	0.14	45,45,45,45	0
57	MG	BA	3296	1/1	0.94	0.38	0,0,0,0	1
57	MG	BA	3090	1/1	0.94	0.41	2,2,2,2	0
57	MG	CA	1640	1/1	0.94	0.84	49,49,49,49	0
57	MG	DA	9653	1/1	0.94	0.41	5,5,5,5	0
57	MG	BA	3096	1/1	0.94	0.42	12,12,12,12	0
57	MG	DA	9582	1/1	0.94	0.88	21,21,21,21	0
57	MG	CA	1664	1/1	0.94	0.45	24,24,24,24	0
57	MG	CA	1703	1/1	0.94	0.45	9,9,9,9	0
57	MG	DA	9454	1/1	0.94	0.44	34,34,34,34	0
57	MG	DD	7102	1/1	0.94	0.28	0,0,0,0	0
57	MG	CA	1618	1/1	0.94	0.22	31,31,31,31	0
57	MG	AA	7064	1/1	0.94	0.28	50,50,50,50	0
57	MG	DA	9428	1/1	0.94	0.41	15,15,15,15	0
57	MG	CV	105	1/1	0.94	0.16	69,69,69,69	0
57	MG	BA	3138	1/1	0.95	0.32	15,15,15,15	0
57	MG	AA	7058	1/1	0.95	0.27	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3228	1/1	0.95	0.61	13,13,13,13	0
57	MG	BA	3068	1/1	0.95	0.11	11,11,11,11	0
57	MG	BA	3147	1/1	0.95	0.59	48,48,48,48	0
57	MG	DA	9384	1/1	0.95	0.29	16,16,16,16	0
57	MG	DA	9459	1/1	0.95	0.52	3,3,3,3	0
57	MG	CA	1631	1/1	0.95	0.89	22,22,22,22	0
57	MG	BA	3312	1/1	0.95	0.30	45,45,45,45	0
57	MG	DA	9345	1/1	0.95	0.52	19,19,19,19	0
57	MG	DU	201	1/1	0.95	0.34	30,30,30,30	1
57	MG	DB	201	1/1	0.95	0.41	22,22,22,22	0
57	MG	BA	3161	1/1	0.95	0.26	11,11,11,11	0
57	MG	AA	7015	1/1	0.95	0.29	4,4,4,4	0
57	MG	DA	9426	1/1	0.95	0.43	9,9,9,9	1
57	MG	BA	3035	1/1	0.95	0.39	0,0,0,0	0
57	MG	DA	9494	1/1	0.95	0.38	39,39,39,39	0
57	MG	D0	101	1/1	0.95	0.44	27,27,27,27	0
57	MG	DA	9330	1/1	0.95	0.35	0,0,0,0	0
57	MG	DA	9311	1/1	0.95	0.46	29,29,29,29	0
57	MG	BA	3064	1/1	0.95	0.26	29,29,29,29	1
57	MG	BB	204	1/1	0.95	0.31	23,23,23,23	0
57	MG	AA	7060	1/1	0.95	0.13	8,8,8,8	0
57	MG	BA	3083	1/1	0.95	0.31	27,27,27,27	1
57	MG	D1	102	1/1	0.95	0.18	9,9,9,9	1
57	MG	DA	9610	1/1	0.95	0.63	19,19,19,19	0
57	MG	DA	9505	1/1	0.95	0.29	0,0,0,0	0
57	MG	BA	3204	1/1	0.95	0.31	3,3,3,3	0
57	MG	DA	9447	1/1	0.95	0.23	68,68,68,68	0
57	MG	DA	9596	1/1	0.95	0.14	27,27,27,27	0
57	MG	CA	1659	1/1	0.95	0.28	28,28,28,28	0
57	MG	DA	9696	1/1	0.95	0.43	34,34,34,34	0
