



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 01:36 pm BST

PDB ID : 4V7Y
Title : Structure of the *Thermus thermophilus* 70S ribosome complexed with azithromycin.
Authors : Bulkley, D.P.; Innis, C.A.; Blaha, G.; Steitz, T.A.
Deposited on : 2010-08-18
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
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

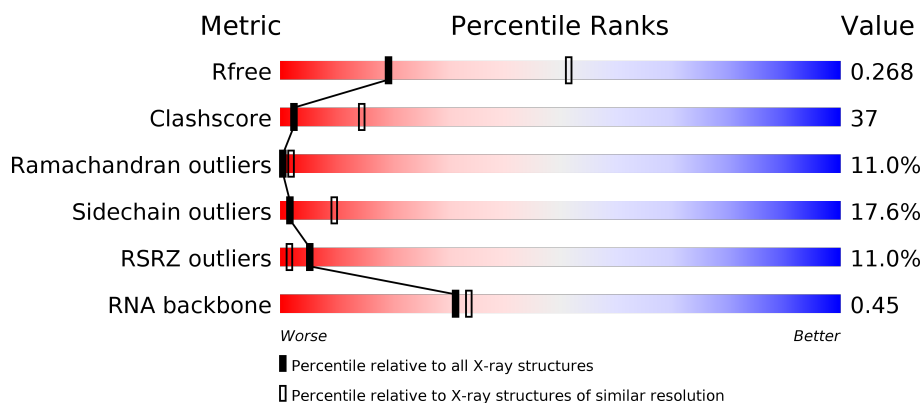
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	AA	1522	
1	CA	1522	
2	AB	256	
2	CB	256	

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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	135	
12	CL	135	
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	B0	85	
22	D0	85	
23	B1	98	
23	D1	98	
24	B2	72	
24	D2	72	
25	B3	60	
25	D3	60	
26	B4	71	
26	D4	71	
27	B5	60	
27	D5	60	



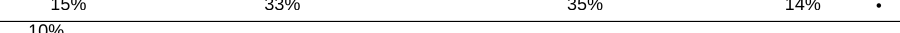

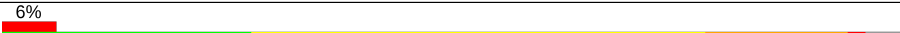
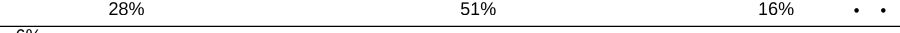
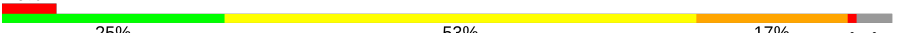
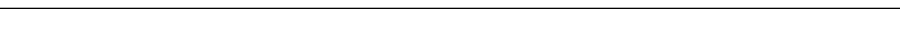
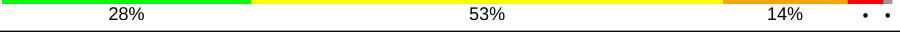
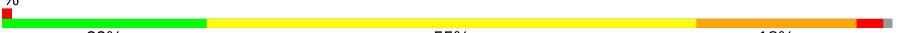
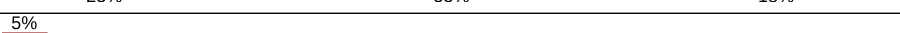


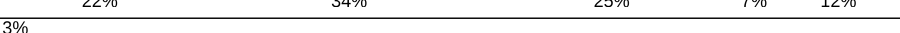
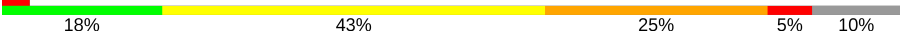

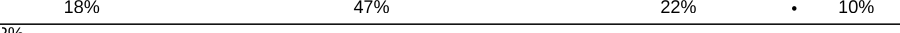



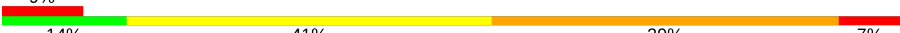


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Mol	Chain	Length	Quality of chain
28	B6	54	
28	D6	54	
29	B7	49	
29	D7	49	
30	B8	65	
30	D8	65	
31	BA	2787	
31	DA	2787	
32	BB	122	
32	DB	122	
33	BD	276	
33	DD	276	
34	BE	206	
34	DE	206	
35	BF	210	
35	DF	210	
36	BG	182	
36	DG	182	
37	BH	180	
37	DH	180	
38	BI	148	
38	DI	148	
39	BN	140	
39	DN	140	
40	BO	122	

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Mol	Chain	Length	Quality of chain
40	DO	122	
41	BP	150	
41	DP	150	
42	BQ	141	
42	DQ	141	
43	BR	118	
43	DR	118	
44	BS	112	
44	DS	112	
45	BT	146	
45	DT	146	
46	BU	118	
46	DU	118	
47	BV	101	
47	DV	101	
48	BW	113	
48	DW	113	
49	BX	96	
49	DX	96	
50	BY	110	
50	DY	110	
51	BZ	206	
51	DZ	206	

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
52	MG	AA	1644	-	-	-	X
52	MG	AA	1650	-	-	-	X
52	MG	BA	3241	-	-	-	X
52	MG	BA	3246	-	-	-	X
52	MG	BA	3296	-	-	-	X
52	MG	BA	3309	-	-	-	X
52	MG	BA	3312	-	-	-	X
52	MG	BA	3336	-	-	-	X
52	MG	BA	3341	-	-	-	X
52	MG	CA	1611	-	-	-	X
52	MG	CA	1626	-	-	-	X
52	MG	CA	1628	-	-	-	X
52	MG	CA	1646	-	-	-	X
52	MG	DA	3198	-	-	-	X
52	MG	DA	3203	-	-	-	X
52	MG	DA	3207	-	-	-	X
52	MG	DA	3216	-	-	-	X
52	MG	DA	3222	-	-	-	X
52	MG	DA	3243	-	-	-	X
52	MG	DA	3255	-	-	-	X
52	MG	DA	3260	-	-	-	X
52	MG	DA	3261	-	-	-	X
52	MG	DA	3267	-	-	-	X
52	MG	DA	3278	-	-	-	X
52	MG	DA	3291	-	-	-	X
54	K	BA	3350	-	-	-	X
54	K	DA	3310	-	-	-	X

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 278000 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
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- 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			
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
			1011	639	198	174			
9	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	CONFLICT	UNP P80374
CI	58	ARG	HIS	CONFLICT	UNP P80374

- 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			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	2	VAL	-	INSERTION	UNP Q5SHN3
AL	3	ALA	-	INSERTION	UNP Q5SHN3
AL	4	LEU	-	INSERTION	UNP Q5SHN3
CL	2	VAL	-	INSERTION	UNP Q5SHN3
CL	3	ALA	-	INSERTION	UNP Q5SHN3
CL	4	LEU	-	INSERTION	UNP Q5SHN3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			
13	CM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			

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

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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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 protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	B0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			
22	D0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	B1	89	Total	C	N	O	0	0	1
			693	435	140	118			
23	D1	89	Total	C	N	O	0	0	1
			693	435	140	118			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	B2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			
24	D2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	B4	32	Total	C	N	O	0	0	0
			157	93	32	32			
26	D4	32	Total	C	N	O	0	0	0
			157	93	32	32			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B5	59	Total	C	N	O	S	9	0	0
			459	288	90	76	5			
27	D5	59	Total	C	N	O	S	9	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

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

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BA	2725	Total	C	N	O	P	0	0	0
			58698	26124	10986	18864	2724			
31	DA	2725	Total	C	N	O	P	0	0	0
			58698	26124	10986	18864	2724			

- Molecule 32 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 33 is a protein called 50S ribosomal protein L2.

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

- Molecule 34 is a protein called 50S ribosomal protein L3.

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

- Molecule 35 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	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
35	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 36 is a protein called 50S ribosomal protein L5.

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

- Molecule 37 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
37	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 38 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
38	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 39 is a protein called 50S ribosomal protein L13.

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

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
41	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 42 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			
42	DQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 43 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
43	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 44 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BS	99	Total	C	N	O	0	0	1
			771	486	155	130			
44	DS	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 45 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BT	132	Total	C	N	O	S	0	0	0
			1100	686	227	186	1			
45	DT	132	Total	C	N	O	S	0	0	0
			1100	686	227	186	1			

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

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

- Molecule 49 is a protein called 50S ribosomal protein L23.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
50	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 51 is a protein called 50S ribosomal protein L25.

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

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

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	BA	349	Total	Mg	0	0
			349	349		
52	CA	48	Total	Mg	0	0
			48	48		
52	DQ	1	Total	Mg	0	0
			1	1		
52	DF	1	Total	Mg	0	0
			1	1		
52	BE	1	Total	Mg	0	0
			1	1		
52	DU	1	Total	Mg	0	0
			1	1		
52	B1	1	Total	Mg	0	0
			1	1		
52	BP	3	Total	Mg	0	0
			3	3		
52	DR	1	Total	Mg	0	0
			1	1		
52	B5	2	Total	Mg	0	0
			2	2		
52	BB	5	Total	Mg	0	0
			5	5		
52	BF	1	Total	Mg	0	0
			1	1		
52	BX	1	Total	Mg	0	0
			1	1		
52	AA	51	Total	Mg	0	0
			51	51		
52	BQ	2	Total	Mg	0	0
			2	2		
52	D7	1	Total	Mg	0	0
			1	1		
52	BU	1	Total	Mg	0	0
			1	1		
52	DD	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	D0	1	Total 1	Mg 1	0	0
52	BR	1	Total 1	Mg 1	0	0
52	DA	309	Total 309	Mg 309	0	0
52	B7	1	Total 1	Mg 1	0	0
52	DE	1	Total 1	Mg 1	0	0
52	D1	1	Total 1	Mg 1	0	0
52	DX	1	Total 1	Mg 1	0	0
52	DP	1	Total 1	Mg 1	0	0
52	D5	2	Total 2	Mg 2	0	0
52	BD	1	Total 1	Mg 1	0	0
52	B0	1	Total 1	Mg 1	0	0
52	DB	3	Total 3	Mg 3	0	0

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 54 is POTASSIUM ION (three-letter code: K) (formula: K).

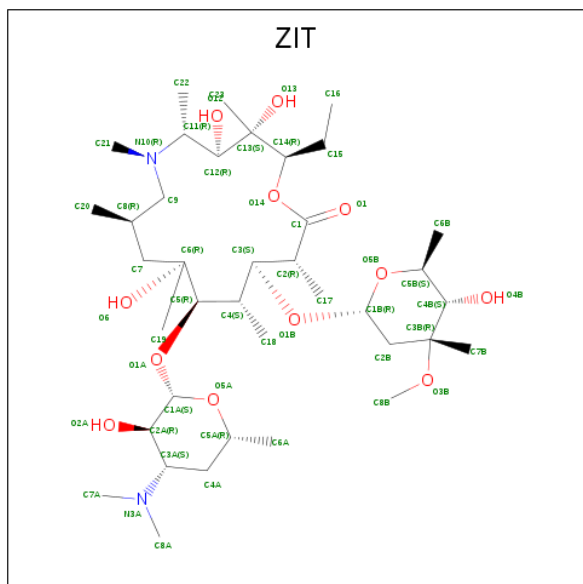
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	DA	1	Total K 1 1	0	0

- Molecule 55 is AZITHROMYCIN (three-letter code: ZIT) (formula: $C_{38}H_{72}N_2O_{12}$).

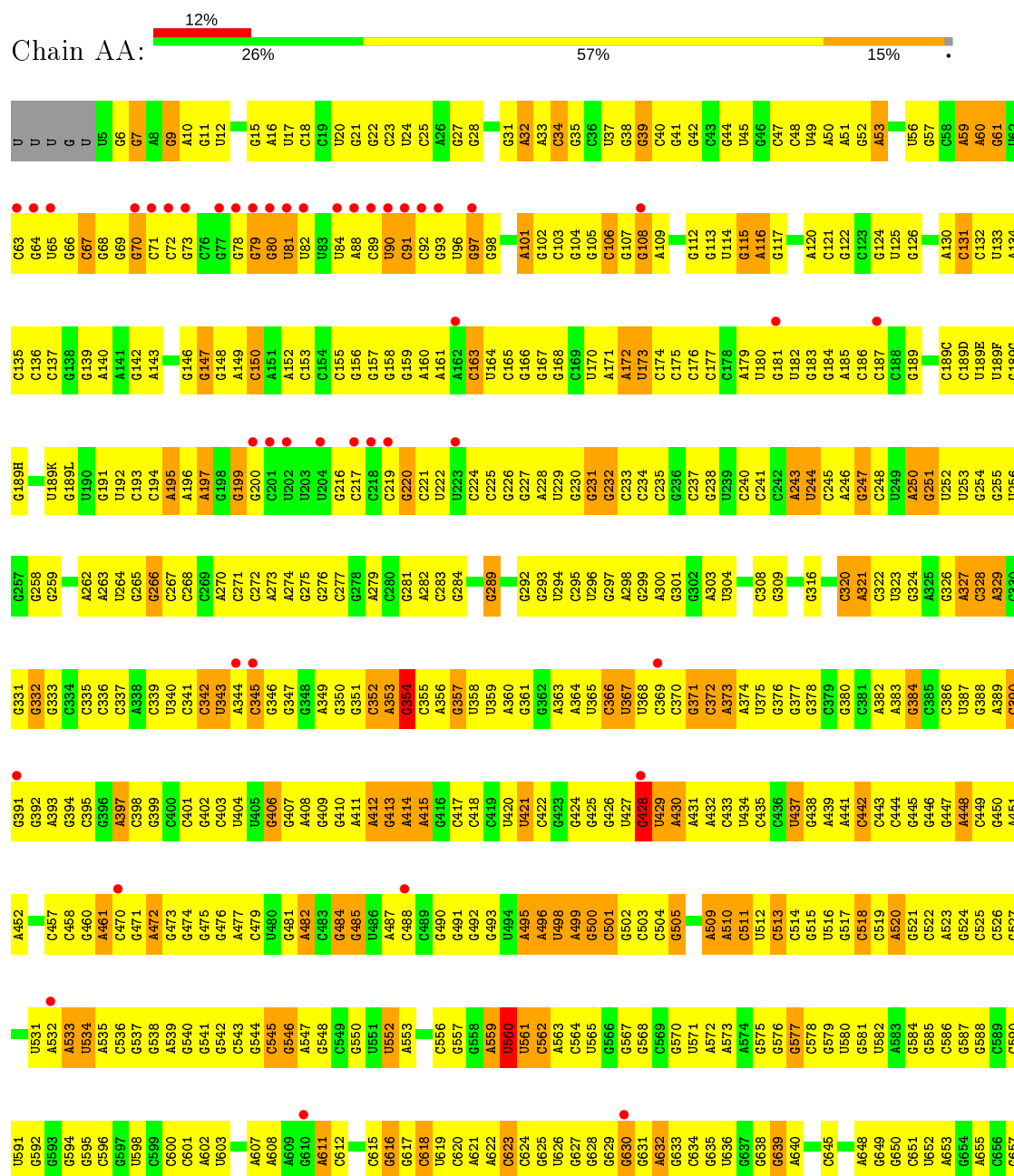


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	BA	1	Total	C	N	O	0	0
			52	38	2	12		
55	DA	1	Total	C	N	O	0	0
			52	38	2	12		

3 Residue-property plots

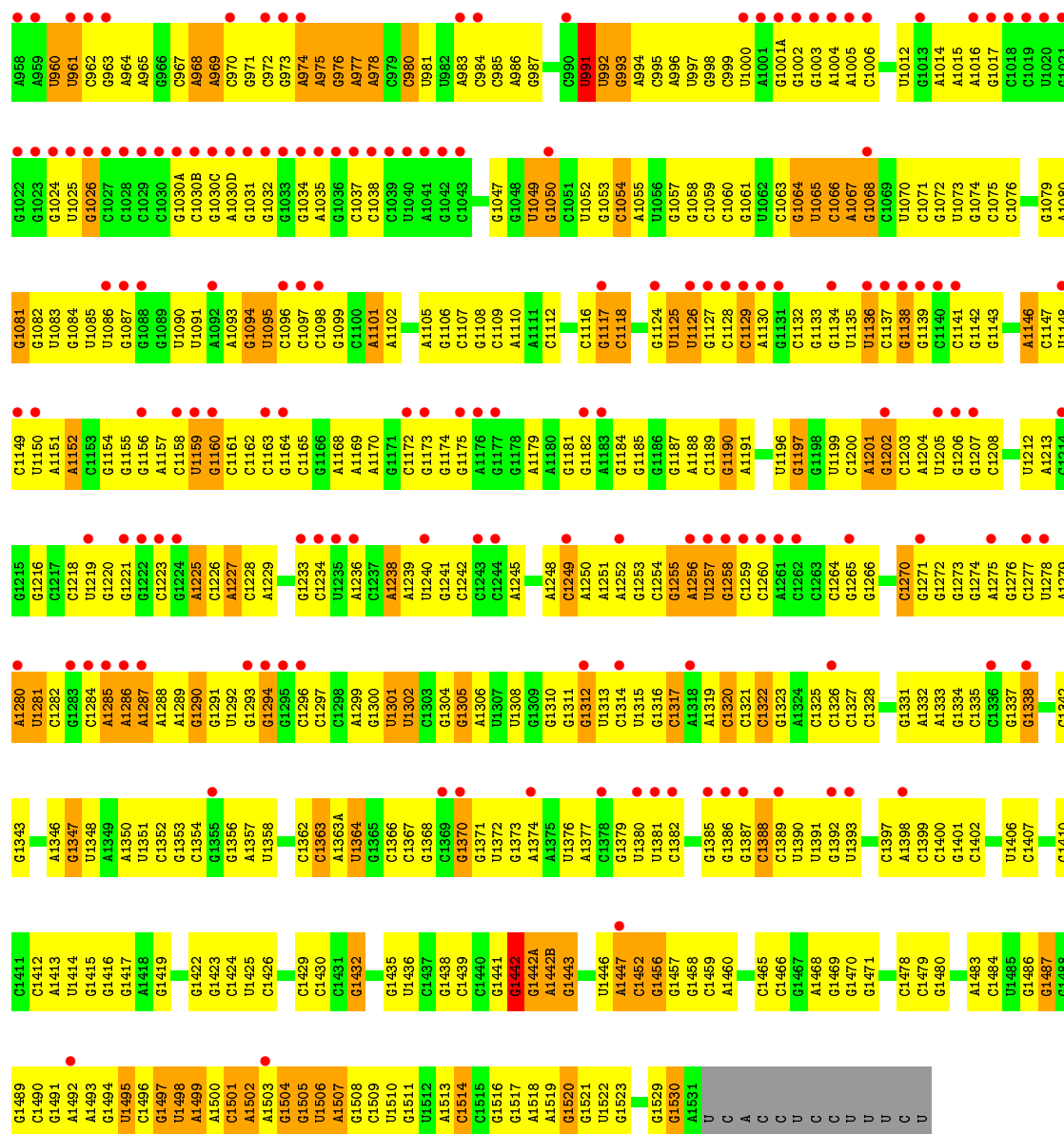
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S rRNA



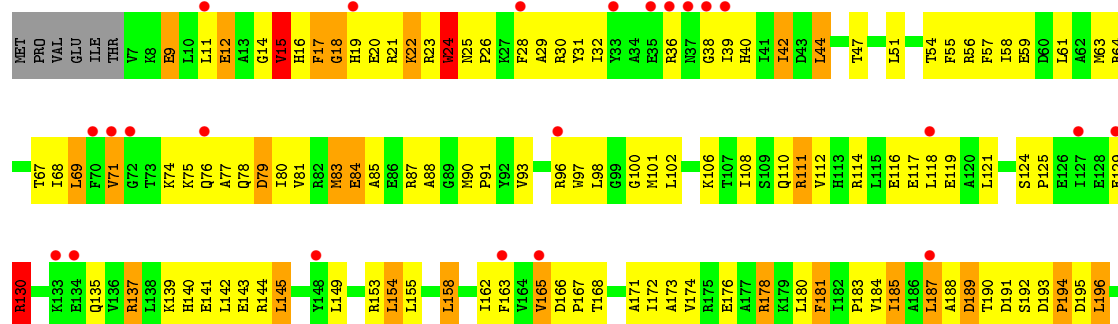
- Molecule 1: 16S rRNA

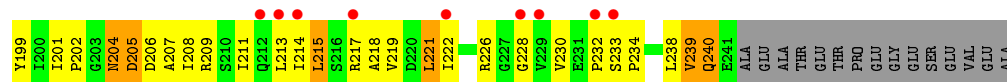




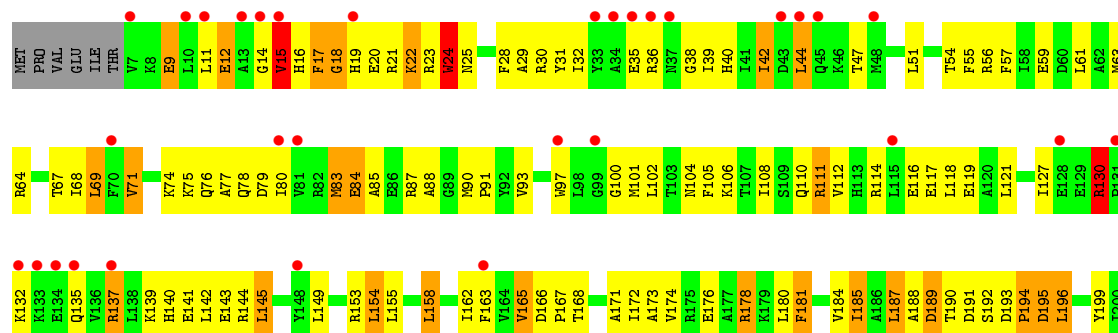
• Molecule 2: 30S ribosomal protein S2

Chain AB: 13% 34% 44% 12% 8%

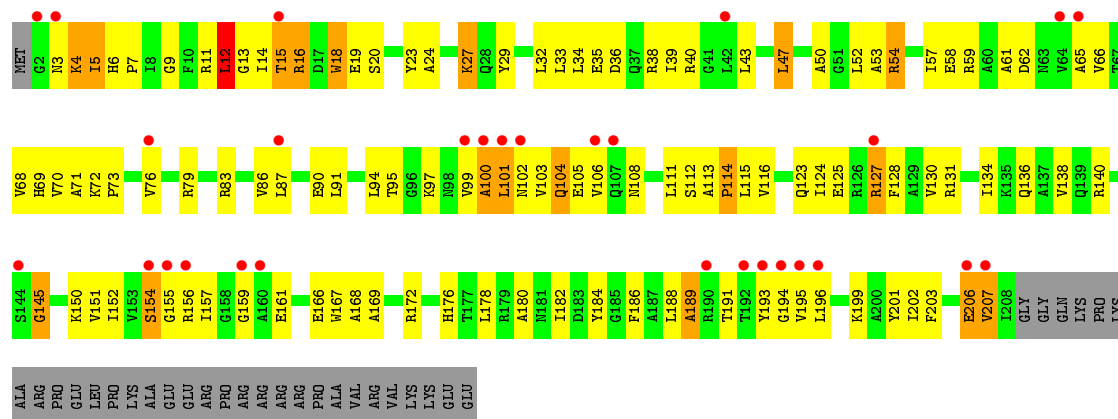




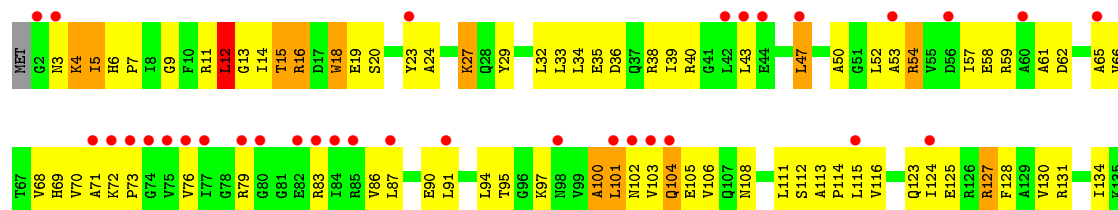
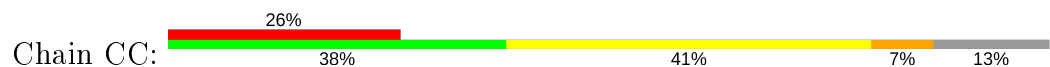
• Molecule 2: 30S ribosomal protein S2

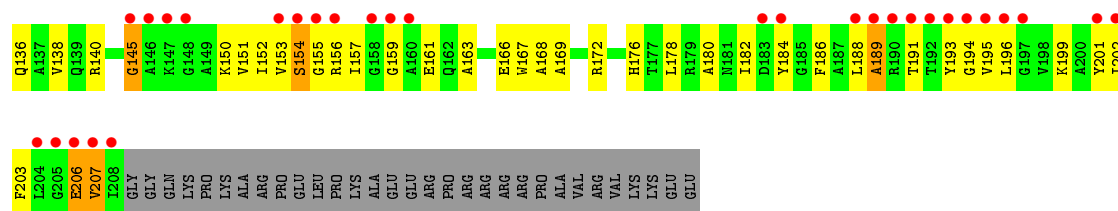


• Molecule 3: 30S ribosomal protein S3

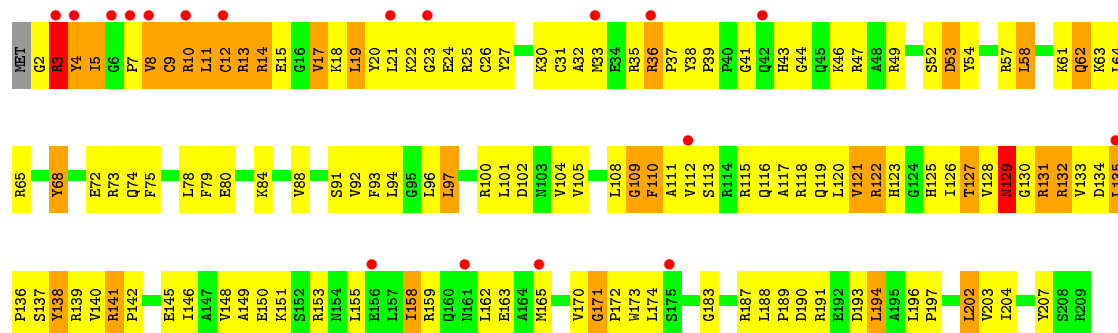


• Molecule 3: 30S ribosomal protein S3

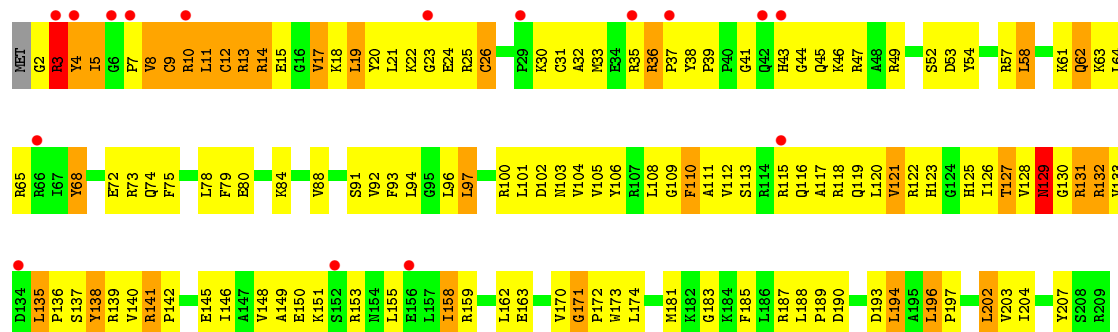




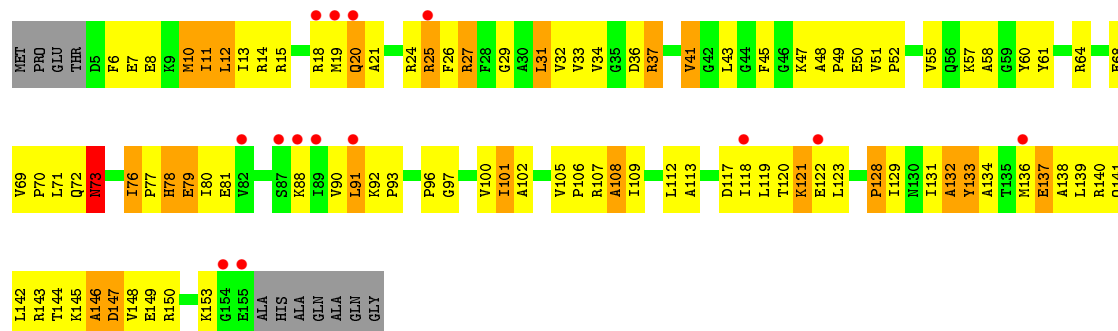
• Molecule 4: 30S ribosomal protein S4



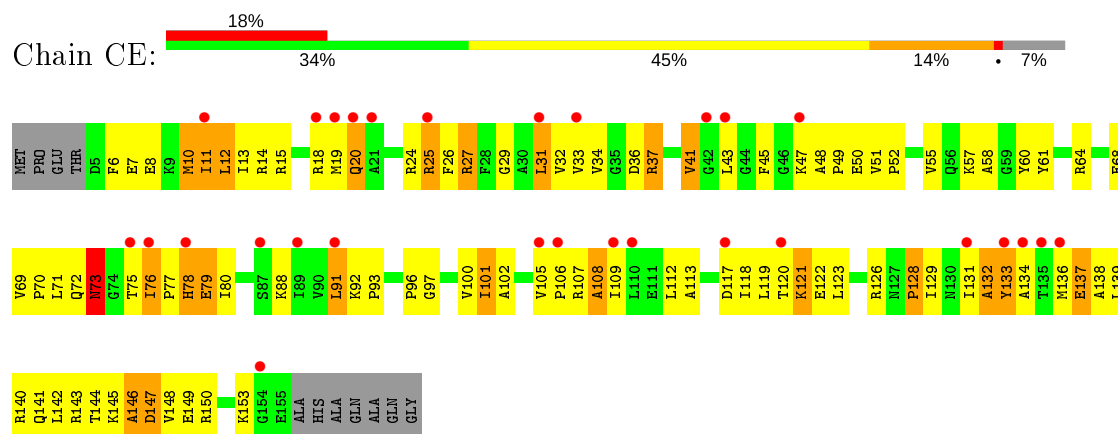
• Molecule 4: 30S ribosomal protein S4



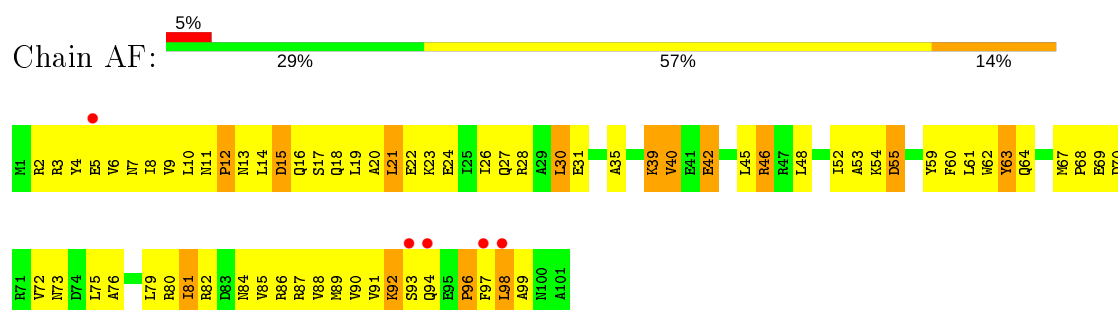
• Molecule 5: 30S ribosomal protein S5



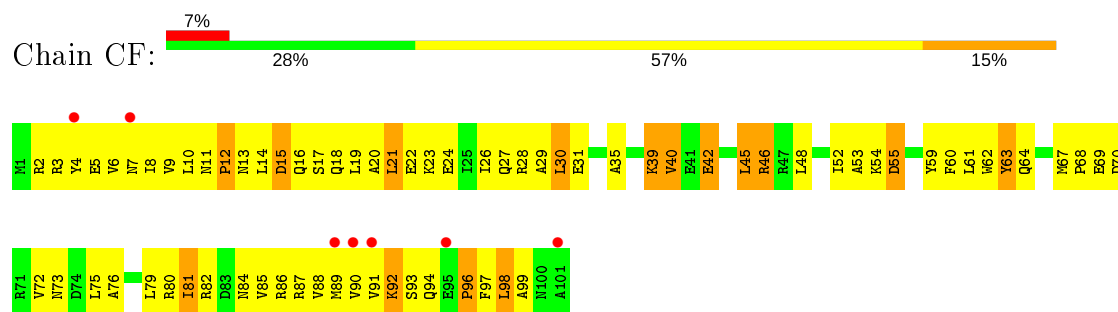
- Molecule 5: 30S ribosomal protein S5



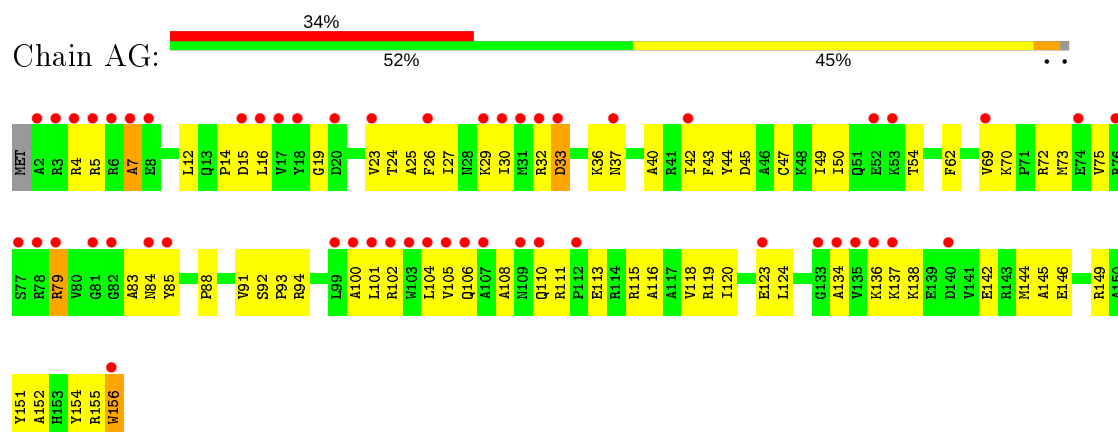
- Molecule 6: 30S ribosomal protein S6



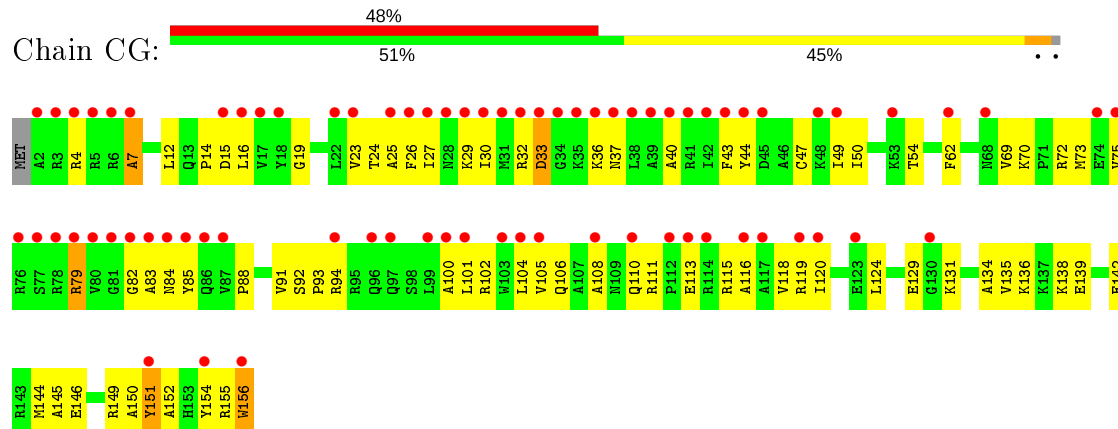
- Molecule 6: 30S ribosomal protein S6



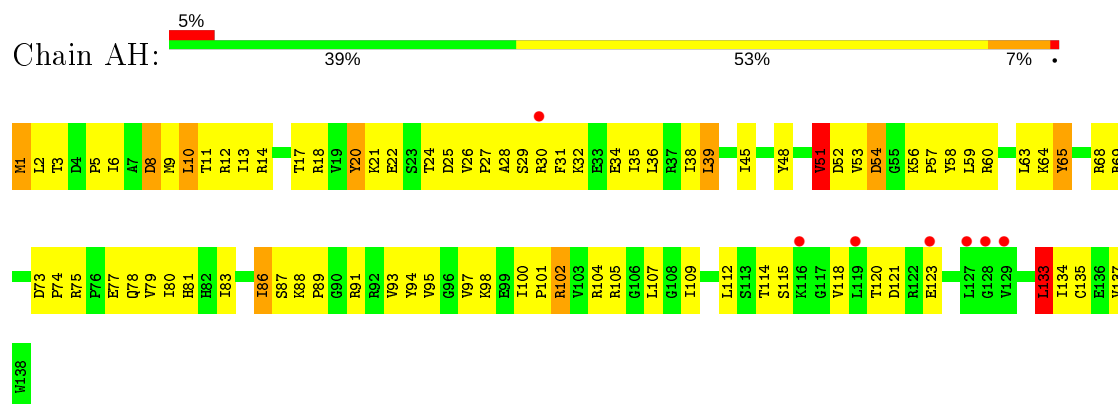
- Molecule 7: 30S ribosomal protein S7



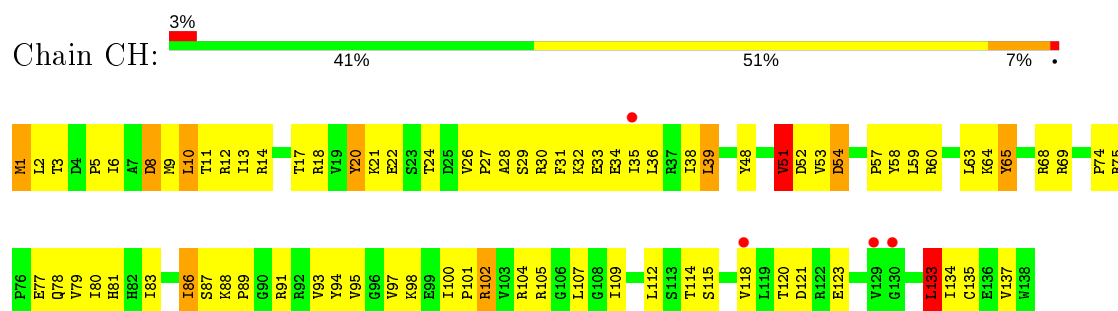
- Molecule 7: 30S ribosomal protein S7



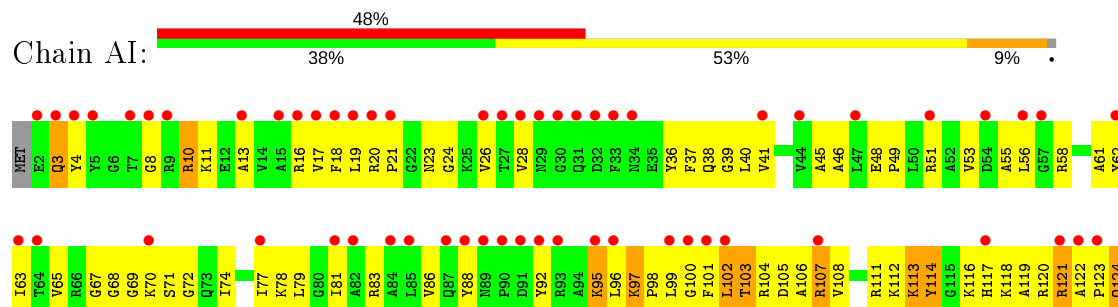
- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8