57	MG	BA	3127	1/1	0.95	0.38	8,8,8,8	0
57	MG	DA	9366	1/1	0.95	0.46	1,1,1,1	0
57	MG	DA	9548	1/1	0.95	0.72	26,26,26,26	0
57	MG	D8	101	1/1	0.95	0.23	3,3,3,3	0
57	MG	BA	3265	1/1	0.95	0.51	43,43,43,43	0
57	MG	AA	7030	1/1	0.95	0.23	2,2,2,2	0
57	MG	DA	9375	1/1	0.95	0.54	0,0,0,0	0
57	MG	BA	3178	1/1	0.95	0.23	28,28,28,28	0
57	MG	DA	9452	1/1	0.95	0.37	10,10,10,10	0
57	MG	DA	9448	1/1	0.95	0.37	18,18,18,18	0
57	MG	DA	9455	1/1	0.95	0.46	0,0,0,0	0
57	MG	CA	1719	1/1	0.95	0.35	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	9356	1/1	0.95	0.32	1,1,1,1	0
57	MG	DA	9497	1/1	0.95	0.36	29,29,29,29	0
57	MG	AA	7044	1/1	0.95	0.35	21,21,21,21	0
57	MG	BA	3043	1/1	0.95	0.21	8,8,8,8	0
57	MG	DA	9424	1/1	0.95	0.51	5,5,5,5	0
57	MG	BA	3005	1/1	0.95	0.26	22,22,22,22	0
57	MG	DA	9580	1/1	0.95	0.46	0,0,0,0	0
57	MG	DA	9463	1/1	0.95	0.26	12,12,12,12	0
57	MG	BA	3223	1/1	0.95	0.19	9,9,9,9	0
57	MG	CA	1711	1/1	0.95	0.12	26,26,26,26	0
57	MG	BA	3309	1/1	0.95	0.79	25,25,25,25	0
57	MG	DA	9507	1/1	0.95	0.55	2,2,2,2	0
57	MG	DA	9510	1/1	0.95	0.52	1,1,1,1	0
57	MG	DA	9682	1/1	0.95	0.42	20,20,20,20	0
57	MG	DA	9326	1/1	0.95	0.24	1,1,1,1	0
57	MG	BA	3181	1/1	0.95	0.49	1,1,1,1	0
57	MG	BA	3311	1/1	0.95	0.43	13,13,13,13	0
57	MG	CE	201	1/1	0.95	0.67	16,16,16,16	0
57	MG	CA	1627	1/1	0.95	0.63	22,22,22,22	0
57	MG	AA	7021	1/1	0.95	0.31	25,25,25,25	0
57	MG	CA	1665	1/1	0.95	0.40	16,16,16,16	0
57	MG	DA	9485	1/1	0.95	0.41	15,15,15,15	0
57	MG	AA	7106	1/1	0.95	0.25	12,12,12,12	0
57	MG	BA	3289	1/1	0.95	0.51	21,21,21,21	0
57	MG	DA	9654	1/1	0.95	0.29	15,15,15,15	0
57	MG	CA	1724	1/1	0.95	0.43	5,5,5,5	0
57	MG	BA	3293	1/1	0.95	0.21	1,1,1,1	0
57	MG	AA	7109	1/1	0.95	0.36	33,33,33,33	0
57	MG	BA	3069	1/1	0.95	0.32	5,5,5,5	0
57	MG	AA	7024	1/1	0.95	0.50	27,27,27,27	0
57	MG	DA	9553	1/1	0.95	0.35	20,20,20,20	0
57	MG	DE	301	1/1	0.95	0.32	1,1,1,1	0
57	MG	BA	3007	1/1	0.95	0.66	4,4,4,4	0
57	MG	D5	102	1/1	0.95	0.33	32,32,32,32	1
57	MG	BA	3018	1/1	0.95	0.17	37,37,37,37	0
57	MG	AA	7095	1/1	0.95	0.08	17,17,17,17	0