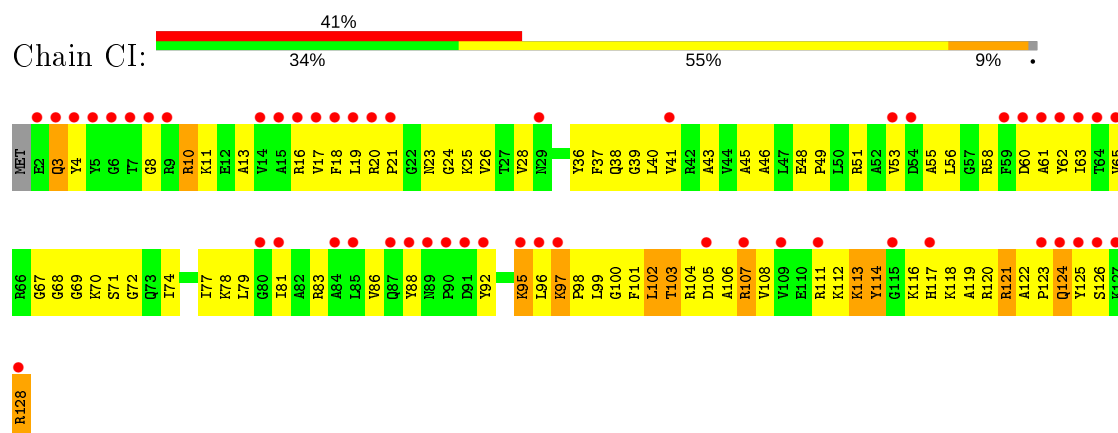


- Molecule 9: 30S ribosomal protein S9

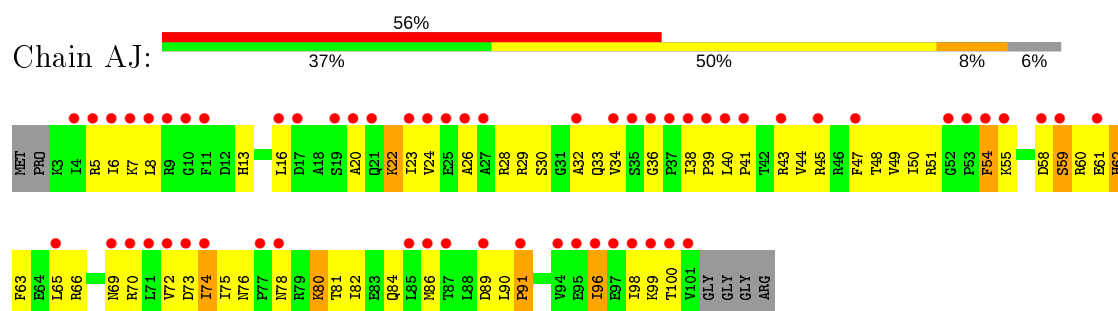




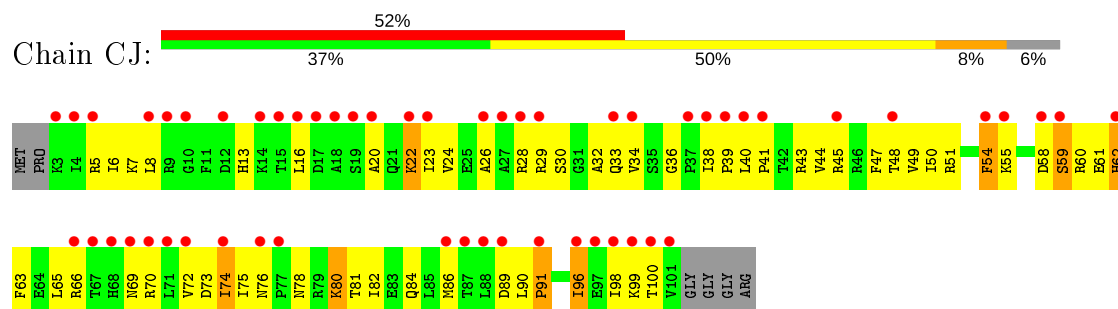
• Molecule 9: 30S ribosomal protein S9



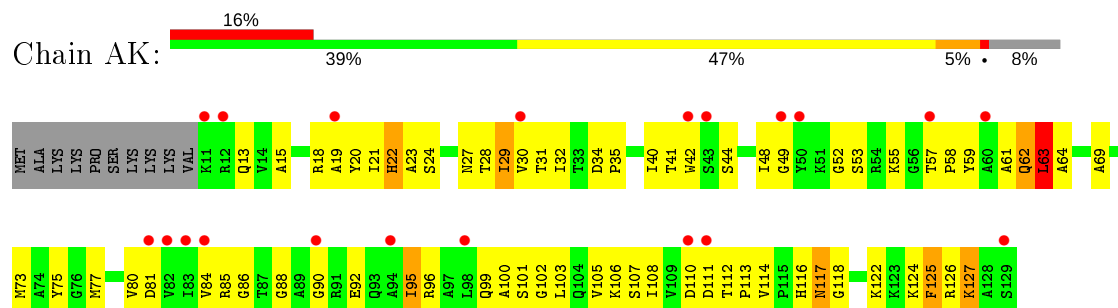
• Molecule 10: 30S ribosomal protein S10




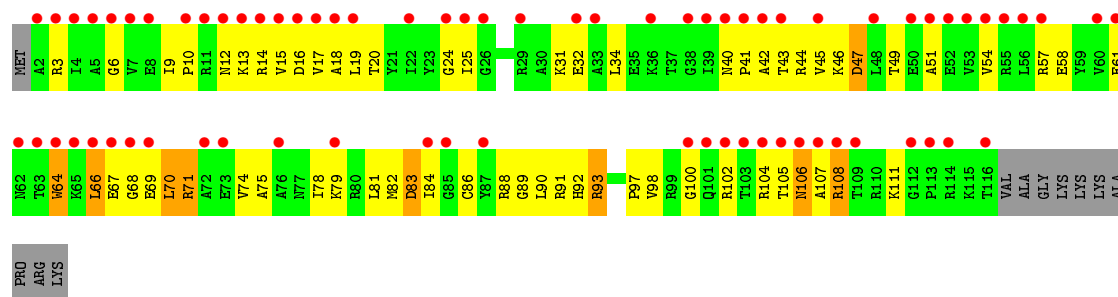
• Molecule 10: 30S ribosomal protein S10



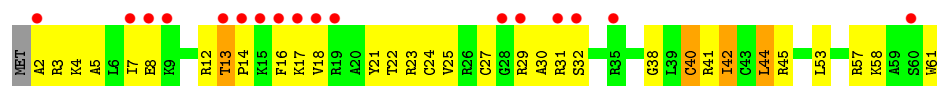
• Molecule 11: 30S ribosomal protein S11



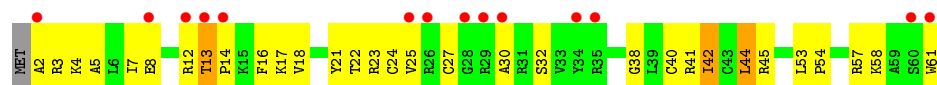
- Chain CM: 



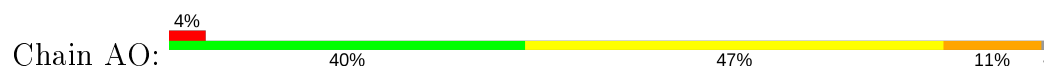
- Molecule 14: 30S ribosomal protein S14



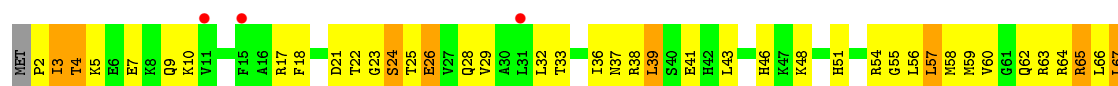
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

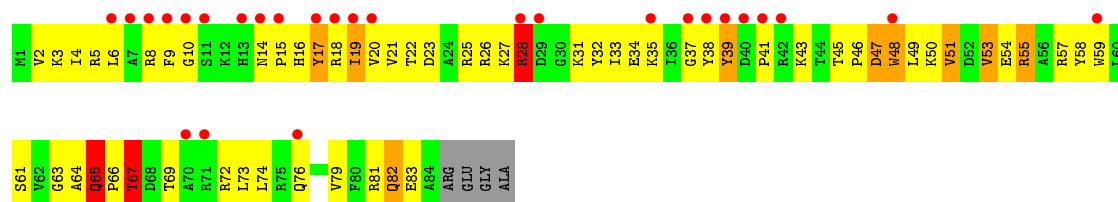


- Molecule 15: 30S ribosomal protein S15

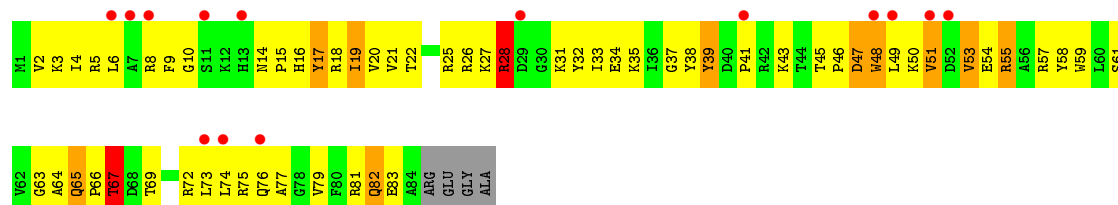


- Molecule 16: 30S ribosomal protein S16

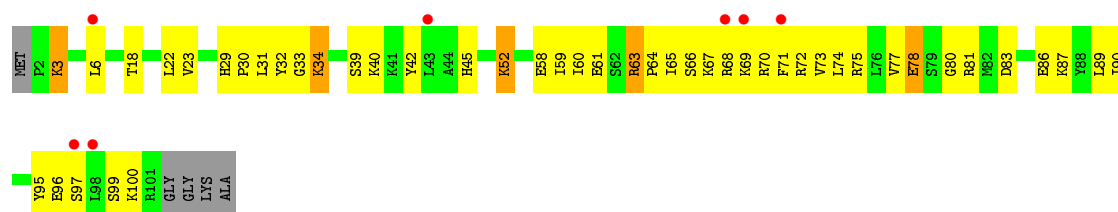




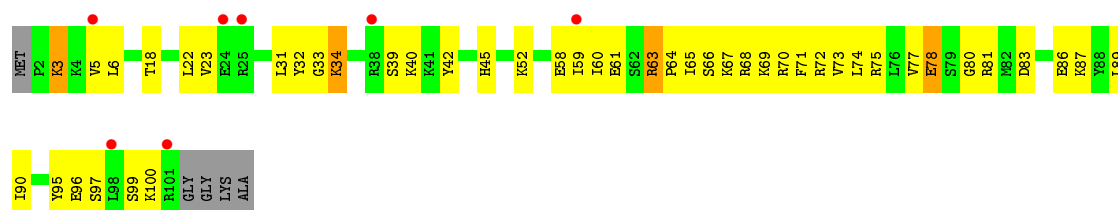
• Molecule 16: 30S ribosomal protein S16



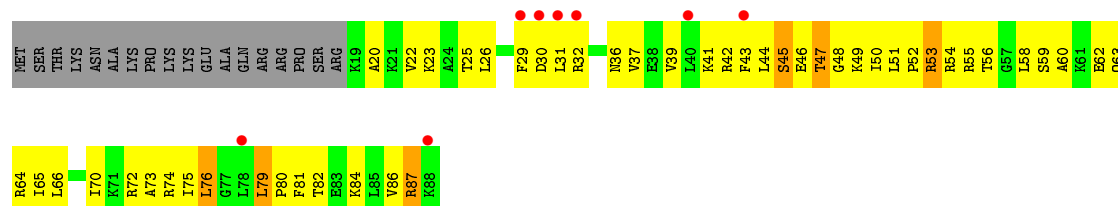
• Molecule 17: 30S ribosomal protein S17



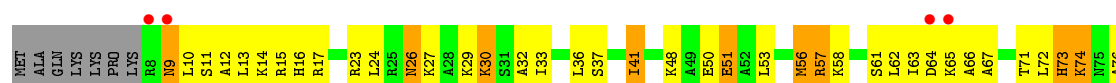
• Molecule 17: 30S ribosomal protein S17



• Molecule 18: 30S ribosomal protein S18

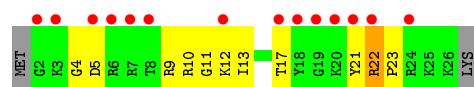


- Chain CR: 





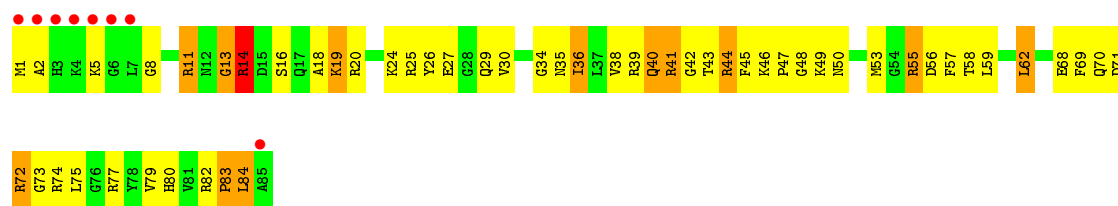
- Molecule 21: 30S ribosomal protein Thx



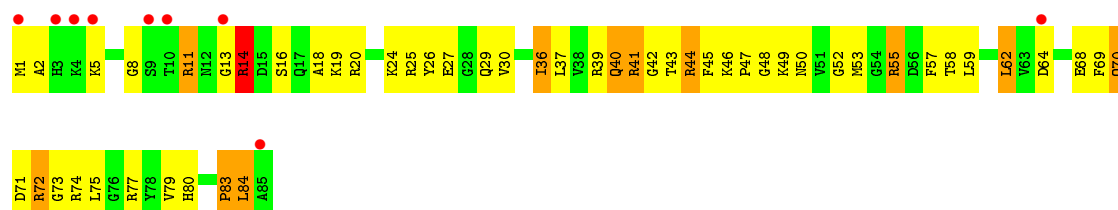
- Molecule 21: 30S ribosomal protein Thx



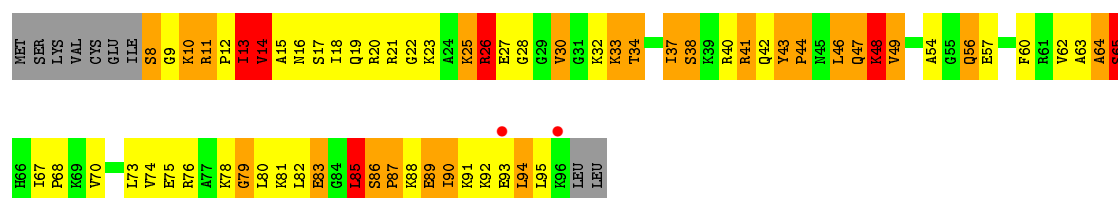
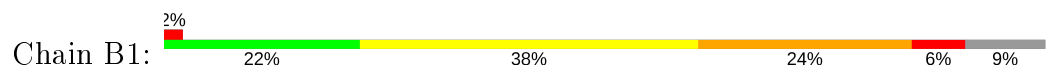
- Molecule 22: 50S ribosomal protein L27




- Molecule 22: 50S ribosomal protein L27

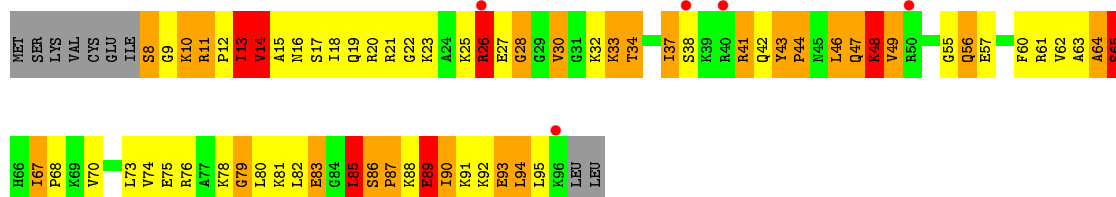


- Molecule 23: 50S ribosomal protein L28



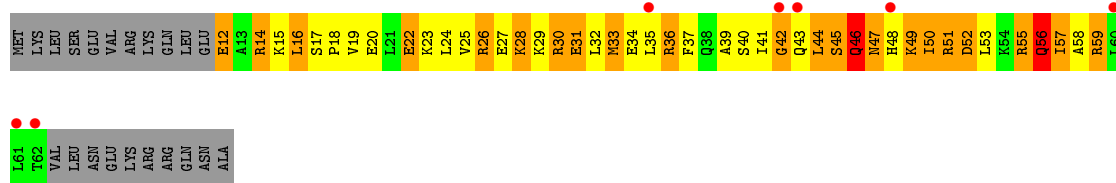
- Molecule 23: 50S ribosomal protein L28

Chain D1: 



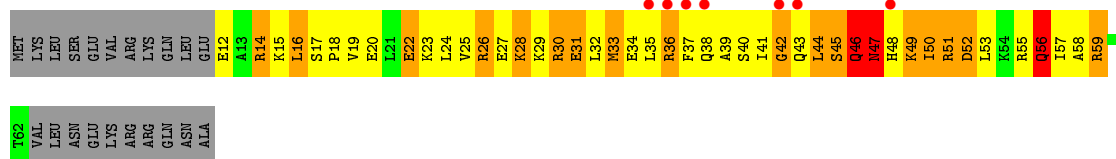
- Molecule 24: 50S ribosomal protein L29

Chain B2: 



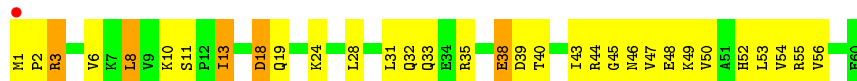
- Molecule 24: 50S ribosomal protein L29

Chain D2: 



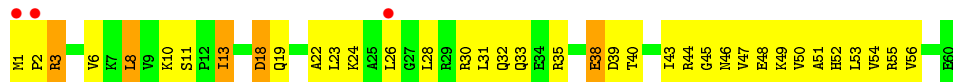
- Molecule 25: 50S ribosomal protein L30

Chain B3: 




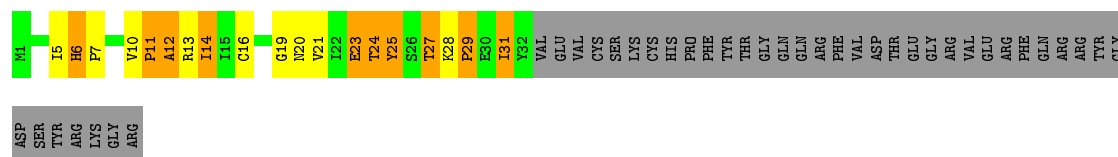
- Molecule 25: 50S ribosomal protein L30

Chain D3: 

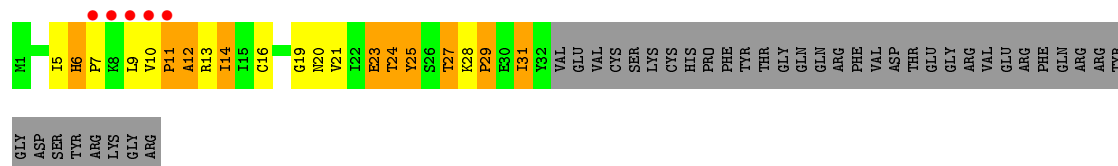
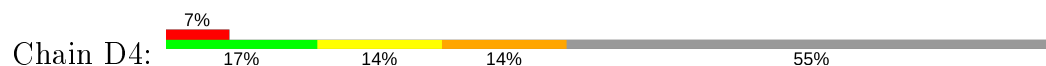


- Molecule 26: 50S ribosomal protein L31

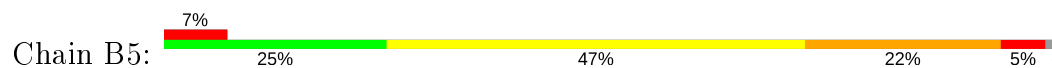
Chain B4: 



- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



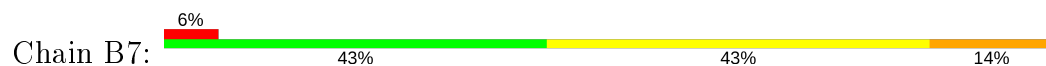
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



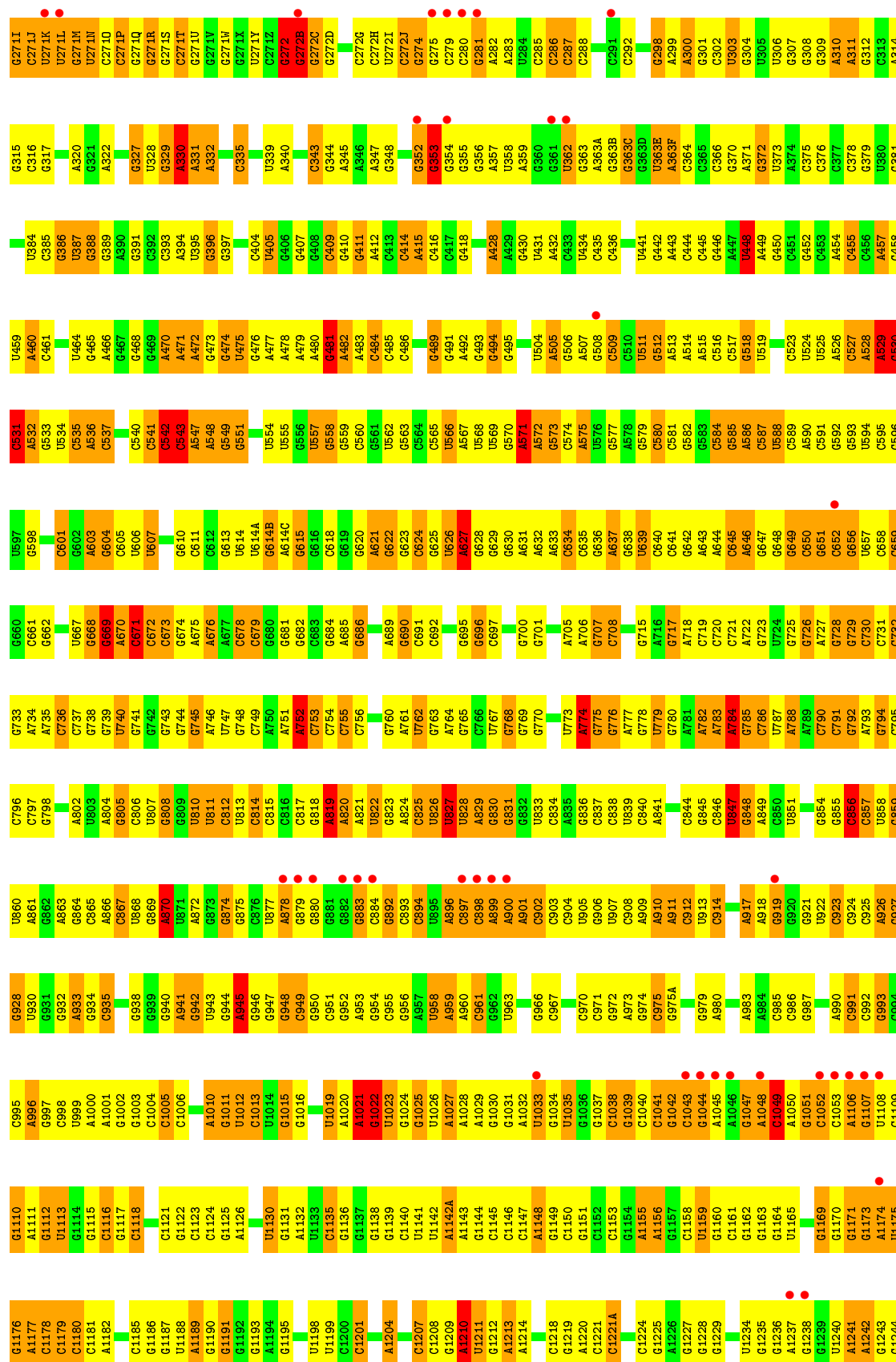
- Molecule 29: 50S ribosomal protein L34