57	MG	DA	9540	1/1	0.95	0.34	0,0,0,0	0
57	MG	DA	9638	1/1	0.95	0.27	8,8,8,8	1
57	MG	CA	1712	1/1	0.95	0.21	34,34,34,34	1
57	MG	CA	1696	1/1	0.95	0.34	49,49,49,49	0
57	MG	CA	1626	1/1	0.95	0.55	28,28,28,28	0
57	MG	BA	3114	1/1	0.95	0.32	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	9592	1/1	0.96	0.17	36,36,36,36	0
57	MG	DA	9545	1/1	0.96	0.43	1,1,1,1	0
57	MG	DA	9363	1/1	0.96	0.23	1,1,1,1	0
57	MG	DA	9491	1/1	0.96	0.45	11,11,11,11	0
57	MG	BA	3261	1/1	0.96	0.31	10,10,10,10	0
57	MG	BA	3041	1/1	0.96	0.51	7,7,7,7	0
57	MG	BA	3194	1/1	0.96	0.28	1,1,1,1	0
57	MG	CA	1603	1/1	0.96	0.16	0,0,0,0	0
57	MG	AA	7091	1/1	0.96	0.23	22,22,22,22	0
57	MG	DA	9543	1/1	0.96	0.30	5,5,5,5	0
57	MG	CA	1707	1/1	0.96	0.83	1,1,1,1	1
57	MG	CA	1679	1/1	0.96	0.28	9,9,9,9	0
57	MG	BA	3004	1/1	0.96	0.59	1,1,1,1	0
57	MG	CA	1693	1/1	0.96	0.39	24,24,24,24	0
57	MG	BA	3016	1/1	0.96	0.35	8,8,8,8	0
57	MG	CA	1649	1/1	0.96	0.10	33,33,33,33	0
57	MG	DA	9642	1/1	0.96	0.30	1,1,1,1	0
57	MG	CA	1698	1/1	0.96	0.14	1,1,1,1	1
57	MG	CA	1715	1/1	0.96	0.51	12,12,12,12	0
57	MG	BA	3071	1/1	0.96	0.31	0,0,0,0	0
57	MG	BA	3244	1/1	0.96	0.20	1,1,1,1	0
57	MG	DA	9613	1/1	0.96	0.23	5,5,5,5	0
57	MG	BA	3303	1/1	0.96	0.29	19,19,19,19	0
57	MG	DA	9675	1/1	0.96	0.29	11,11,11,11	0
57	MG	DA	9536	1/1	0.96	0.44	0,0,0,0	0
57	MG	AA	7087	1/1	0.96	0.13	24,24,24,24	0
57	MG	DA	9387	1/1	0.96	0.76	1,1,1,1	0
57	MG	CA	1648	1/1	0.96	0.42	23,23,23,23	0
57	MG	BA	3139	1/1	0.96	0.46	0,0,0,0	0
57	MG	BA	3056	1/1	0.96	0.24	5,5,5,5	0
57	MG	DA	9647	1/1	0.96	0.61	1,1,1,1	0
57	MG	BA	3152	1/1	0.96	0.32	18,18,18,18	0
57	MG	AA	7038	1/1	0.96	0.63	10,10,10,10	0
57	MG	DA	9664	1/1	0.96	0.54	1,1,1,1	0
57	MG	BA	3191	1/1	0.96	0.41	2,2,2,2	0
57	MG	DP	201	1/1	0.96	0.12	7,7,7,7	0
57	MG	AA	7028	1/1	0.96	0.85	30,30,30,30	0
57	MG	BA	3222	1/1	0.96	0.39	5,5,5,5	0
57	MG	BA	3307	1/1	0.96	0.54	25,25,25,25	0
57	MG	BA	3146	1/1	0.96	0.71	0,0,0,0	0
57	MG	BA	3054	1/1	0.96	0.33	14,14,14,14	0