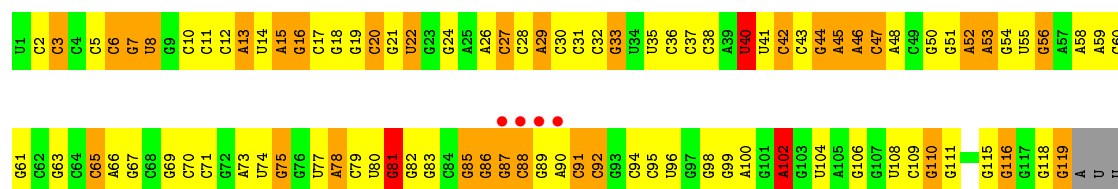












Chain DB:

8% 18% 52% 27%

U1 U2 U3 U4 U5 U6 U7 U8 U9 U10 U11 U12 U13 U14 U15 U16 U17 U18 U19 U20 U21 U22 U23 U24 U25 U26 U27 U28 U29 U30 U31 U32 U33 U34 U35 U36 U37 U38 U39 U40 U41 U42 U43 U44 U45 U46 U47 U48 U49 U50 U51 U52 U53 U54 U55 U56 U57 U58 U59 U60

G61 G62 G63 G64 G65 G66 G67 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 G129 G130 G131 G132 G133 G134 G135 G136 G137 G138 G139 G140 G141 G142 G143 G144 G145 G146 G147 G148 G149 G150 G151 G152 G153 G154 G155 G156 G157 G158 G159 G160

[illegible]

Chain DD:

Category	Percentage
A209	30%
G210	30%
R211	30%
S212	30%
R213	30%
E214	30%
I215	30%
G216	30%
R217	30%
R218	30%
P219	30%
H220	30%
V221	30%
R222	30%
G223	30%
A224	30%
A225	30%
G226	30%
I227	30%
P228	30%
V229	30%
D230	30%
H231	30%
P232	30%
R233	30%
G234	30%
G235	30%
G236	30%
E237	30%
G238	30%
R239	30%
A240	30%
P241	30%
R242	30%
G243	30%
R244	30%
P245	30%
A246	30%
G247	30%
S248	30%
P249	30%
V250	30%
G253	30%
T254	30%
R255	30%
G256	30%
L257	30%
R258	30%
T259	30%
S266	30%
S267	30%
R268	30%
P269	30%
I270	30%
I271	30%
A272	30%
G273	30%
R274	30%
R69	30%
A70	30%
K4	30%
R5	30%
R6	30%
K7	30%
P8	30%
Y9	30%
T10	30%
P11	30%
S12	30%
R13	30%
R14	30%
F15	30%
Y16	30%
T17	30%
V18	30%
A19	30%
D20	30%
I24	30%
T25	30%
R26	30%
T27	30%
E28	30%
P29	30%
Y30	30%
R31	30%
S32	30%
L33	30%
V34	30%
R35	30%
K38	30%
R39	30%
R43	30%
N44	30%
N45	30%
O46	30%
G47	30%
R48	30%
T49	30%
T50	30%
V51	30%
R52	30%
F53	30%
R54	30%
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E101	30%
K102	30%
R103	30%
Y104	30%
I105	30%
I106	30%
A107	30%
P108	30%
D109	30%
G110	30%
L111	30%
V117	30%
V118	30%
A119	30%
I125	30%
G126	30%
V127	30%
G128	30%
N129	30%
A130	30%
L131	30%
P132	30%
L133	30%
L136	30%
P137	30%
L165	30%
P166	30%
V138	30%
R69	30%
A70	30%
K4	30%
R5	30%
R6	30%
K7	30%
P8	30%
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T10	30%
P11	30%
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R14	30%
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Y16	30%
T17	30%
V18	30%
A19	30%
D20	30%
I24	30%
T25	30%
R26	30%
T27	30%
E28	30%
P29	30%
Y30	30%
R31	30%
S32	30%
L33	30%
V34	30%
R35	30%
K38	30%
R39	30%
R43	30%
N44	30%
N45	30%
O46	30%
G47	30%
R48	30%
T49	30%
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V51	30%
R52	30%
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I105	30%
I106	30%
A107	30%
P108	30%
D109	30%
G110	30%
L111	30%
V117	30%
V118	30%
A119	30%
I125	30%
G126	30%
V127	30%
G128	30%
N129	30%
A130	30%
L131	30%
P132	30%
L133	30%
L136	30%
P137	30%

Chain BE:

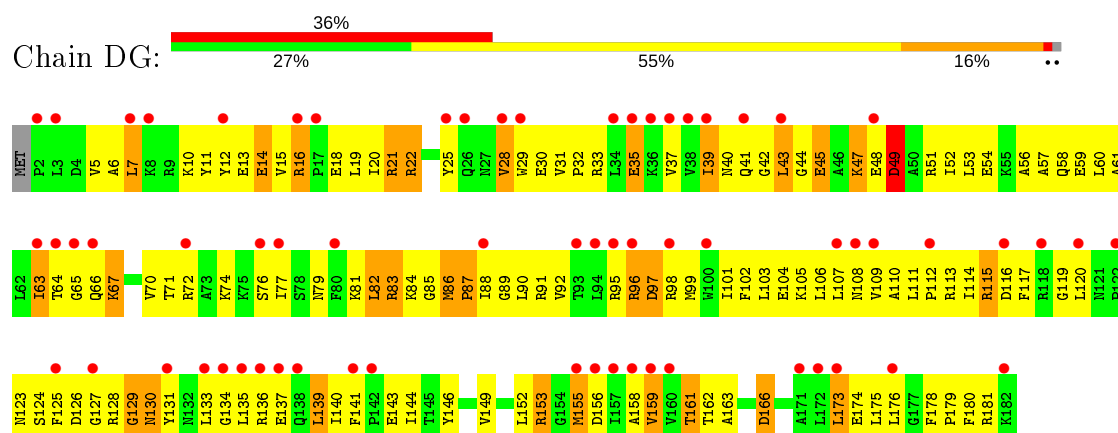
Category	Percentage
R199	3%
E200	29%
T201	46%
K202	21%
A204	1%
A205	1%
LYS	1%

Chain DE:

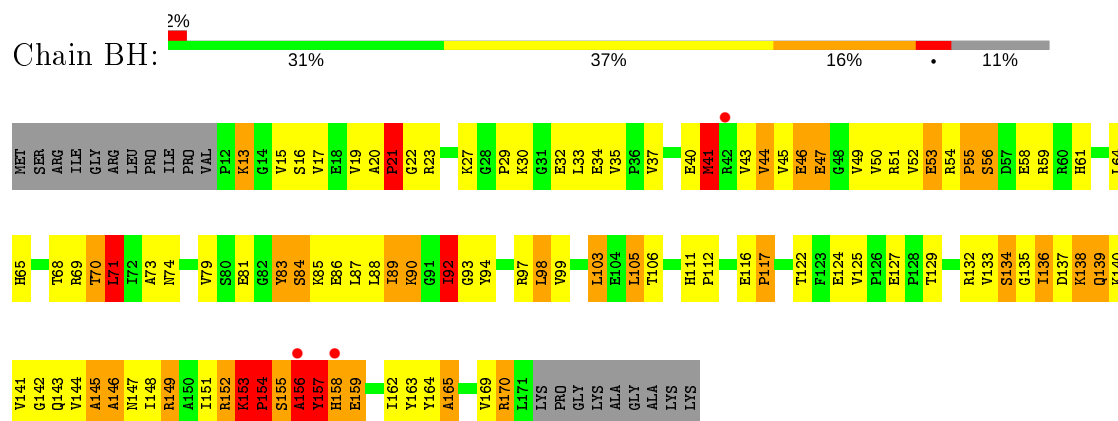
Category	Value
L195	5%
V196	28%
I197	47%
V198	21%
R199	5%
E200	28%
T201	47%
K202	21%
K203	5%
A204	28%
A205	47%
L205	21%
M1	5%
K2	28%
G3	47%
I4	21%
V7	5%
K8	28%
V9	47%
G10	21%
M11	5%
T12	28%
R13	47%
I14	21%
D17	5%
D18	28%
R19	47%
A20	21%
V21	5%
P22	28%
V23	47%
T24	21%
V25	5%
T26	28%
L27	47%
A28	21%
G29	5%
P30	28%
G31	47%
P32	21%
V33	5%
V34	28%
Q35	47%
R36	21%
R37	5%
T38	28%
P39	47%
E40	21%
Y44	5%
T45	28%
A46	47%
V47	21%
Q48	5%
L49	28%
G50	47%
F51	21%
L52	5%
P53	28%
Q54	47%
N55	21%
P56	5%
M17	28%
X18	47%
R58	21%
V59	5%
N60	28%
R61	47%
P62	21%
L63	5%
V64	28%
S128	47%
G85	21%
H86	5%
F87	28%
A88	47%
K89	21%
A90	5%
G91	28%
V92	47%
E93	21%
T94	5%
R95	28%
F96	47%
K97	21%
P98	5%
G99	28%
E100	47%
R101	21%
V102	5%
D103	28%
V104	47%
T105	21%
G106	5%
T107	28%
S108	47%
K109	21%
G110	5%
R111	28%
G112	47%
F113	21%
A114	5%
G115	28%
V116	47%
M117	21%
X118	5%
R119	28%
W120	47%
N121	21%
F122	5%
F123	28%
S128	47%
H129	21%
G130	5%
A131	28%
K132	47%
K133	21%
I134	5%
H135	28%
K136	47%
H137	21%
P138	5%
I141	28%
G142	47%
R144	21%
T146	5%
P147	28%
G148	47%
R149	21%
K152	5%
G153	28%
K154	47%
K155	21%
M156	5%
A157	28%
G158	47%
H159	21%
Y160	5%
E163	28%
R164	47%
V165	21%
T166	5%
V167	28%
M168	47%
L170	21%
E171	5%
V172	28%
V173	47%
D174	21%
V175	5%
I176	28%
E179	47%
M180	21%
L181	5%
L182	28%
L183	47%
V184	21%
K185	5%
G186	28%
A187	47%
V188	21%
P189	5%
M192	28%

Chain BF:

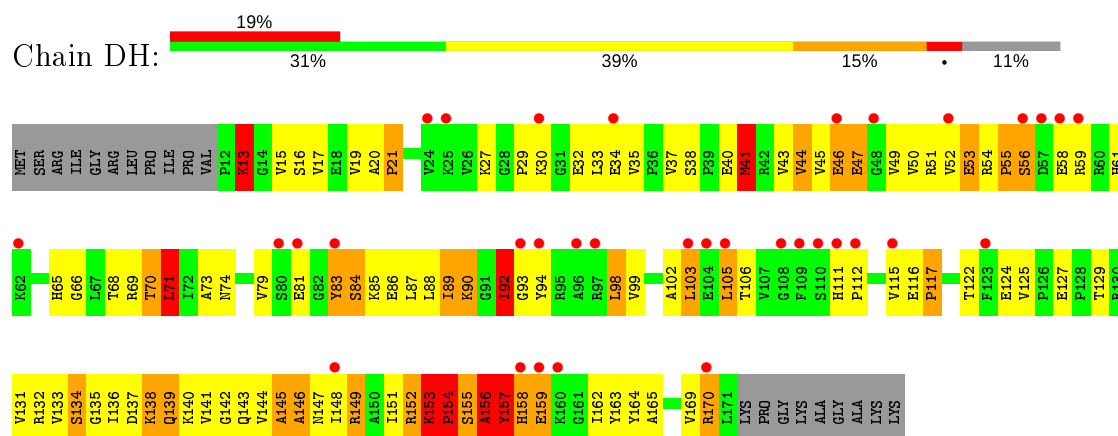
Iteration	Chain BF
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3	0.00
4	0.00
5	0.00
6	0.00
7	0.00
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9	0.00
10	0.00
11	0.00
12	0.00
13	0.00
14	0.00
15	0.00
16	0.00
17	0.00
18	0.00
19	0.00
20	0.00
21	0.00
22	0.00
23	0.00
24	0.00
25	0.00
26	0.00
27	0.00
28	0.00
29	0.00
30	0.00
31	0.00
32	0.00
33	0.00
34	0.00
35	0.00
36	0.00
37	0.00
38	0.00
39	0.00
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54	0.00
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56	0.00
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60	0.00
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113	0.00
114	0.00
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122	0.00
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125	0.00
126	0.00
127	0.00
128	0.00
129	0.00
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135	0.00
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139	0.00
140	0.00
141	0.00
142	0.00
143	0.00
144	0.00
145	0.00
146	0.00
147	0.00
148	0.00
149	0.00
150	0.00
151	0.00
152	0.00
153	0.00
154	0.00
155	0.00
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157	0.00
158	0.00
159	0.00
160	0.00
161	0.00
162	0.00
163	0.00
164	0.00
165	0.00
166	0.00
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169	0.00
170	0.00
171	0.00
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175	0.00
176	0.00
177	0.00
178	0.00
179	0.00
180	0.00



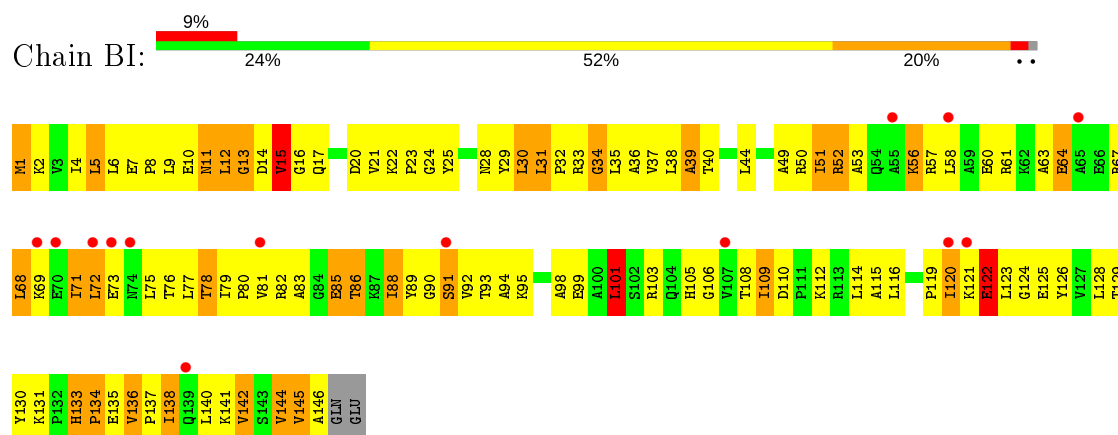
- Molecule 37: 50S ribosomal protein L6



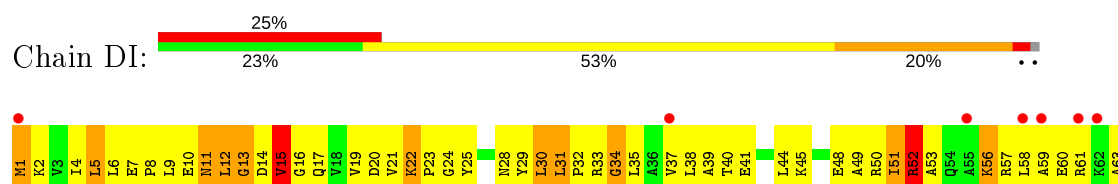
- Molecule 37: 50S ribosomal protein L6

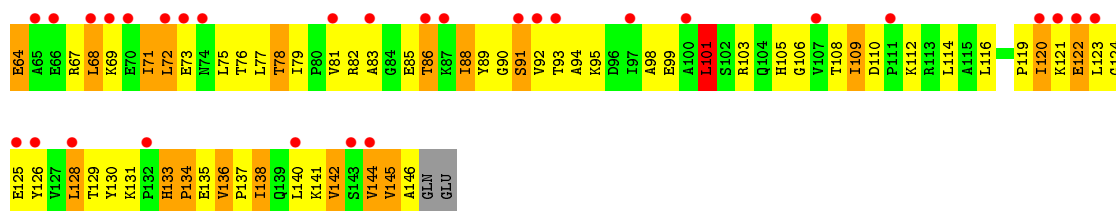


- Molecule 38: 50S ribosomal protein L9

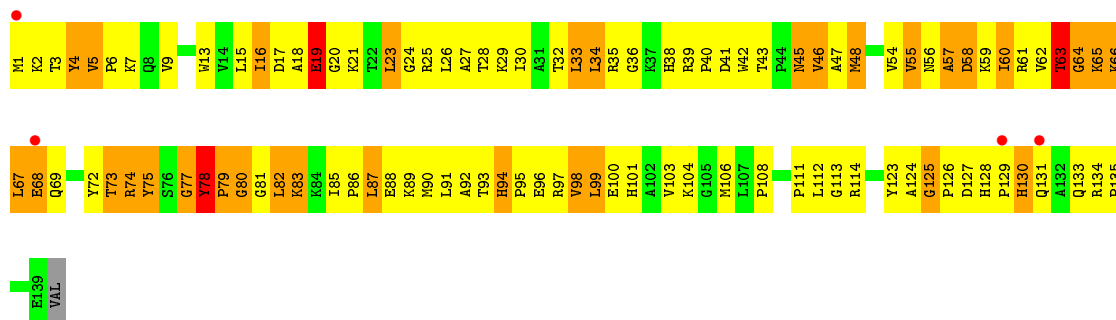


- Molecule 38: 50S ribosomal protein L9





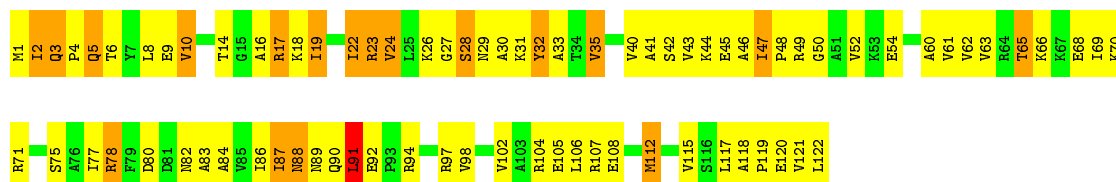
• Molecule 39: 50S ribosomal protein L13



• Molecule 39: 50S ribosomal protein L13

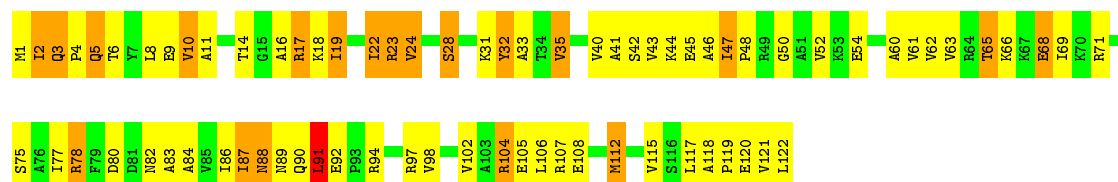


• Molecule 40: 50S ribosomal protein L14

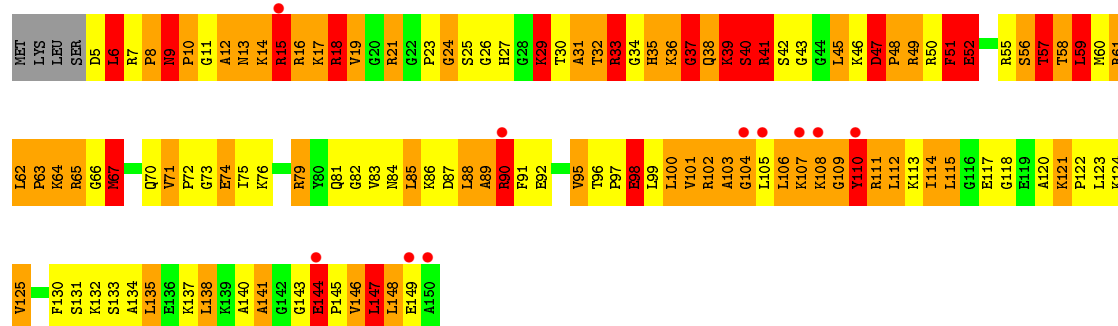


• Molecule 40: 50S ribosomal protein L14

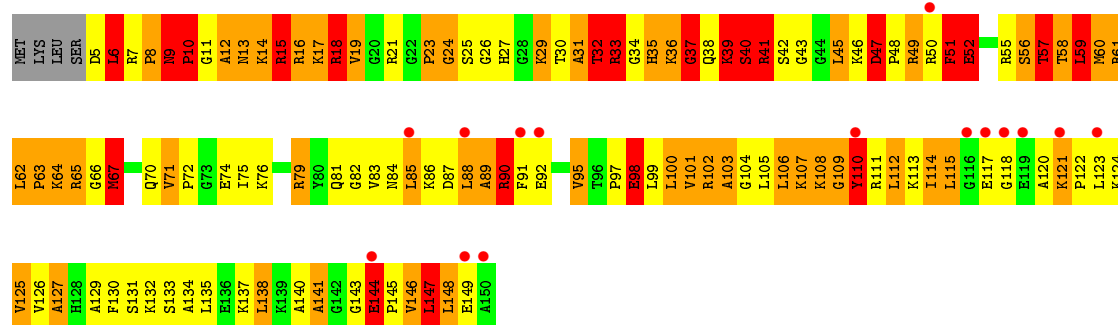




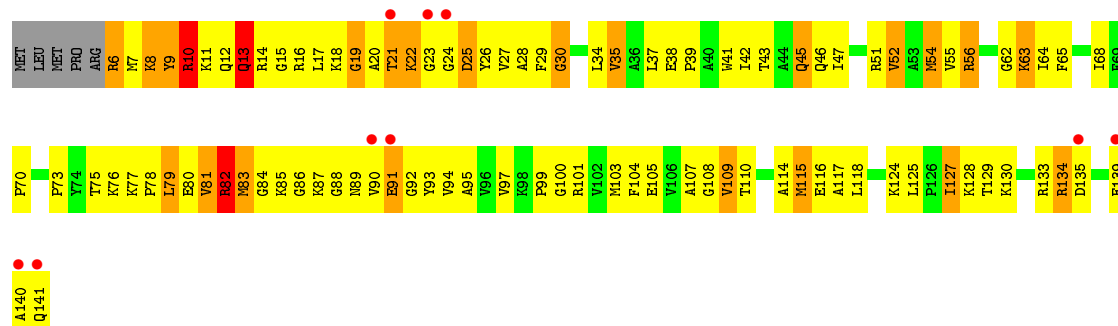
• Molecule 41: 50S ribosomal protein L15