57	MG	DA	9318	1/1	0.96	0.40	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	9353	1/1	0.96	0.55	24,24,24,24	0
57	MG	BA	3219	1/1	0.96	0.18	19,19,19,19	0
57	MG	DA	9538	1/1	0.96	0.46	1,1,1,1	0
57	MG	DA	9357	1/1	0.96	0.37	0,0,0,0	0
57	MG	AA	7017	1/1	0.96	0.08	29,29,29,29	0
57	MG	DA	9478	1/1	0.96	0.40	13,13,13,13	0
57	MG	CA	1602	1/1	0.96	0.16	14,14,14,14	0
57	MG	DA	9474	1/1	0.96	0.30	28,28,28,28	0
57	MG	DA	9391	1/1	0.96	0.17	1,1,1,1	0
57	MG	DA	9599	1/1	0.96	0.34	20,20,20,20	0
57	MG	CA	1667	1/1	0.96	0.29	12,12,12,12	0
57	MG	BA	3092	1/1	0.96	0.17	1,1,1,1	0
57	MG	DA	9492	1/1	0.96	0.11	76,76,76,76	0
57	MG	DA	9646	1/1	0.96	0.22	31,31,31,31	0
57	MG	DA	9498	1/1	0.96	0.50	2,2,2,2	0
57	MG	DA	9529	1/1	0.96	0.29	0,0,0,0	0
57	MG	BA	3211	1/1	0.96	0.17	2,2,2,2	0
57	MG	CA	1742	1/1	0.96	0.44	10,10,10,10	0
57	MG	BA	3175	1/1	0.96	0.28	4,4,4,4	0
57	MG	BA	3188	1/1	0.96	0.35	0,0,0,0	0
57	MG	DA	9349	1/1	0.96	0.61	3,3,3,3	0
57	MG	BA	3010	1/1	0.96	0.89	28,28,28,28	0
57	MG	BA	3305	1/1	0.96	0.25	24,24,24,24	0
57	MG	DA	9508	1/1	0.96	0.25	0,0,0,0	0
57	MG	DA	9560	1/1	0.96	0.26	4,4,4,4	0
57	MG	DA	9547	1/1	0.96	0.22	3,3,3,3	0
57	MG	AV	101	1/1	0.96	0.14	2,2,2,2	0
57	MG	BA	3086	1/1	0.96	0.23	1,1,1,1	0
57	MG	DA	9401	1/1	0.96	0.55	21,21,21,21	1
57	MG	DA	9575	1/1	0.96	0.12	35,35,35,35	0
57	MG	CA	1613	1/1	0.96	0.95	31,31,31,31	0
57	MG	CA	1629	1/1	0.96	0.34	37,37,37,37	0
57	MG	BA	3156	1/1	0.96	0.33	19,19,19,19	0
57	MG	DA	9305	1/1	0.96	0.46	0,0,0,0	0
57	MG	BA	3198	1/1	0.96	0.34	0,0,0,0	0
57	MG	DA	9342	1/1	0.96	0.10	0,0,0,0	0
57	MG	DA	9612	1/1	0.96	0.70	1,1,1,1	1
57	MG	BA	3189	1/1	0.96	0.46	1,1,1,1	0
57	MG	AA	7057	1/1	0.96	0.18	44,44,44,44	0
57	MG	CA	1604	1/1	0.96	0.43	15,15,15,15	0
57	MG	AA	7110	1/1	0.96	0.33	31,31,31,31	0
57	MG	BA	3167	1/1	0.96	0.17	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	9506	1/1	0.96	0.23	0,0,0,0	0
57	MG	DA	9516	1/1	0.96	0.46	1,1,1,1	0
57	MG	BA	3025	1/1	0.96	0.16	37,37,37,37	0
57	MG	D5	101	1/1	0.96	0.36	7,7,7,7	0
57	MG	BD	302	1/1	0.96	0.27	4,4,4,4	0
57	MG	BA	3275	1/1	0.97	0.27	1,1,1,1	1
57	MG	BA	3270	1/1	0.97	0.51	0,0,0,0	1
57	MG	DA	9644	1/1	0.97	0.16	25,25,25,25	0
57	MG	BA	3151	1/1	0.97	0.13	12,12,12,12	0
57	MG	DA	9601	1/1	0.97	0.35	31,31,31,31	0
57	MG	BA	3040	1/1	0.97	0.27	0,0,0,0	0
57	MG	DA	9587	1/1	0.97	0.28	2,2,2,2	0
57	MG	DA	9307	1/1	0.97	0.38	12,12,12,12	0
57	MG	DD	7103	1/1	0.97	0.42	0,0,0,0	0
57	MG	BA	3252	1/1	0.97	0.48	56,56,56,56	0
57	MG	AA	7056	1/1	0.97	0.34	12,12,12,12	0
57	MG	DA	9522	1/1	0.97	0.47	2,2,2,2	0
57	MG	BA	3255	1/1	0.97	0.44	45,45,45,45	0
57	MG	DA	9668	1/1	0.97	0.50	4,4,4,4	0
57	MG	DA	9566	1/1	0.97	0.30	18,18,18,18	0
57	MG	DA	9623	1/1	0.97	0.37	13,13,13,13	0
57	MG	DA	9500	1/1	0.97	0.22	1,1,1,1	0
57	MG	AA	7037	1/1	0.97	0.32	7,7,7,7	0
57	MG	DA	9495	1/1	0.97	0.74	3,3,3,3	0
57	MG	BA	3172	1/1	0.97	0.28	58,58,58,58	0
57	MG	AA	7099	1/1	0.97	0.36	6,6,6,6	0
57	MG	DA	9590	1/1	0.97	0.49	1,1,1,1	0
57	MG	BA	3247	1/1	0.97	0.81	55,55,55,55	0
57	MG	AA	7033	1/1	0.97	0.18	35,35,35,35	0
57	MG	DA	9414	1/1	0.97	0.81	16,16,16,16	0
57	MG	BA	3055	1/1	0.97	0.20	11,11,11,11	0
57	MG	BA	3047	1/1	0.97	0.29	0,0,0,0	0
57	MG	AA	7007	1/1	0.97	0.14	1,1,1,1	0
57	MG	BA	3200	1/1	0.97	0.51	5,5,5,5	0
57	MG	DA	9343	1/1	0.97	0.27	2,2,2,2	0
57	MG	CA	1623	1/1	0.97	0.27	19,19,19,19	0
57	MG	BA	3100	1/1	0.97	0.15	21,21,21,21	0
57	MG	DA	9523	1/1	0.97	0.77	9,9,9,9	0
57	MG	DA	9571	1/1	0.97	0.44	0,0,0,0	0
57	MG	BA	3280	1/1	0.97	0.28	19,19,19,19	1
57	MG	DA	9546	1/1	0.97	0.34	2,2,2,2	0
57	MG	BA	3243	1/1	0.97	0.45	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3020	1/1	0.97	0.48	1,1,1,1	0
57	MG	BA	3190	1/1	0.97	0.47	8,8,8,8	0
57	MG	BA	3011	1/1	0.97	0.52	36,36,36,36	0
57	MG	BA	3121	1/1	0.97	0.60	1,1,1,1	0
57	MG	BA	3250	1/1	0.97	0.32	18,18,18,18	0
57	MG	CA	1622	1/1	0.97	0.09	37,37,37,37	0
57	MG	DA	9621	1/1	0.97	0.59	0,0,0,0	1
57	MG	BA	3240	1/1	0.97	0.13	21,21,21,21	0
57	MG	DA	9322	1/1	0.97	0.24	8,8,8,8	0
57	MG	DA	9617	1/1	0.97	0.29	11,11,11,11	0