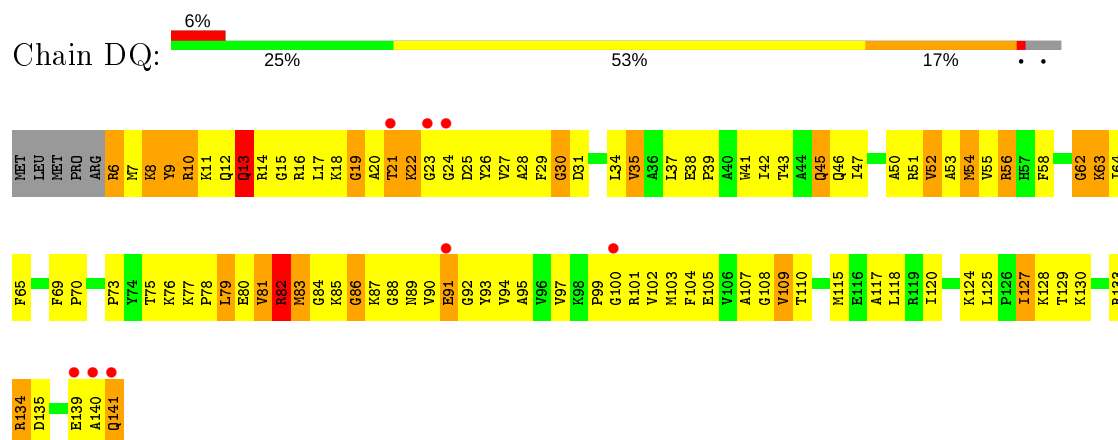
• Molecule 41: 50S ribosomal protein L15



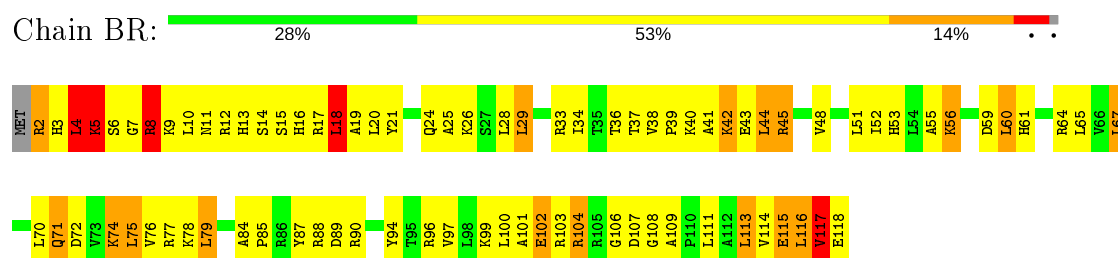
• Molecule 42: 50S ribosomal protein L16



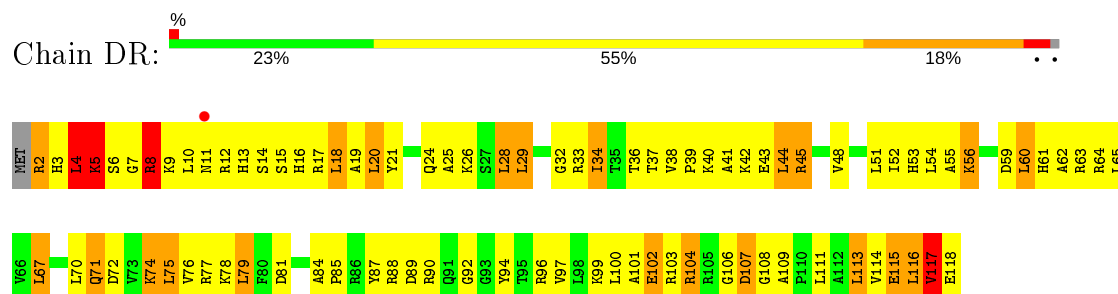
- Molecule 42: 50S ribosomal protein L16



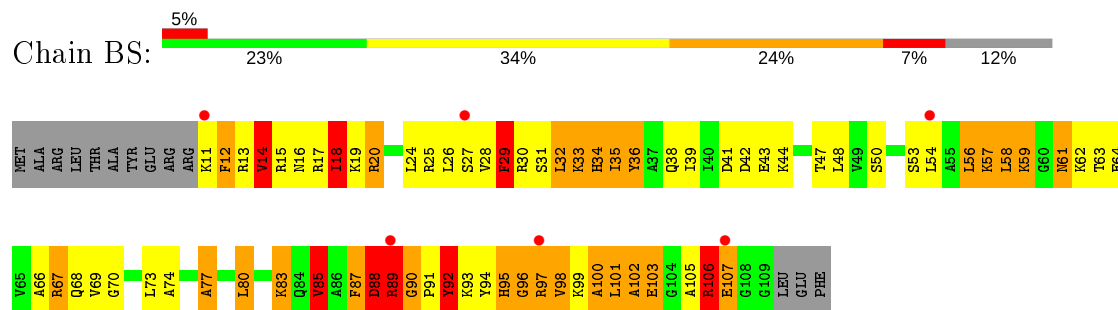
- Molecule 43: 50S ribosomal protein L17



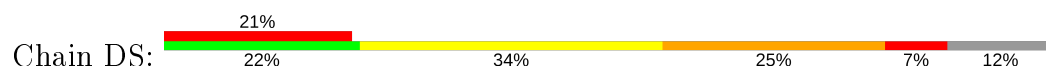
- Molecule 43: 50S ribosomal protein L17

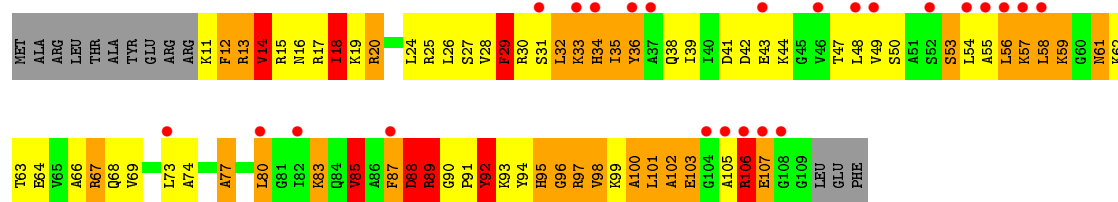


- Molecule 44: 50S ribosomal protein L18

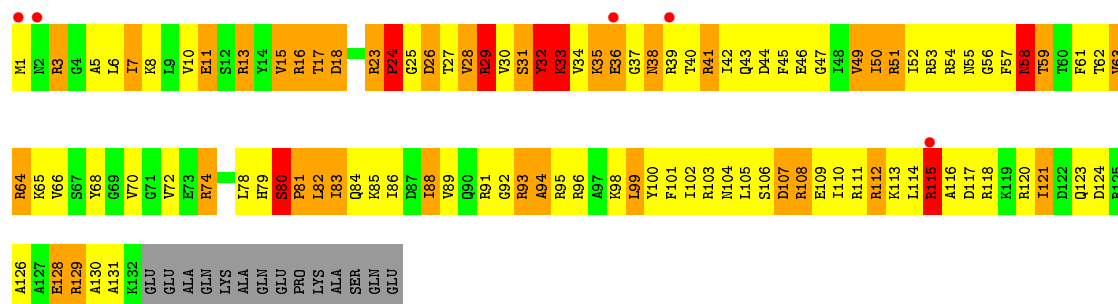
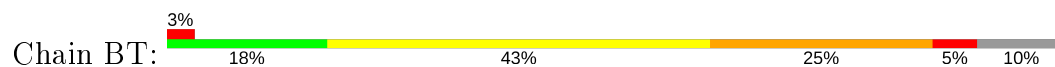


- Molecule 44: 50S ribosomal protein L18

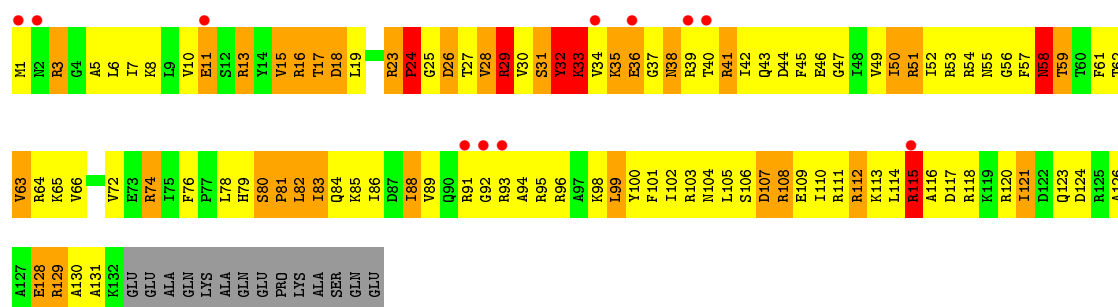
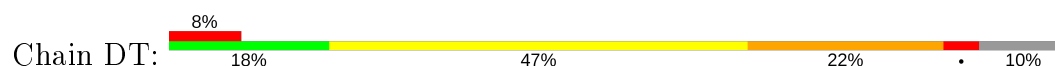




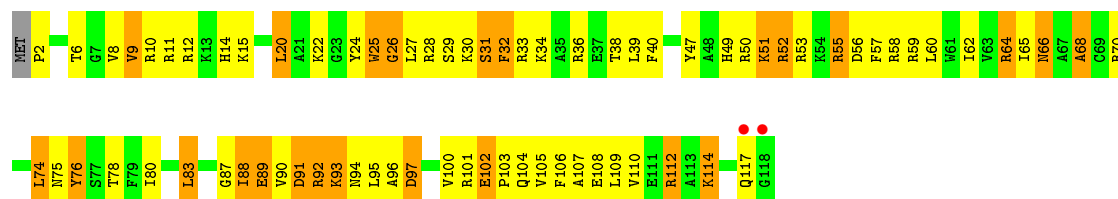
• Molecule 45: 50S ribosomal protein L19



• Molecule 45: 50S ribosomal protein L19

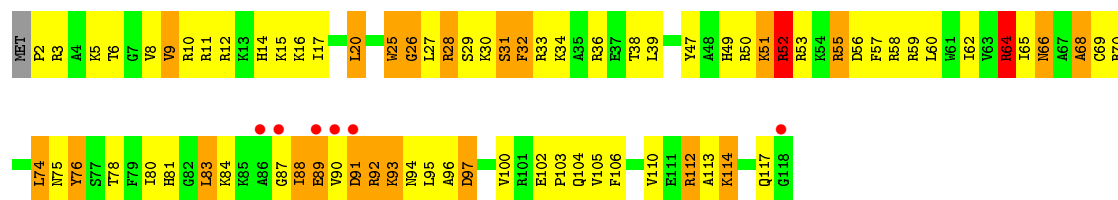


• Molecule 46: 50S ribosomal protein L20

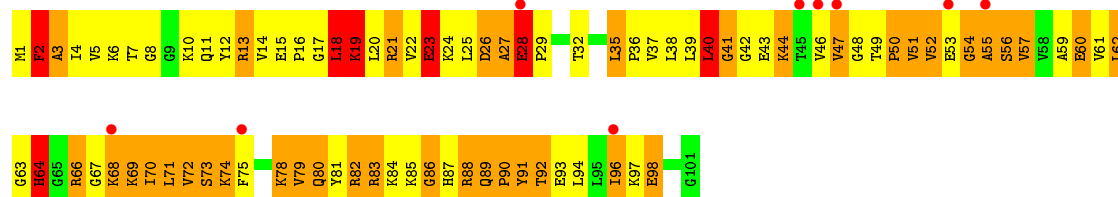


• Molecule 46: 50S ribosomal protein L20

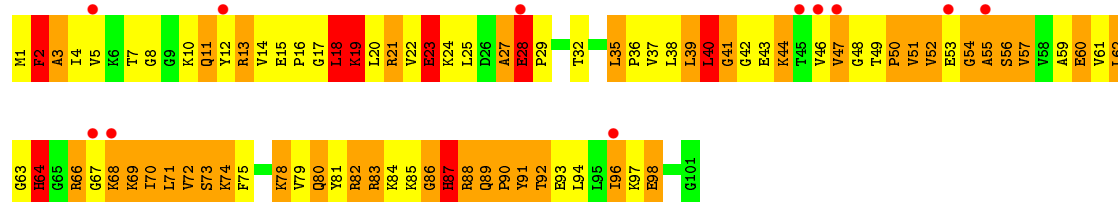
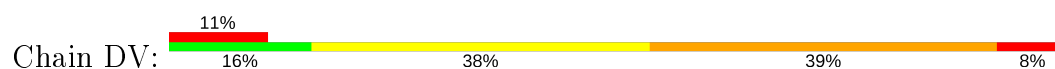




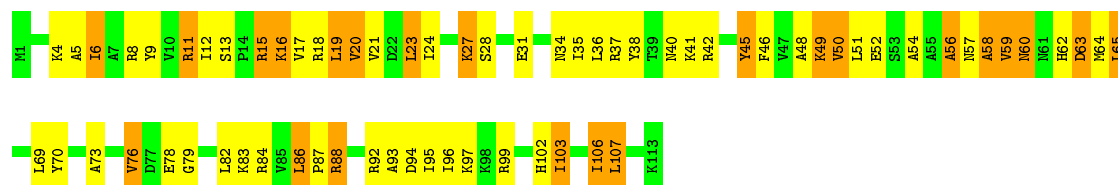
• Molecule 47: 50S ribosomal protein L21



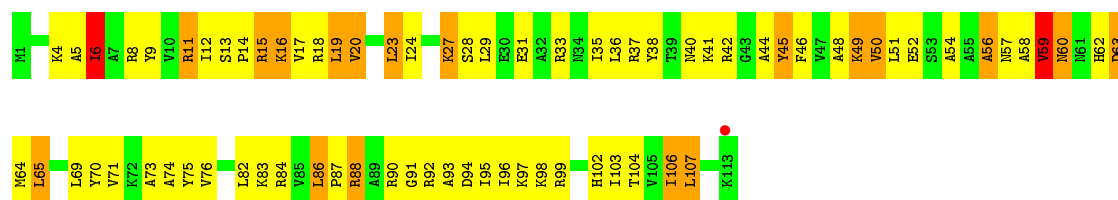
• Molecule 47: 50S ribosomal protein L21



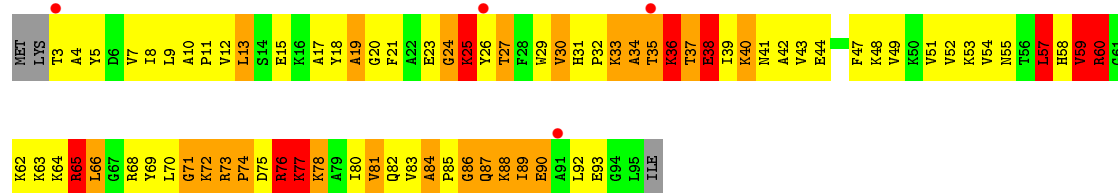
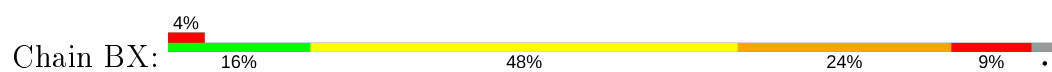
• Molecule 48: 50S ribosomal protein L22



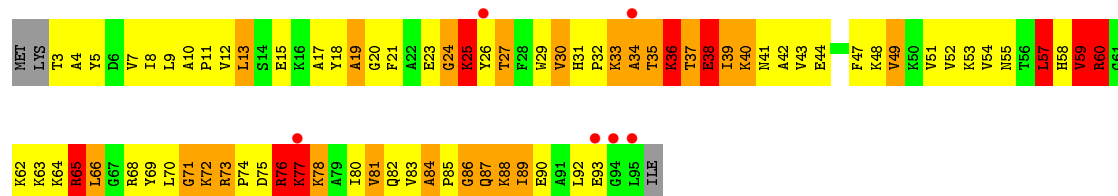
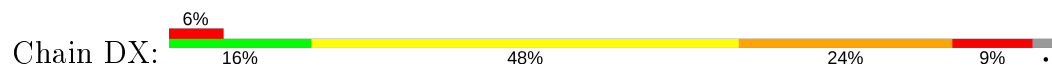
• Molecule 48: 50S ribosomal protein L22



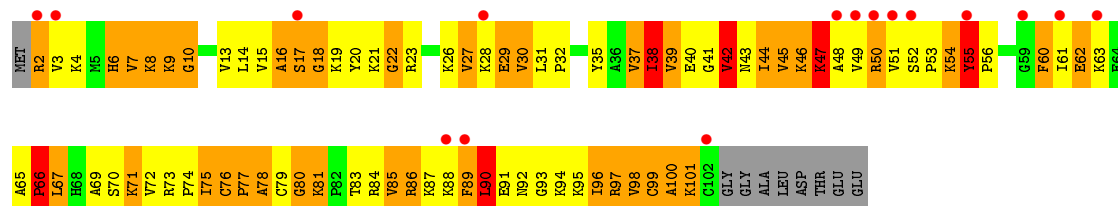
• Molecule 49: 50S ribosomal protein L23



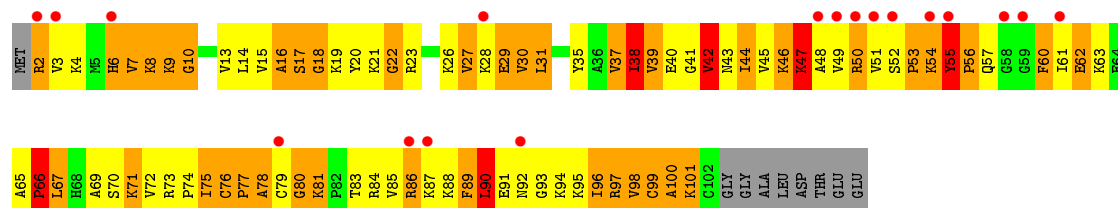
- Molecule 49: 50S ribosomal protein L23



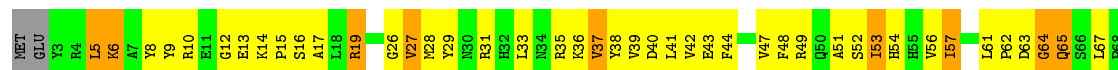
- Molecule 50: 50S ribosomal protein L24