57	MG	BA	3089	1/1	0.97	0.23	18,18,18,18	0
57	MG	DA	9517	1/1	0.97	0.29	0,0,0,0	0
57	MG	DA	9520	1/1	0.97	0.47	2,2,2,2	0
57	MG	DA	9586	1/1	0.97	0.20	3,3,3,3	0
57	MG	CA	1611	1/1	0.97	0.54	0,0,0,0	0
57	MG	DA	9697	1/1	0.97	0.22	41,41,41,41	0
57	MG	DA	9404	1/1	0.97	0.31	12,12,12,12	0
57	MG	CA	1647	1/1	0.97	0.36	6,6,6,6	0
57	MG	BA	3085	1/1	0.97	0.26	29,29,29,29	0
57	MG	AA	7003	1/1	0.97	0.10	27,27,27,27	0
57	MG	BA	3180	1/1	0.97	0.60	2,2,2,2	0
57	MG	AA	7025	1/1	0.97	0.21	1,1,1,1	0
57	MG	DA	9315	1/1	0.97	0.10	26,26,26,26	0
57	MG	CA	1624	1/1	0.97	0.33	18,18,18,18	0
57	MG	BA	3048	1/1	0.97	0.29	17,17,17,17	0
57	MG	CA	1652	1/1	0.97	0.60	6,6,6,6	0
57	MG	BA	3065	1/1	0.97	0.65	2,2,2,2	0
57	MG	DA	9515	1/1	0.97	0.32	10,10,10,10	0
57	MG	DA	9534	1/1	0.97	0.51	1,1,1,1	0
57	MG	DA	9509	1/1	0.97	0.44	17,17,17,17	0
57	MG	DA	9562	1/1	0.97	0.60	2,2,2,2	0
57	MG	BA	3080	1/1	0.97	0.56	0,0,0,0	0
57	MG	DA	9411	1/1	0.97	0.27	2,2,2,2	0
57	MG	BA	3165	1/1	0.97	0.57	0,0,0,0	0
57	MG	DA	9521	1/1	0.97	0.57	2,2,2,2	0
57	MG	DA	9678	1/1	0.97	0.19	33,33,33,33	0
57	MG	DA	9649	1/1	0.97	0.42	1,1,1,1	0
57	MG	AA	7068	1/1	0.97	0.09	34,34,34,34	0
57	MG	DA	9637	1/1	0.97	0.37	18,18,18,18	0
57	MG	DA	9499	1/1	0.97	0.15	29,29,29,29	0
57	MG	DA	9427	1/1	0.97	0.20	91,91,91,91	0
57	MG	DA	9316	1/1	0.97	0.23	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	7042	1/1	0.97	0.08	31,31,31,31	0
57	MG	DA	9650	1/1	0.97	0.26	7,7,7,7	0
57	MG	DA	9344	1/1	0.97	0.44	33,33,33,33	0
59	ZN	AN	101	1/1	0.97	0.10	147,147,147,147	0
57	MG	BA	3215	1/1	0.97	0.41	1,1,1,1	0
57	MG	DD	7101	1/1	0.97	0.48	3,3,3,3	0
57	MG	BD	301	1/1	0.97	0.57	7,7,7,7	0
57	MG	BA	3288	1/1	0.98	0.14	18,18,18,18	0
57	MG	CA	1718	1/1	0.98	0.27	27,27,27,27	0
57	MG	BA	3046	1/1	0.98	0.64	1,1,1,1	0
57	MG	DA	9309	1/1	0.98	0.34	6,6,6,6	0
57	MG	DA	9324	1/1	0.98	0.48	2,2,2,2	0
57	MG	BA	3072	1/1	0.98	0.17	25,25,25,25	0
57	MG	BA	3179	1/1	0.98	0.31	10,10,10,10	0
57	MG	DA	9359	1/1	0.98	0.38	0,0,0,0	0