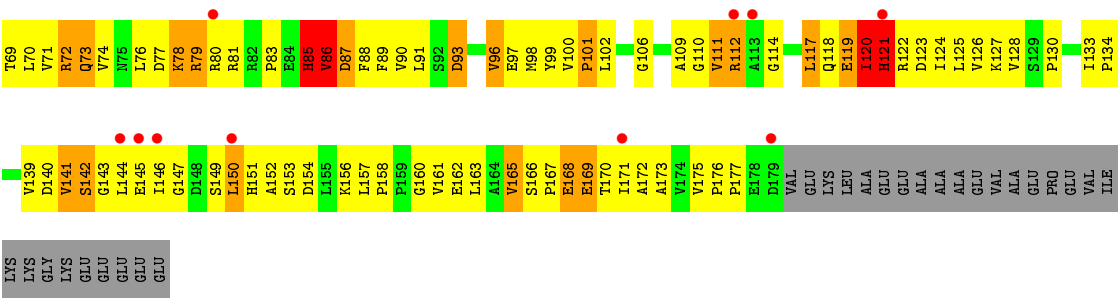


- Molecule 50: 50S ribosomal protein L24

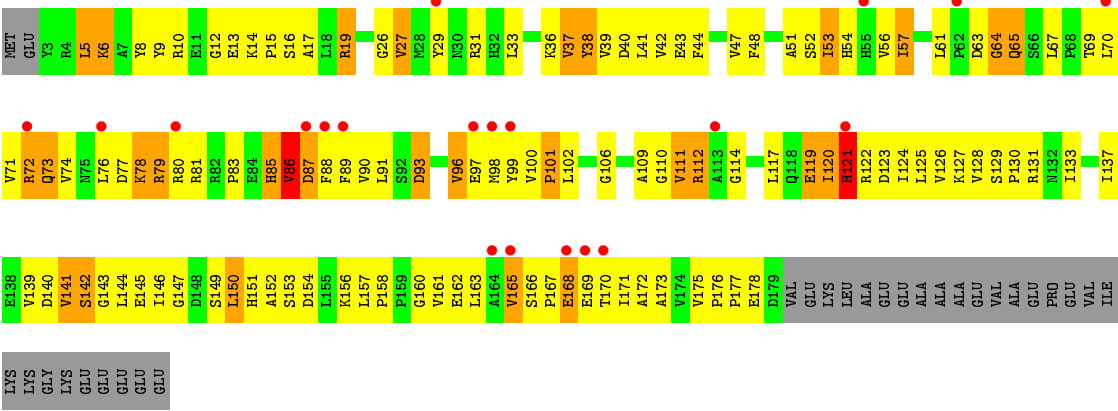


- Molecule 51: 50S ribosomal protein L25





• Molecule 51: 50S ribosomal protein L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.22Å 450.25Å 623.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 3.00 49.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.80-3.00) 88.7 (49.80-3.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.235 , 0.269 0.234 , 0.268	Depositor DCC
R_{free} test set	51892 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 92.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	278000	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.51	0/36190	0.87	34/56486 (0.1%)
1	CA	0.50	0/36190	0.88	40/56486 (0.1%)
2	AB	0.29	0/1936	0.51	0/2611
2	CB	0.29	0/1936	0.50	0/2611
3	AC	0.27	0/1637	0.45	0/2207
3	CC	0.27	0/1637	0.45	0/2207
4	AD	0.34	0/1733	0.52	0/2318
4	CD	0.34	0/1733	0.53	0/2318
5	AE	0.34	0/1163	0.55	0/1566
5	CE	0.34	0/1163	0.55	0/1566
6	AF	0.35	0/856	0.54	0/1154
6	CF	0.36	0/856	0.54	0/1154
7	AG	0.25	0/1276	0.44	0/1709
7	CG	0.26	0/1276	0.44	0/1709
8	AH	0.34	0/1136	0.55	0/1527
8	CH	0.33	0/1136	0.54	0/1527
9	AI	0.27	0/1028	0.44	0/1375
9	CI	0.27	0/1028	0.44	0/1375
10	AJ	0.29	0/808	0.48	0/1087
10	CJ	0.29	0/808	0.48	0/1087
11	AK	0.32	0/900	0.52	0/1213
11	CK	0.32	0/900	0.52	0/1213
12	AL	0.38	0/987	0.61	1/1322 (0.1%)
12	CL	0.39	0/987	0.62	0/1322
13	AM	0.26	0/928	0.47	0/1238
13	CM	0.27	0/928	0.47	0/1238
14	AN	0.27	0/501	0.45	0/664
14	CN	0.28	0/501	0.44	0/664
15	AO	0.35	0/745	0.56	0/992
15	CO	0.33	0/745	0.56	0/992
16	AP	0.33	0/717	0.55	0/965
16	CP	0.33	0/717	0.55	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.33	0/837	0.57	0/1119
17	CQ	0.34	0/837	0.56	0/1119
18	AR	0.35	0/579	0.57	0/768
18	CR	0.37	0/579	0.57	0/768
19	AS	0.28	0/643	0.46	0/867
19	CS	0.28	0/643	0.46	0/867
20	AT	0.34	0/765	0.56	0/1007
20	CT	0.34	0/765	0.55	0/1007
21	AU	0.27	0/213	0.43	0/279
21	CU	0.28	0/213	0.43	0/279
22	B0	0.58	0/658	0.76	1/878 (0.1%)
22	D0	0.52	0/658	0.74	0/878
23	B1	0.74	0/700	0.98	0/931
23	D1	0.65	0/700	0.95	1/931 (0.1%)
24	B2	0.68	0/423	0.92	0/560
24	D2	0.59	0/423	0.89	0/560
25	B3	0.62	0/473	0.71	0/636
25	D3	0.47	0/473	0.69	0/636
26	B4	0.31	0/156	0.59	0/215
26	D4	0.33	0/156	0.57	0/215
27	B5	0.86	1/473 (0.2%)	1.17	2/639 (0.3%)
27	D5	0.74	0/473	1.07	2/639 (0.3%)
28	B6	0.86	1/387 (0.3%)	1.05	2/517 (0.4%)
28	D6	0.70	0/387	0.97	1/517 (0.2%)
29	B7	0.65	0/427	0.79	0/563
29	D7	0.59	0/427	0.78	0/563
30	B8	0.76	0/516	1.08	3/681 (0.4%)
30	D8	0.64	0/516	1.02	3/681 (0.4%)
31	BA	1.11	98/65745 (0.1%)	1.45	1072/102639 (1.0%)
31	DA	0.84	36/65745 (0.1%)	1.38	904/102639 (0.9%)
32	BB	0.87	0/2853	1.26	29/4451 (0.7%)
32	DB	0.69	0/2853	1.18	27/4451 (0.6%)
33	BD	0.61	0/2155	0.82	1/2907 (0.0%)
33	DD	0.56	0/2155	0.80	1/2907 (0.0%)
34	BE	0.64	0/1597	0.82	2/2155 (0.1%)
34	DE	0.57	0/1597	0.80	0/2155
35	BF	0.63	1/1659 (0.1%)	0.77	0/2246
35	DF	0.53	0/1659	0.75	2/2246 (0.1%)
36	BG	0.33	0/1498	0.55	0/2013
36	DG	0.31	0/1498	0.53	0/2013
37	BH	0.64	0/1246	0.77	0/1684
37	DH	0.47	0/1246	0.70	0/1684
38	BI	0.39	0/1147	0.64	0/1553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DI	0.38	0/1147	0.63	0/1553
39	BN	0.70	0/1132	0.88	1/1527 (0.1%)
39	DN	0.54	0/1132	0.79	0/1527
40	BO	0.57	0/943	0.71	0/1269
40	DO	0.50	0/943	0.69	0/1269
41	BP	0.72	1/1131 (0.1%)	1.03	4/1504 (0.3%)
41	DP	0.63	0/1131	0.95	4/1504 (0.3%)
42	BQ	0.65	0/1100	0.84	1/1470 (0.1%)
42	DQ	0.58	0/1100	0.80	0/1470
43	BR	0.63	0/974	0.91	4/1302 (0.3%)
43	DR	0.56	0/974	0.87	3/1302 (0.2%)
44	BS	0.56	0/779	0.83	0/1038
44	DS	0.49	0/779	0.78	0/1038
45	BT	0.58	0/1114	0.83	1/1488 (0.1%)
45	DT	0.53	0/1114	0.80	0/1488
46	BU	0.71	0/975	0.77	0/1297
46	DU	0.59	0/975	0.71	0/1297
47	BV	0.76	0/789	0.96	1/1054 (0.1%)
47	DV	0.58	0/789	0.89	1/1054 (0.1%)
48	BW	0.67	0/907	0.84	0/1216
48	DW	0.58	0/907	0.79	0/1216
49	BX	0.74	0/740	0.99	3/995 (0.3%)
49	DX	0.64	0/740	0.90	2/995 (0.2%)
50	BY	0.67	1/789 (0.1%)	0.88	1/1053 (0.1%)
50	DY	0.56	0/789	0.82	1/1053 (0.1%)
51	BZ	0.46	0/1436	0.64	2/1951 (0.1%)
51	DZ	0.40	0/1436	0.62	2/1951 (0.1%)
All	All	0.75	139/301000 (0.0%)	1.13	2159/449812 (0.5%)

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
23	B1	0	1
23	D1	0	1
24	B2	0	3
24	D2	0	1
27	B5	0	1
27	D5	0	1
31	BA	21	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	DA	21	0
33	BD	0	2
33	DD	0	2
34	BE	0	2
34	DE	0	2
35	BF	0	1
37	BH	0	2
37	DH	0	2
41	BP	0	5
41	DP	0	4
42	BQ	0	1
42	DQ	0	1
43	BR	0	1
43	DR	0	1
44	BS	0	1
44	DS	0	1
45	BT	0	1
45	DT	0	1
47	BV	0	1
47	DV	0	2
49	BX	0	3
49	DX	0	3
All	All	42	47

The worst 5 of 139 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BA	783	A	N9-C4	-12.00	1.30	1.37
31	BA	669	G	C4'-C3'	-11.54	1.40	1.53
31	DA	528	A	N9-C4	-11.40	1.31	1.37
31	BA	2346	A	N3-C4	-10.07	1.28	1.34
31	DA	669	G	C4'-C3'	-9.54	1.42	1.53

The worst 5 of 2159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	DA	1779	U	C5-C6-N1	-19.83	112.78	122.70
31	DA	2447	G	N1-C6-O6	16.89	130.03	119.90
31	BA	1779	U	C5-C6-N1	-16.70	114.35	122.70
31	DA	2447	G	C5-C6-O6	-16.69	118.58	128.60
31	BA	676	A	C5-N7-C8	-15.75	96.03	103.90

5 of 42 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	BA	100	G	C1'
31	BA	472	A	C3'
31	BA	669	G	C4',C3',C1'
31	BA	945	A	C1'
31	BA	1300	U	C4',C3',C1'

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	B1	30	VAL	Peptide
24	B2	55	ARG	Peptide
24	B2	56	GLN	Peptide
24	B2	57	ILE	Peptide
27	B5	51	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1409	0
1	CA	32329	0	16318	1381	0
2	AB	1901	0	1951	169	0
2	CB	1901	0	1951	167	0
3	AC	1613	0	1677	116	0
3	CC	1613	0	1677	117	0
4	AD	1703	0	1763	158	0
4	CD	1703	0	1763	160	0
5	AE	1147	0	1207	103	0
5	CE	1147	0	1207	107	0
6	AF	843	0	857	80	0
6	CF	843	0	857	86	0
7	AG	1257	0	1296	60	0
7	CG	1257	0	1296	62	0
8	AH	1116	0	1177	83	0
8	CH	1116	0	1177	82	0
9	AI	1011	0	1042	84	0
9	CI	1011	0	1042	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	795	0	840	80	0
10	CJ	795	0	840	82	0
11	AK	885	0	904	64	0
11	CK	885	0	904	69	0
12	AL	971	0	1057	104	0
12	CL	971	0	1057	106	0
13	AM	921	0	976	60	0
13	CM	921	0	976	63	0
14	AN	492	0	530	35	0
14	CN	492	0	529	33	0
15	AO	734	0	771	54	0
15	CO	734	0	771	56	0
16	AP	701	0	720	88	0
16	CP	701	0	720	91	0
17	AQ	824	0	891	46	0
17	CQ	824	0	891	49	0
18	AR	574	0	644	63	0
18	CR	574	0	644	64	0
19	AS	630	0	652	40	0
19	CS	630	0	652	34	0
20	AT	763	0	861	78	0
20	CT	763	0	861	75	0
21	AU	209	0	221	11	0
21	CU	209	0	221	11	0
22	B0	650	0	654	67	0
22	D0	650	0	654	64	0
23	B1	693	0	764	143	0
23	D1	693	0	764	144	0
24	B2	421	0	461	119	1
24	D2	421	0	461	125	0
25	B3	468	0	523	37	0
25	D3	468	0	523	56	0
26	B4	157	0	69	12	0
26	D4	157	0	69	12	0
27	B5	459	0	478	82	0
27	D5	459	0	480	85	0
28	B6	381	0	390	96	0
28	D6	381	0	390	92	0
29	B7	419	0	467	37	0
29	D7	419	0	467	38	0
30	B8	508	0	576	156	0
30	D8	508	0	576	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BA	58698	0	29590	2392	0
31	DA	58698	0	29591	2578	1
32	BB	2551	0	1295	156	0
32	DB	2551	0	1295	173	0
33	BD	2105	0	2182	336	0
33	DD	2105	0	2182	333	0
34	BE	1564	0	1629	214	0
34	DE	1564	0	1629	213	0
35	BF	1624	0	1677	171	0
35	DF	1624	0	1677	178	0
36	BG	1474	0	1534	149	0
36	DG	1474	0	1534	149	0
37	BH	1223	0	1282	141	0
37	DH	1223	0	1282	129	0
38	BI	1132	0	1218	142	0
38	DI	1132	0	1218	156	0
39	BN	1105	0	1180	184	0
39	DN	1105	0	1180	183	0
40	BO	933	0	996	86	0
40	DO	933	0	996	76	0
41	BP	1114	0	1187	271	0
41	DP	1114	0	1187	260	0
42	BQ	1080	0	1127	157	0
42	DQ	1080	0	1127	162	0
43	BR	960	0	1021	115	0
43	DR	960	0	1021	117	0
44	BS	771	0	832	148	0
44	DS	771	0	832	150	0
45	BT	1100	0	1164	173	0
45	DT	1100	0	1164	166	0
46	BU	958	0	1015	142	0
46	DU	958	0	1015	151	0
47	BV	779	0	851	210	0
47	DV	779	0	851	215	0
48	BW	896	0	953	76	0
48	DW	896	0	953	80	0
49	BX	726	0	778	163	0
49	DX	726	0	778	168	0
50	BY	776	0	870	179	0
50	DY	776	0	870	187	0
51	BZ	1404	0	1432	140	0
51	DZ	1404	0	1432	139	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	AA	51	0	0	0	0
52	B0	1	0	0	0	0
52	B1	1	0	0	0	0
52	B5	2	0	0	0	0
52	B7	1	0	0	0	0
52	BA	349	0	0	0	0
52	BB	5	0	0	0	0
52	BD	1	0	0	0	0
52	BE	1	0	0	0	0
52	BF	1	0	0	0	0
52	BP	3	0	0	0	0
52	BQ	2	0	0	0	0
52	BR	1	0	0	0	0
52	BU	1	0	0	0	0
52	BX	1	0	0	0	0
52	CA	48	0	0	0	0
52	D0	1	0	0	0	0
52	D1	1	0	0	0	0
52	D5	2	0	0	0	0
52	D7	1	0	0	0	0
52	DA	309	0	0	0	0
52	DB	3	0	0	0	0
52	DD	1	0	0	0	0
52	DE	1	0	0	0	0
52	DF	1	0	0	0	0
52	DP	1	0	0	0	0
52	DQ	1	0	0	0	0
52	DR	1	0	0	0	0
52	DU	1	0	0	0	0
52	DX	1	0	0	0	0
53	AD	1	0	0	0	0
53	AN	1	0	0	0	0
53	CD	1	0	0	0	0
53	CN	1	0	0	0	0
54	BA	1	0	0	0	0
54	DA	1	0	0	0	0
55	BA	52	0	72	3	0
55	DA	52	0	72	3	0
All	All	278000	0	189246	17418	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

The worst 5 of 17418 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)
42:BQ:81:VAL:O	42:BQ:82:ARG:HG2	1.13	1.31
42:DQ:81:VAL:O	42:DQ:82:ARG:HG2	1.25	1.27
41:BP:59:LEU:HA	41:BP:61:ARG:NH1	1.49	1.25
41:DP:59:LEU:HA	41:DP:61:ARG:NH1	1.55	1.20
31:DA:2206:G:N2	31:DA:2207:G:H5'	1.58	1.19

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B2:12:GLU:CB	31:DA:306:U:OP1[1_455]	2.15	0.05

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%)	178 (76%)	38 (16%)	17 (7%)	1	5
2	CB	233/256 (91%)	177 (76%)	39 (17%)	17 (7%)	1	5
3	AC	205/239 (86%)	155 (76%)	36 (18%)	14 (7%)	1	6
3	CC	205/239 (86%)	155 (76%)	37 (18%)	13 (6%)	1	7
4	AD	206/209 (99%)	138 (67%)	52 (25%)	16 (8%)	1	4
4	CD	206/209 (99%)	137 (66%)	55 (27%)	14 (7%)	1	6
5	AE	149/162 (92%)	105 (70%)	31 (21%)	13 (9%)	1	3
5	CE	149/162 (92%)	103 (69%)	33 (22%)	13 (9%)	1	3
6	AF	99/101 (98%)	76 (77%)	15 (15%)	8 (8%)	1	4
6	CF	99/101 (98%)	76 (77%)	14 (14%)	9 (9%)	1	3
7	AG	153/156 (98%)	130 (85%)	19 (12%)	4 (3%)	5	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	CG	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	5	27
8	AH	136/138 (99%)	98 (72%)	31 (23%)	7 (5%)	2	12
8	CH	136/138 (99%)	98 (72%)	31 (23%)	7 (5%)	2	12
9	AI	123/128 (96%)	92 (75%)	24 (20%)	7 (6%)	1	10
9	CI	123/128 (96%)	94 (76%)	22 (18%)	7 (6%)	1	10
10	AJ	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	2	12
10	CJ	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	2	12
11	AK	117/129 (91%)	87 (74%)	26 (22%)	4 (3%)	3	20
11	CK	117/129 (91%)	86 (74%)	27 (23%)	4 (3%)	3	20
12	AL	123/135 (91%)	82 (67%)	31 (25%)	10 (8%)	1	4
12	CL	123/135 (91%)	83 (68%)	29 (24%)	11 (9%)	1	3
13	AM	107/126 (85%)	84 (78%)	17 (16%)	6 (6%)	2	10
13	CM	107/126 (85%)	84 (78%)	17 (16%)	6 (6%)	2	10
14	AN	58/61 (95%)	45 (78%)	11 (19%)	2 (3%)	3	20
14	CN	58/61 (95%)	44 (76%)	12 (21%)	2 (3%)	3	20
15	AO	86/89 (97%)	62 (72%)	19 (22%)	5 (6%)	1	10
15	CO	86/89 (97%)	61 (71%)	21 (24%)	4 (5%)	2	14
16	AP	82/88 (93%)	48 (58%)	27 (33%)	7 (8%)	1	4
16	CP	82/88 (93%)	47 (57%)	29 (35%)	6 (7%)	1	5
17	AQ	98/105 (93%)	74 (76%)	18 (18%)	6 (6%)	1	8
17	CQ	98/105 (93%)	73 (74%)	19 (19%)	6 (6%)	1	8
18	AR	68/88 (77%)	52 (76%)	11 (16%)	5 (7%)	1	5
18	CR	68/88 (77%)	51 (75%)	13 (19%)	4 (6%)	1	9
19	AS	77/93 (83%)	58 (75%)	13 (17%)	6 (8%)	1	4
19	CS	77/93 (83%)	59 (77%)	12 (16%)	6 (8%)	1	4
20	AT	97/106 (92%)	69 (71%)	19 (20%)	9 (9%)	0	3
20	CT	97/106 (92%)	65 (67%)	23 (24%)	9 (9%)	0	3
21	AU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	15
21	CU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	15
22	B0	83/85 (98%)	65 (78%)	14 (17%)	4 (5%)	2	13
22	D0	83/85 (98%)	64 (77%)	15 (18%)	4 (5%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	B1	87/98 (89%)	48 (55%)	17 (20%)	22 (25%)	0	0
23	D1	87/98 (89%)	45 (52%)	19 (22%)	23 (26%)	0	0
24	B2	49/72 (68%)	23 (47%)	19 (39%)	7 (14%)	0	1
24	D2	49/72 (68%)	23 (47%)	18 (37%)	8 (16%)	0	1
25	B3	58/60 (97%)	52 (90%)	4 (7%)	2 (3%)	3	20
25	D3	58/60 (97%)	51 (88%)	5 (9%)	2 (3%)	3	20
26	B4	30/71 (42%)	5 (17%)	11 (37%)	14 (47%)	0	0
26	D4	30/71 (42%)	5 (17%)	10 (33%)	15 (50%)	0	0
27	B5	57/60 (95%)	38 (67%)	11 (19%)	8 (14%)	0	1
27	D5	57/60 (95%)	36 (63%)	14 (25%)	7 (12%)	0	1
28	B6	41/54 (76%)	21 (51%)	6 (15%)	14 (34%)	0	0
28	D6	41/54 (76%)	19 (46%)	8 (20%)	14 (34%)	0	0
29	B7	47/49 (96%)	41 (87%)	4 (8%)	2 (4%)	2	15
29	D7	47/49 (96%)	40 (85%)	4 (8%)	3 (6%)	1	7
30	B8	62/65 (95%)	42 (68%)	11 (18%)	9 (14%)	0	1
30	D8	62/65 (95%)	41 (66%)	12 (19%)	9 (14%)	0	1
33	BD	270/276 (98%)	208 (77%)	45 (17%)	17 (6%)	1	7
33	DD	270/276 (98%)	207 (77%)	47 (17%)	16 (6%)	1	9
34	BE	203/206 (98%)	138 (68%)	37 (18%)	28 (14%)	0	1
34	DE	203/206 (98%)	138 (68%)	38 (19%)	27 (13%)	0	1
35	BF	206/210 (98%)	160 (78%)	30 (15%)	16 (8%)	1	4
35	DF	206/210 (98%)	156 (76%)	33 (16%)	17 (8%)	1	4
36	BG	177/182 (97%)	128 (72%)	35 (20%)	14 (8%)	1	4
36	DG	177/182 (97%)	127 (72%)	36 (20%)	14 (8%)	1	4
37	BH	158/180 (88%)	92 (58%)	41 (26%)	25 (16%)	0	1
37	DH	158/180 (88%)	93 (59%)	39 (25%)	26 (16%)	0	0
38	BI	144/148 (97%)	88 (61%)	32 (22%)	24 (17%)	0	0
38	DI	144/148 (97%)	87 (60%)	35 (24%)	22 (15%)	0	1
39	BN	137/140 (98%)	87 (64%)	32 (23%)	18 (13%)	0	1
39	DN	137/140 (98%)	88 (64%)	32 (23%)	17 (12%)	0	1
40	BO	120/122 (98%)	101 (84%)	16 (13%)	3 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	DO	120/122 (98%)	99 (82%)	17 (14%)	4 (3%)	4	21
41	BP	144/150 (96%)	77 (54%)	17 (12%)	50 (35%)	0	0
41	DP	144/150 (96%)	76 (53%)	18 (12%)	50 (35%)	0	0
42	BQ	134/141 (95%)	92 (69%)	28 (21%)	14 (10%)	0	2
42	DQ	134/141 (95%)	96 (72%)	23 (17%)	15 (11%)	0	2
43	BR	115/118 (98%)	78 (68%)	29 (25%)	8 (7%)	1	6
43	DR	115/118 (98%)	82 (71%)	24 (21%)	9 (8%)	1	4
44	BS	97/112 (87%)	49 (50%)	24 (25%)	24 (25%)	0	0
44	DS	97/112 (87%)	49 (50%)	23 (24%)	25 (26%)	0	0
45	BT	130/146 (89%)	89 (68%)	21 (16%)	20 (15%)	0	1
45	DT	130/146 (89%)	90 (69%)	21 (16%)	19 (15%)	0	1
46	BU	115/118 (98%)	77 (67%)	27 (24%)	11 (10%)	0	3
46	DU	115/118 (98%)	74 (64%)	29 (25%)	12 (10%)	0	2
47	BV	97/101 (96%)	54 (56%)	15 (16%)	28 (29%)	0	0
47	DV	97/101 (96%)	52 (54%)	18 (19%)	27 (28%)	0	0
48	BW	111/113 (98%)	88 (79%)	15 (14%)	8 (7%)	1	5
48	DW	111/113 (98%)	89 (80%)	15 (14%)	7 (6%)	1	7
49	BX	91/96 (95%)	47 (52%)	22 (24%)	22 (24%)	0	0
49	DX	91/96 (95%)	48 (53%)	22 (24%)	21 (23%)	0	0
50	BY	99/110 (90%)	45 (46%)	22 (22%)	32 (32%)	0	0
50	DY	99/110 (90%)	46 (46%)	21 (21%)	32 (32%)	0	0
51	BZ	175/206 (85%)	113 (65%)	43 (25%)	19 (11%)	0	2
51	DZ	175/206 (85%)	113 (65%)	44 (25%)	18 (10%)	0	2
All	All	11148/12060 (92%)	7735 (69%)	2187 (20%)	1226 (11%)	0	2

5 of 1226 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	24	TRP
2	AB	154	LEU
2	AB	165	VAL
2	AB	194	PRO

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%)	176 (87%)	26 (13%)	4	19
2	CB	202/220 (92%)	176 (87%)	26 (13%)	4	19
3	AC	160/188 (85%)	152 (95%)	8 (5%)	24	60
3	CC	160/188 (85%)	152 (95%)	8 (5%)	24	60
4	AD	180/181 (99%)	157 (87%)	23 (13%)	4	19
4	CD	180/181 (99%)	156 (87%)	24 (13%)	4	17
5	AE	115/123 (94%)	100 (87%)	15 (13%)	4	19
5	CE	115/123 (94%)	100 (87%)	15 (13%)	4	19
6	AF	90/90 (100%)	79 (88%)	11 (12%)	5	21
6	CF	90/90 (100%)	79 (88%)	11 (12%)	5	21
7	AG	126/127 (99%)	121 (96%)	5 (4%)	31	68
7	CG	126/127 (99%)	121 (96%)	5 (4%)	31	68
8	AH	119/119 (100%)	107 (90%)	12 (10%)	7	29
8	CH	119/119 (100%)	107 (90%)	12 (10%)	7	29
9	AI	98/99 (99%)	88 (90%)	10 (10%)	7	28
9	CI	98/99 (99%)	88 (90%)	10 (10%)	7	28
10	AJ	88/92 (96%)	81 (92%)	7 (8%)	12	40
10	CJ	88/92 (96%)	81 (92%)	7 (8%)	12	40
11	AK	90/99 (91%)	79 (88%)	11 (12%)	5	21
11	CK	90/99 (91%)	80 (89%)	10 (11%)	6	25
12	AL	104/111 (94%)	96 (92%)	8 (8%)	13	42
12	CL	104/111 (94%)	96 (92%)	8 (8%)	13	42
13	AM	93/101 (92%)	86 (92%)	7 (8%)	13	43
13	CM	93/101 (92%)	86 (92%)	7 (8%)	13	43
14	AN	49/50 (98%)	46 (94%)	3 (6%)	18	53
14	CN	49/50 (98%)	47 (96%)	2 (4%)	30	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	79/80 (99%)	69 (87%)	10 (13%)	4	19
15	CO	79/80 (99%)	69 (87%)	10 (13%)	4	19
16	AP	72/74 (97%)	60 (83%)	12 (17%)	2	11
16	CP	72/74 (97%)	60 (83%)	12 (17%)	2	11
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	39	74
17	CQ	94/97 (97%)	91 (97%)	3 (3%)	39	74
18	AR	61/77 (79%)	56 (92%)	5 (8%)	11	39
18	CR	61/77 (79%)	55 (90%)	6 (10%)	8	30
19	AS	69/80 (86%)	62 (90%)	7 (10%)	7	29
19	CS	69/80 (86%)	62 (90%)	7 (10%)	7	29
20	AT	76/82 (93%)	65 (86%)	11 (14%)	3	15
20	CT	76/82 (93%)	66 (87%)	10 (13%)	4	18
21	AU	19/22 (86%)	19 (100%)	0	100	100
21	CU	19/22 (86%)	19 (100%)	0	100	100
22	B0	61/67 (91%)	49 (80%)	12 (20%)	1	7
22	D0	61/67 (91%)	47 (77%)	14 (23%)	1	4
23	B1	73/83 (88%)	55 (75%)	18 (25%)	0	3
23	D1	73/83 (88%)	55 (75%)	18 (25%)	0	3
24	B2	46/67 (69%)	29 (63%)	17 (37%)	0	0
24	D2	46/67 (69%)	30 (65%)	16 (35%)	0	1
25	B3	51/52 (98%)	44 (86%)	7 (14%)	3	17
25	D3	51/52 (98%)	44 (86%)	7 (14%)	3	17
27	B5	51/52 (98%)	38 (74%)	13 (26%)	0	3
27	D5	51/52 (98%)	36 (71%)	15 (29%)	0	1
28	B6	43/52 (83%)	27 (63%)	16 (37%)	0	0
28	D6	43/52 (83%)	27 (63%)	16 (37%)	0	0
29	B7	41/42 (98%)	35 (85%)	6 (15%)	3	15
29	D7	41/42 (98%)	35 (85%)	6 (15%)	3	15
30	B8	53/55 (96%)	38 (72%)	15 (28%)	0	2
30	D8	53/55 (96%)	41 (77%)	12 (23%)	1	4
33	BD	213/218 (98%)	163 (76%)	50 (24%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DD	213/218 (98%)	162 (76%)	51 (24%)	0	3
34	BE	165/166 (99%)	126 (76%)	39 (24%)	1	3
34	DE	165/166 (99%)	126 (76%)	39 (24%)	1	3
35	BF	165/166 (99%)	132 (80%)	33 (20%)	1	7
35	DF	165/166 (99%)	135 (82%)	30 (18%)	1	9
36	BG	155/156 (99%)	132 (85%)	23 (15%)	3	14
36	DG	155/156 (99%)	131 (84%)	24 (16%)	2	13
37	BH	132/148 (89%)	107 (81%)	25 (19%)	1	8
37	DH	132/148 (89%)	108 (82%)	24 (18%)	1	9
38	BI	122/124 (98%)	103 (84%)	19 (16%)	2	13
38	DI	122/124 (98%)	103 (84%)	19 (16%)	2	13
39	BN	117/119 (98%)	93 (80%)	24 (20%)	1	6
39	DN	117/119 (98%)	92 (79%)	25 (21%)	1	5
40	BO	100/100 (100%)	75 (75%)	25 (25%)	0	3
40	DO	100/100 (100%)	74 (74%)	26 (26%)	0	2
41	BP	112/116 (97%)	63 (56%)	49 (44%)	0	0
41	DP	112/116 (97%)	65 (58%)	47 (42%)	0	0
42	BQ	106/111 (96%)	88 (83%)	18 (17%)	2	10
42	DQ	106/111 (96%)	87 (82%)	19 (18%)	2	9
43	BR	100/101 (99%)	76 (76%)	24 (24%)	0	3
43	DR	100/101 (99%)	75 (75%)	25 (25%)	0	3
44	BS	77/88 (88%)	54 (70%)	23 (30%)	0	1
44	DS	77/88 (88%)	54 (70%)	23 (30%)	0	1
45	BT	116/127 (91%)	84 (72%)	32 (28%)	0	2
45	DT	116/127 (91%)	84 (72%)	32 (28%)	0	2
46	BU	92/94 (98%)	75 (82%)	17 (18%)	1	8
46	DU	92/94 (98%)	74 (80%)	18 (20%)	1	7
47	BV	82/82 (100%)	53 (65%)	29 (35%)	0	1
47	DV	82/82 (100%)	52 (63%)	30 (37%)	0	1
48	BW	91/92 (99%)	70 (77%)	21 (23%)	1	4
48	DW	91/92 (99%)	69 (76%)	22 (24%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BX	74/78 (95%)	54 (73%)	20 (27%)	0	2
49	DX	74/78 (95%)	54 (73%)	20 (27%)	0	2
50	BY	84/91 (92%)	58 (69%)	26 (31%)	0	1
50	DY	84/91 (92%)	59 (70%)	25 (30%)	0	1
51	BZ	155/179 (87%)	130 (84%)	25 (16%)	2	12
51	DZ	155/179 (87%)	130 (84%)	25 (16%)	2	12
All	All	9322/9876 (94%)	7681 (82%)	1641 (18%)	2	10

5 of 1641 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BW	76	VAL
8	CH	95	VAL
46	DU	102	GLU
49	BX	65	ARG
2	CB	130	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 272 such sidechains are listed below:

Mol	Chain	Res	Type
47	BV	89	GLN
6	CF	18	GLN
45	DT	123	GLN
48	BW	61	ASN
2	CB	40	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	287 (19%)	31 (2%)
1	CA	1503/1522 (98%)	288 (19%)	31 (2%)
31	BA	2723/2787 (97%)	735 (26%)	71 (2%)
31	DA	2723/2787 (97%)	729 (26%)	70 (2%)
32	BB	118/122 (96%)	35 (29%)	1 (0%)
32	DB	118/122 (96%)	35 (29%)	0
All	All	8688/8862 (98%)	2109 (24%)	204 (2%)

5 of 2109 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 204 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	BA	2506	U
1	CA	484	G
31	DA	1992	G
31	BA	2611	U
1	CA	60	A

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 802 ligands modelled in this entry, 800 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
55	ZIT	DA	3311	-	54,54,54	1.38	6 (11%)	82,83,83	1.08	4 (4%)
55	ZIT	BA	3351	-	54,54,54	1.38	6 (11%)	82,83,83	1.08	4 (4%)

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
55	ZIT	DA	3311	-	-	3/72/107/107	0/3/3/3
55	ZIT	BA	3351	-	-	3/72/107/107	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BA	3351	ZIT	C22-C11	3.30	1.58	1.52
55	DA	3311	ZIT	C22-C11	3.28	1.58	1.52
55	DA	3311	ZIT	C13-C14	3.20	1.60	1.54
55	BA	3351	ZIT	C13-C14	3.16	1.60	1.54
55	DA	3311	ZIT	O13-C13	2.61	1.48	1.44

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BA	3351	ZIT	C9-N10-C11	-3.01	106.95	112.05
55	DA	3311	ZIT	C9-N10-C11	-2.99	106.99	112.05
55	DA	3311	ZIT	C7-C8-C9	2.83	116.09	112.06
55	BA	3351	ZIT	C7-C8-C9	2.82	116.09	112.06
55	BA	3351	ZIT	C4A-C3A-C2A	-2.12	106.91	109.97

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

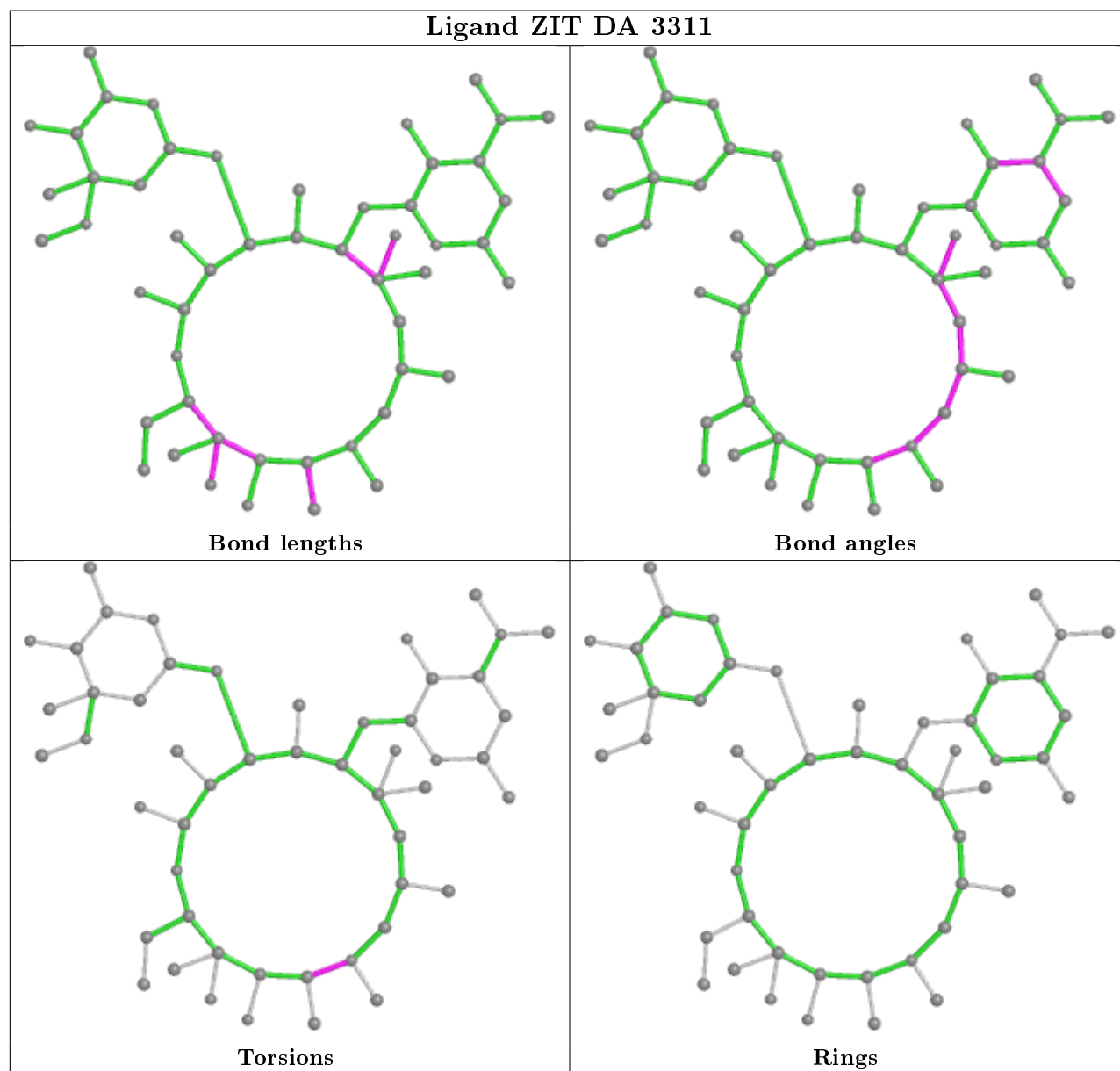
Mol	Chain	Res	Type	Atoms
55	BA	3351	ZIT	C12-C11-N10-C21
55	BA	3351	ZIT	C22-C11-N10-C21
55	DA	3311	ZIT	C12-C11-N10-C21
55	DA	3311	ZIT	C22-C11-N10-C21
55	BA	3351	ZIT	C12-C11-N10-C9

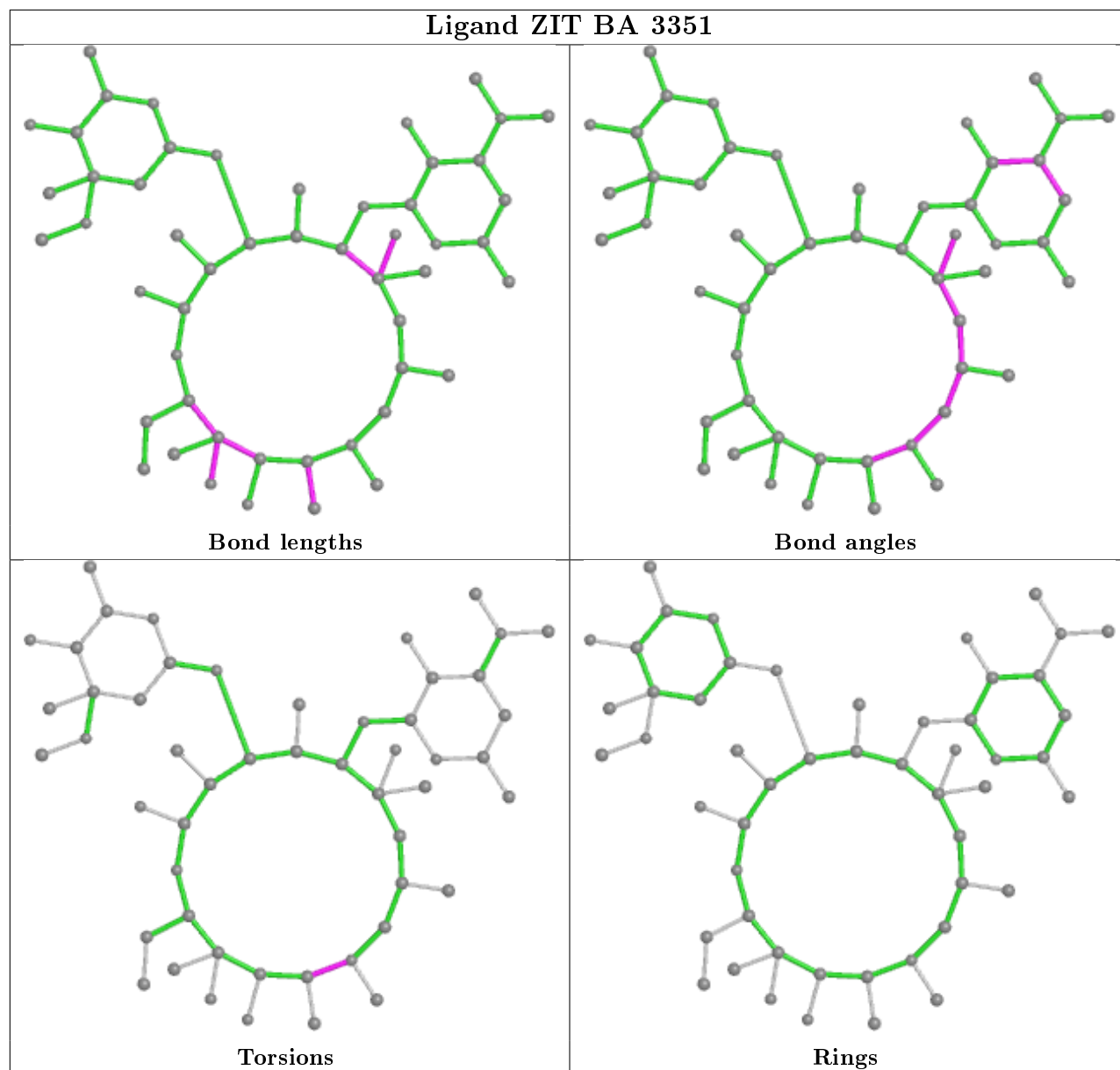
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	DA	3311	ZIT	3	0
55	BA	3351	ZIT	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
13	CM	3
13	AM	3
47	DV	1

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Mol	Chain	Number of breaks
36	DG	1
36	BG	1
9	AI	1
9	CI	1
47	BV	1
28	D6	1
28	B6	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CM	69:GLU	C	70:LEU	N	5.29
1	AM	69:GLU	C	70:LEU	N	5.28
1	DG	112:PRO	C	113:ARG	N	4.77
1	BG	112:PRO	C	113:ARG	N	4.76
1	AM	112:GLY	C	113:PRO	N	4.20