57	MG	BA	3197	1/1	0.98	0.22	1,1,1,1	0
57	MG	DA	9364	1/1	0.98	0.82	1,1,1,1	0
57	MG	BA	3125	1/1	0.98	0.29	20,20,20,20	0
57	MG	DA	9481	1/1	0.98	0.09	0,0,0,0	0
57	MG	BA	3279	1/1	0.98	0.24	31,31,31,31	0
57	MG	DA	9641	1/1	0.98	0.07	11,11,11,11	0
57	MG	DA	9542	1/1	0.98	0.35	6,6,6,6	0
57	MG	DA	9386	1/1	0.98	0.46	2,2,2,2	0
57	MG	CA	1645	1/1	0.98	0.35	20,20,20,20	0
57	MG	DA	9437	1/1	0.98	0.19	14,14,14,14	0
57	MG	DA	9619	1/1	0.98	0.15	0,0,0,0	0
57	MG	BA	3060	1/1	0.98	0.57	1,1,1,1	0
57	MG	BA	3206	1/1	0.98	0.45	29,29,29,29	0
57	MG	CA	1615	1/1	0.98	0.27	0,0,0,0	0
57	MG	DA	9554	1/1	0.98	0.27	10,10,10,10	0
57	MG	DA	9449	1/1	0.98	0.43	0,0,0,0	0
57	MG	DA	9310	1/1	0.98	0.29	0,0,0,0	0
59	ZN	CD	301	1/1	0.98	0.32	44,44,44,44	0
57	MG	BA	3260	1/1	0.98	0.57	8,8,8,8	0
57	MG	CA	1619	1/1	0.98	0.52	11,11,11,11	0
57	MG	DA	9493	1/1	0.98	0.26	1,1,1,1	0
57	MG	CA	1733	1/1	0.98	0.46	11,11,11,11	0
57	MG	BA	3009	1/1	0.98	0.15	2,2,2,2	0
57	MG	BA	3182	1/1	0.98	0.57	2,2,2,2	0
57	MG	BA	3078	1/1	0.98	0.43	2,2,2,2	0
57	MG	DA	9406	1/1	0.98	0.18	32,32,32,32	0
57	MG	DA	9408	1/1	0.98	0.25	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3034	1/1	0.98	0.22	7,7,7,7	0
57	MG	DA	9524	1/1	0.98	0.36	2,2,2,2	0
57	MG	BA	3238	1/1	0.98	0.33	9,9,9,9	0
57	MG	CA	1729	1/1	0.98	0.43	35,35,35,35	0
57	MG	DA	9558	1/1	0.98	0.15	6,6,6,6	0
57	MG	DA	9488	1/1	0.98	0.56	0,0,0,0	0
57	MG	BA	3234	1/1	0.98	0.56	10,10,10,10	0
57	MG	BA	3218	1/1	0.98	0.30	24,24,24,24	0
57	MG	BA	3027	1/1	0.98	0.34	4,4,4,4	0
57	MG	BA	3176	1/1	0.98	0.33	0,0,0,0	0
57	MG	BA	3105	1/1	0.98	0.69	26,26,26,26	0
57	MG	DA	9472	1/1	0.98	0.41	16,16,16,16	0
57	MG	DA	9537	1/1	0.98	0.38	0,0,0,0	0
57	MG	BA	3091	1/1	0.98	0.19	0,0,0,0	0
57	MG	DA	9390	1/1	0.98	0.28	0,0,0,0	0
57	MG	DA	9355	1/1	0.98	0.67	0,0,0,0	0
57	MG	DA	9564	1/1	0.98	0.58	17,17,17,17	0
57	MG	DA	9430	1/1	0.98	0.39	0,0,0,0	0
57	MG	BA	3015	1/1	0.98	0.20	3,3,3,3	0
57	MG	DA	9360	1/1	0.98	0.36	7,7,7,7	0
57	MG	BA	3316	1/1	0.98	0.42	7,7,7,7	0
57	MG	BA	3051	1/1	0.98	0.40	6,6,6,6	0
57	MG	BA	3237	1/1	0.98	0.24	43,43,43,43	0
57	MG	DA	9479	1/1	0.98	0.63	0,0,0,0	0
57	MG	DA	9346	1/1	0.98	0.30	0,0,0,0	0
57	MG	DA	9672	1/1	0.98	0.37	5,5,5,5	0
57	MG	AA	7077	1/1	0.98	0.16	22,22,22,22	0
57	MG	BA	3073	1/1	0.98	0.67	8,8,8,8	0
57	MG	DA	9308	1/1	0.98	0.44	2,2,2,2	0
57	MG	DU	202	1/1	0.98	0.15	6,6,6,6	0
57	MG	DA	9400	1/1	0.98	0.41	0,0,0,0	0
57	MG	BA	3142	1/1	0.98	0.43	10,10,10,10	0
57	MG	DA	9312	1/1	0.98	0.67	4,4,4,4	0
57	MG	AA	7035	1/1	0.98	0.11	42,42,42,42	0
57	MG	CA	1620	1/1	0.98	0.27	1,1,1,1	0
57	MG	BA	3210	1/1	0.98	0.74	11,11,11,11	0
57	MG	BA	3207	1/1	0.98	0.38	1,1,1,1	0
57	MG	DA	9584	1/1	0.98	0.36	0,0,0,0	0
57	MG	BA	3008	1/1	0.98	0.46	2,2,2,2	0
57	MG	DA	9362	1/1	0.98	0.34	5,5,5,5	0
57	MG	DA	9627	1/1	0.98	0.29	0,0,0,0	1
57	MG	DA	9392	1/1	0.98	0.70	12,12,12,12	0

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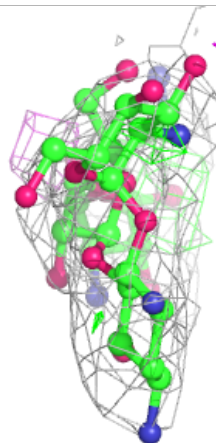
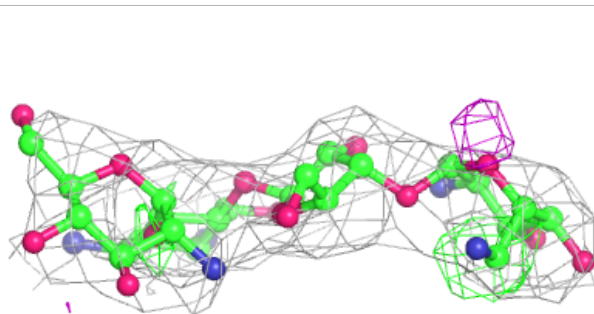
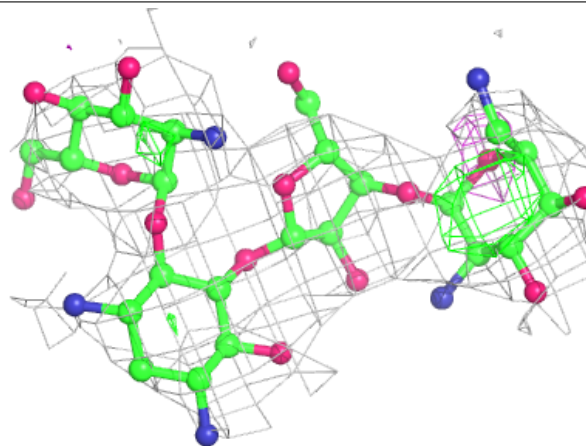
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3124	1/1	0.98	0.20	17,17,17,17	0
57	MG	DU	203	1/1	0.99	0.14	0,0,0,0	1
57	MG	BA	3299	1/1	0.99	0.48	10,10,10,10	0
57	MG	BA	3224	1/1	0.99	0.17	5,5,5,5	0
57	MG	DA	9354	1/1	0.99	0.49	2,2,2,2	0
57	MG	BA	3013	1/1	0.99	0.30	16,16,16,16	0
57	MG	AA	7006	1/1	0.99	0.37	20,20,20,20	0
57	MG	BA	3239	1/1	0.99	0.35	1,1,1,1	0
57	MG	AA	7019	1/1	0.99	0.56	16,16,16,16	0
57	MG	BE	303	1/1	0.99	0.15	1,1,1,1	0
57	MG	BA	3084	1/1	0.99	0.50	1,1,1,1	0
57	MG	BA	3259	1/1	0.99	0.32	18,18,18,18	0
57	MG	DA	9369	1/1	0.99	0.59	0,0,0,0	0
57	MG	DA	9398	1/1	0.99	0.44	0,0,0,0	0
57	MG	DA	9518	1/1	0.99	0.35	0,0,0,0	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around PAR CA 1741:**

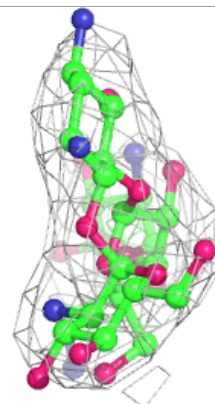
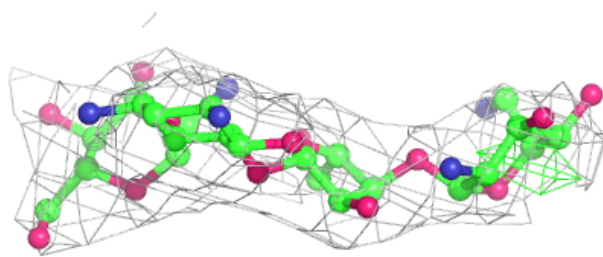
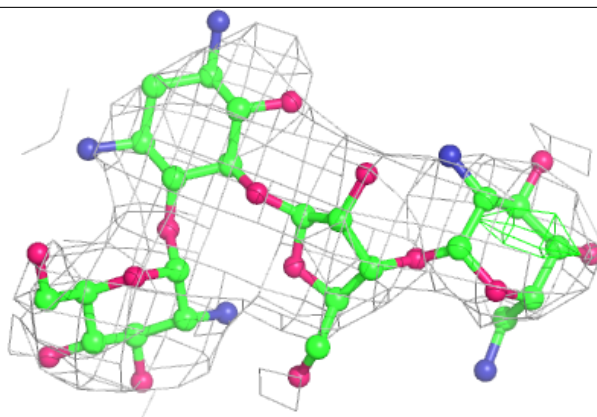
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PAR AA 7111:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.