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	0.63	189 (12%) 3 1	60, 125, 191, 194	0
1	CA	1504/1522 (98%)	0.63	194 (12%) 3 1	61, 125, 191, 194	0
2	AB	235/256 (91%)	0.52	32 (13%) 3 1	107, 156, 184, 191	0
2	CB	235/256 (91%)	0.91	46 (19%) 1 0	107, 158, 185, 191	0
3	AC	207/239 (86%)	0.60	29 (14%) 2 1	115, 163, 184, 189	0
3	CC	207/239 (86%)	1.36	63 (30%) 0 0	119, 166, 184, 191	0
4	AD	208/209 (99%)	0.41	18 (8%) 10 3	83, 131, 170, 181	0
4	CD	208/209 (99%)	0.34	16 (7%) 13 4	82, 131, 168, 182	0
5	AE	151/162 (93%)	0.44	14 (9%) 8 3	83, 116, 160, 188	0
5	CE	151/162 (93%)	0.78	29 (19%) 1 0	84, 117, 162, 189	0
6	AF	101/101 (100%)	0.22	5 (4%) 28 10	85, 132, 164, 180	0
6	CF	101/101 (100%)	0.20	7 (6%) 16 5	86, 132, 165, 182	0
7	AG	155/156 (99%)	1.43	53 (34%) 0 0	140, 171, 188, 191	0
7	CG	155/156 (99%)	2.45	75 (48%) 0 0	140, 171, 188, 190	0
8	AH	138/138 (100%)	0.08	7 (5%) 28 10	85, 121, 155, 164	0
8	CH	138/138 (100%)	0.02	4 (2%) 51 23	85, 123, 156, 162	0
9	AI	127/128 (99%)	2.37	62 (48%) 0 0	142, 182, 190, 192	0
9	CI	127/128 (99%)	2.31	52 (40%) 0 0	143, 183, 190, 191	0
10	AJ	99/105 (94%)	3.02	59 (59%) 0 0	130, 176, 189, 191	0
10	CJ	99/105 (94%)	2.84	55 (55%) 0 0	130, 177, 190, 193	0
11	AK	119/129 (92%)	0.73	20 (16%) 1 0	82, 123, 164, 187	0
11	CK	119/129 (92%)	0.85	15 (12%) 3 1	84, 123, 165, 186	0
12	AL	125/135 (92%)	0.60	15 (12%) 4 1	80, 108, 163, 189	0
12	CL	125/135 (92%)	0.63	15 (12%) 4 1	82, 109, 164, 189	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	AM	115/126 (91%)	3.06	71 (61%)	0	0	150, 185, 190, 193	0
13	CM	115/126 (91%)	2.85	72 (62%)	0	0	149, 185, 190, 192	0
14	AN	60/61 (98%)	1.33	17 (28%)	0	0	131, 168, 185, 189	0
14	CN	60/61 (98%)	1.08	14 (23%)	0	0	132, 170, 186, 189	0
15	AO	88/89 (98%)	0.14	4 (4%)	33	12	74, 111, 157, 162	0
15	CO	88/89 (98%)	0.40	6 (6%)	17	5	74, 112, 159, 165	0
16	AP	84/88 (95%)	1.15	27 (32%)	0	0	91, 118, 161, 179	0
16	CP	84/88 (95%)	0.82	14 (16%)	1	0	89, 116, 160, 180	0
17	AQ	100/105 (95%)	0.35	7 (7%)	16	5	80, 109, 153, 163	0
17	CQ	100/105 (95%)	0.23	7 (7%)	16	5	85, 110, 153, 159	0
18	AR	70/88 (79%)	0.62	8 (11%)	5	1	93, 121, 170, 183	0
18	CR	70/88 (79%)	1.48	20 (28%)	0	0	93, 122, 171, 183	0
19	AS	79/93 (84%)	3.39	51 (64%)	0	0	142, 186, 190, 191	0
19	CS	79/93 (84%)	3.34	54 (68%)	0	0	142, 186, 191, 192	0
20	AT	99/106 (93%)	0.65	11 (11%)	5	1	84, 119, 157, 177	0
20	CT	99/106 (93%)	0.39	9 (9%)	9	3	84, 119, 157, 179	0
21	AU	25/27 (92%)	3.24	14 (56%)	0	0	143, 174, 188, 190	0
21	CU	25/27 (92%)	2.67	15 (60%)	0	0	141, 172, 188, 189	0
22	B0	85/85 (100%)	0.41	8 (9%)	8	3	49, 70, 175, 187	0
22	D0	85/85 (100%)	0.51	9 (10%)	6	2	54, 74, 173, 188	0
23	B1	89/98 (90%)	0.21	2 (2%)	62	33	50, 79, 150, 187	0
23	D1	89/98 (90%)	0.12	5 (5%)	24	8	51, 81, 151, 190	0
24	B2	51/72 (70%)	0.75	7 (13%)	3	1	59, 99, 175, 186	0
24	D2	51/72 (70%)	0.53	7 (13%)	3	1	62, 100, 175, 188	0
25	B3	60/60 (100%)	-0.13	1 (1%)	70	41	46, 69, 132, 168	0
25	D3	60/60 (100%)	0.29	3 (5%)	28	10	51, 72, 136, 161	0
26	B4	32/71 (45%)	-0.22	0	100	100	133, 161, 182, 184	0
26	D4	32/71 (45%)	0.31	5 (15%)	2	1	133, 164, 182, 186	0
27	B5	58/60 (96%)	0.35	4 (6%)	16	5	34, 61, 165, 188	0
27	D5	58/60 (96%)	0.05	5 (8%)	10	3	39, 63, 163, 190	0
28	B6	45/54 (83%)	0.68	3 (6%)	17	5	49, 85, 141, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/54 (83%)	0.61	7 (15%) 2 1	52, 87, 142, 172	0
29	B7	49/49 (100%)	0.26	3 (6%) 21 7	36, 45, 119, 172	0
29	D7	49/49 (100%)	0.36	4 (8%) 11 3	38, 49, 120, 173	0
30	B8	64/65 (98%)	0.30	5 (7%) 13 4	46, 68, 140, 165	0
30	D8	64/65 (98%)	0.09	0 100 100	49, 73, 141, 169	0
31	BA	2725/2787 (97%)	0.02	59 (2%) 62 33	33, 59, 153, 194	0
31	DA	2725/2787 (97%)	-0.16	101 (3%) 41 17	38, 64, 157, 194	0
32	BB	119/122 (97%)	0.16	4 (3%) 45 19	50, 101, 149, 184	0
32	DB	119/122 (97%)	0.38	10 (8%) 11 3	59, 105, 157, 184	0
33	BD	272/276 (98%)	-0.19	4 (1%) 73 46	37, 62, 120, 168	0
33	DD	272/276 (98%)	-0.29	3 (1%) 80 56	40, 65, 122, 165	0
34	BE	205/206 (99%)	-0.01	6 (2%) 51 23	36, 65, 153, 181	0
34	DE	205/206 (99%)	0.06	10 (4%) 29 11	40, 69, 154, 182	0
35	BF	208/210 (99%)	0.15	14 (6%) 17 5	35, 77, 175, 189	0
35	DF	208/210 (99%)	0.28	13 (6%) 20 6	39, 79, 176, 188	0
36	BG	181/182 (99%)	1.16	49 (27%) 0 0	100, 152, 186, 192	0
36	DG	181/182 (99%)	1.84	65 (35%) 0 0	106, 159, 189, 191	0
37	BH	160/180 (88%)	0.22	3 (1%) 66 37	69, 111, 151, 182	0
37	DH	160/180 (88%)	0.93	34 (21%) 0 0	74, 114, 157, 185	0
38	BI	146/148 (98%)	0.47	14 (9%) 8 2	67, 152, 187, 190	0
38	DI	146/148 (98%)	1.07	37 (25%) 0 0	69, 156, 189, 191	0
39	BN	139/140 (99%)	0.01	4 (2%) 51 23	45, 75, 143, 182	0
39	DN	139/140 (99%)	-0.16	3 (2%) 62 33	49, 78, 143, 183	0
40	BO	122/122 (100%)	-0.25	0 100 100	45, 67, 123, 147	0
40	DO	122/122 (100%)	-0.55	0 100 100	48, 69, 125, 149	0
41	BP	146/150 (97%)	0.46	10 (6%) 17 5	29, 93, 149, 190	0
41	DP	146/150 (97%)	0.45	15 (10%) 6 2	38, 95, 152, 188	0
42	BQ	136/141 (96%)	0.42	9 (6%) 18 5	50, 77, 147, 183	0
42	DQ	136/141 (96%)	0.38	8 (5%) 22 7	52, 79, 147, 183	0
43	BR	117/118 (99%)	-0.07	0 100 100	40, 60, 130, 139	0
43	DR	117/118 (99%)	-0.28	1 (0%) 84 63	42, 62, 131, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BS	99/112 (88%)	0.40	6 (6%) 21 7	54, 111, 148, 165	0
44	DS	99/112 (88%)	1.19	24 (24%) 0 0	62, 113, 154, 170	0
45	BT	132/146 (90%)	0.17	5 (3%) 40 16	55, 87, 154, 181	0
45	DT	132/146 (90%)	0.14	11 (8%) 11 3	58, 90, 156, 179	0
46	BU	117/118 (99%)	0.09	2 (1%) 70 41	40, 62, 124, 176	0
46	DU	117/118 (99%)	0.14	6 (5%) 28 10	44, 67, 130, 175	0
47	BV	101/101 (100%)	0.60	9 (8%) 9 3	38, 103, 176, 189	0
47	DV	101/101 (100%)	0.63	11 (10%) 5 2	44, 109, 177, 188	0
48	BW	113/113 (100%)	-0.38	0 100 100	38, 51, 112, 179	0
48	DW	113/113 (100%)	-0.46	1 (0%) 84 63	41, 54, 119, 181	0
49	BX	93/96 (96%)	0.11	4 (4%) 35 13	47, 74, 145, 179	0
49	DX	93/96 (96%)	0.02	6 (6%) 18 5	52, 76, 146, 179	0
50	BY	101/110 (91%)	0.89	16 (15%) 2 1	57, 107, 184, 192	0
50	DY	101/110 (91%)	0.79	18 (17%) 1 0	60, 108, 183, 193	0
51	BZ	177/206 (85%)	0.15	10 (5%) 24 8	68, 113, 158, 169	0
51	DZ	177/206 (85%)	0.51	20 (11%) 5 1	74, 117, 161, 168	0
All	All	20062/20922 (95%)	0.44	2198 (10%) 5 2	29, 99, 187, 194	0

The worst 5 of 2198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	DQ	141	GLN	19.8
31	DA	2802	G	19.5
42	BQ	140	ALA	18.9
42	BQ	141	GLN	17.8
35	DF	208	GLY	16.1

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	K	BA	3350	1/1	0.54	0.46	95,95,95,95	0
52	MG	BA	3246	1/1	0.55	0.45	75,75,75,75	0
52	MG	DA	3278	1/1	0.57	0.54	68,68,68,68	0
52	MG	DA	3291	1/1	0.61	1.07	86,86,86,86	0
52	MG	BA	3312	1/1	0.62	0.66	87,87,87,87	0
52	MG	DA	3305	1/1	0.63	0.34	76,76,76,76	0
52	MG	DA	3255	1/1	0.64	0.44	75,75,75,75	0
52	MG	BA	3341	1/1	0.65	0.71	63,63,63,63	0
52	MG	DA	3261	1/1	0.66	0.52	95,95,95,95	0
52	MG	AA	1644	1/1	0.66	1.26	99,99,99,99	0
52	MG	CA	1622	1/1	0.67	0.28	78,78,78,78	0
52	MG	BA	3196	1/1	0.67	0.21	65,65,65,65	0
52	MG	BA	3148	1/1	0.69	0.34	58,58,58,58	0
52	MG	DA	3219	1/1	0.69	0.36	75,75,75,75	0
52	MG	DA	3267	1/1	0.69	0.58	72,72,72,72	0
52	MG	DA	3216	1/1	0.69	0.61	85,85,85,85	0
52	MG	DA	3294	1/1	0.70	0.34	67,67,67,67	0
52	MG	DQ	201	1/1	0.70	0.39	78,78,78,78	0
52	MG	BA	3241	1/1	0.71	0.61	79,79,79,79	0
52	MG	DA	3245	1/1	0.71	0.19	78,78,78,78	0
52	MG	BA	3295	1/1	0.71	0.23	70,70,70,70	0
52	MG	DA	3260	1/1	0.71	0.81	73,73,73,73	0
52	MG	CA	1626	1/1	0.71	0.54	78,78,78,78	0
52	MG	DA	3226	1/1	0.71	0.35	64,64,64,64	0
52	MG	DA	3306	1/1	0.72	0.38	87,87,87,87	0
52	MG	DA	3223	1/1	0.73	0.12	65,65,65,65	0
52	MG	DA	3191	1/1	0.73	0.26	91,91,91,91	0
52	MG	DA	3059	1/1	0.74	0.40	53,53,53,53	0
52	MG	CA	1628	1/1	0.75	0.45	75,75,75,75	0
52	MG	BA	3229	1/1	0.75	0.29	50,50,50,50	0
52	MG	DA	3222	1/1	0.75	0.84	67,67,67,67	0
52	MG	DA	3198	1/1	0.76	0.78	70,70,70,70	0
52	MG	DA	3126	1/1	0.77	0.22	73,73,73,73	0
52	MG	BA	3296	1/1	0.77	0.72	67,67,67,67	0
52	MG	CA	1646	1/1	0.77	0.52	80,80,80,80	0
52	MG	DA	3203	1/1	0.78	0.65	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	AA	1650	1/1	0.78	0.53	68,68,68,68	0
54	K	DA	3310	1/1	0.78	0.48	106,106,106,106	0
52	MG	DA	3243	1/1	0.78	0.48	70,70,70,70	0
52	MG	CA	1611	1/1	0.78	0.61	81,81,81,81	0
52	MG	BA	3298	1/1	0.78	0.33	61,61,61,61	0
52	MG	DA	3120	1/1	0.79	0.31	71,71,71,71	0
52	MG	BA	3309	1/1	0.79	0.97	61,61,61,61	0
52	MG	DA	3244	1/1	0.79	0.28	86,86,86,86	0
52	MG	DA	3246	1/1	0.79	0.26	87,87,87,87	0
52	MG	DA	3248	1/1	0.79	0.33	74,74,74,74	0
52	MG	BA	3336	1/1	0.79	0.48	65,65,65,65	0
52	MG	DA	3207	1/1	0.79	0.80	78,78,78,78	0
52	MG	DA	3067	1/1	0.80	0.37	81,81,81,81	0
52	MG	AA	1640	1/1	0.80	0.62	83,83,83,83	0
52	MG	BA	3144	1/1	0.81	0.27	53,53,53,53	0
52	MG	BA	3190	1/1	0.81	0.30	53,53,53,53	0
52	MG	D5	102	1/1	0.81	0.64	79,79,79,79	0
52	MG	DA	3100	1/1	0.81	0.71	50,50,50,50	0
52	MG	BA	3178	1/1	0.81	0.53	78,78,78,78	0
52	MG	AA	1619	1/1	0.82	0.36	56,56,56,56	0
52	MG	DA	3268	1/1	0.82	1.51	81,81,81,81	0
52	MG	DA	3157	1/1	0.82	0.50	65,65,65,65	0
52	MG	DA	3264	1/1	0.82	0.83	80,80,80,80	0
52	MG	AA	1633	1/1	0.82	0.10	81,81,81,81	0
52	MG	DA	3284	1/1	0.82	0.70	65,65,65,65	0
52	MG	AA	1639	1/1	0.82	0.21	95,95,95,95	0
52	MG	BA	3240	1/1	0.82	0.46	60,60,60,60	0
52	MG	DA	3195	1/1	0.82	0.51	56,56,56,56	0
52	MG	BA	3192	1/1	0.83	0.34	58,58,58,58	0
52	MG	BA	3304	1/1	0.83	1.20	86,86,86,86	0
52	MG	BA	3238	1/1	0.83	0.47	49,49,49,49	0
52	MG	BA	3302	1/1	0.83	0.27	72,72,72,72	0
52	MG	CA	1623	1/1	0.83	0.51	67,67,67,67	0
52	MG	DA	3102	1/1	0.83	0.28	80,80,80,80	0
52	MG	D7	101	1/1	0.83	0.36	62,62,62,62	0
52	MG	CA	1632	1/1	0.83	0.25	79,79,79,79	0
52	MG	BB	201	1/1	0.84	0.45	42,42,42,42	0
52	MG	AA	1604	1/1	0.84	0.46	95,95,95,95	0
52	MG	DA	3038	1/1	0.84	0.60	48,48,48,48	0
52	MG	DA	3108	1/1	0.84	0.33	48,48,48,48	0
52	MG	DA	3175	1/1	0.84	0.69	67,67,67,67	0
52	MG	BA	3237	1/1	0.84	0.32	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3306	1/1	0.84	0.26	56,56,56,56	0
52	MG	AA	1637	1/1	0.85	0.29	69,69,69,69	0
52	MG	DA	3270	1/1	0.85	0.67	65,65,65,65	0
52	MG	DA	3258	1/1	0.85	0.14	61,61,61,61	0
52	MG	BA	3334	1/1	0.85	0.32	53,53,53,53	0
52	MG	DA	3302	1/1	0.85	0.68	86,86,86,86	0
52	MG	DA	3145	1/1	0.85	0.91	88,88,88,88	0
52	MG	DA	3247	1/1	0.85	0.70	87,87,87,87	0
52	MG	BA	3096	1/1	0.85	0.33	55,55,55,55	0
52	MG	DA	3129	1/1	0.85	0.12	87,87,87,87	0
52	MG	DA	3150	1/1	0.85	0.56	77,77,77,77	0
52	MG	BA	3200	1/1	0.85	0.86	59,59,59,59	0
52	MG	BA	3303	1/1	0.85	0.44	68,68,68,68	0
52	MG	DA	3280	1/1	0.85	0.55	77,77,77,77	0
52	MG	CA	1634	1/1	0.85	0.52	87,87,87,87	0
52	MG	DA	3309	1/1	0.85	0.14	84,84,84,84	0
52	MG	BA	3232	1/1	0.86	0.38	70,70,70,70	0
52	MG	DA	3106	1/1	0.86	0.52	76,76,76,76	0
52	MG	BA	3188	1/1	0.86	0.67	62,62,62,62	0
52	MG	DA	3194	1/1	0.86	0.31	60,60,60,60	0
52	MG	DX	101	1/1	0.86	0.30	77,77,77,77	0
52	MG	CA	1605	1/1	0.86	0.56	61,61,61,61	0
52	MG	BA	3219	1/1	0.86	0.11	38,38,38,38	0
52	MG	DA	3070	1/1	0.86	0.62	74,74,74,74	0
52	MG	BA	3114	1/1	0.86	0.44	56,56,56,56	0
52	MG	DA	3262	1/1	0.86	0.87	77,77,77,77	0
52	MG	BA	3343	1/1	0.86	0.45	58,58,58,58	0
52	MG	DA	3119	1/1	0.86	0.07	64,64,64,64	0
52	MG	CA	1617	1/1	0.86	0.32	61,61,61,61	0
52	MG	BA	3307	1/1	0.86	0.44	76,76,76,76	0
52	MG	CA	1633	1/1	0.86	1.26	87,87,87,87	0
52	MG	BA	3157	1/1	0.87	0.77	74,74,74,74	0
52	MG	DA	3257	1/1	0.87	0.91	63,63,63,63	0
52	MG	BA	3318	1/1	0.87	0.54	60,60,60,60	0
52	MG	DA	3017	1/1	0.87	0.32	47,47,47,47	0
52	MG	BA	3138	1/1	0.87	0.12	74,74,74,74	0
52	MG	DA	3201	1/1	0.87	0.30	59,59,59,59	0
52	MG	BA	3149	1/1	0.87	0.11	51,51,51,51	0
52	MG	DA	3182	1/1	0.87	0.28	55,55,55,55	0
52	MG	BA	3274	1/1	0.87	0.16	81,81,81,81	0
52	MG	BA	3249	1/1	0.87	0.26	40,40,40,40	0
52	MG	BA	3294	1/1	0.87	0.54	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3279	1/1	0.87	0.44	50,50,50,50	0
52	MG	AA	1641	1/1	0.87	0.15	69,69,69,69	0
52	MG	DA	3231	1/1	0.87	0.35	79,79,79,79	0
52	MG	DA	3115	1/1	0.87	0.40	72,72,72,72	0
52	MG	BA	3280	1/1	0.88	0.35	75,75,75,75	0
52	MG	DA	3179	1/1	0.88	0.85	77,77,77,77	0
52	MG	BA	3189	1/1	0.88	0.41	45,45,45,45	0
52	MG	DA	3013	1/1	0.88	0.49	77,77,77,77	0
52	MG	DA	3295	1/1	0.88	0.17	88,88,88,88	0
52	MG	DA	3288	1/1	0.88	0.20	72,72,72,72	0
52	MG	BA	3349	1/1	0.88	0.09	61,61,61,61	0
52	MG	DA	3208	1/1	0.88	0.68	62,62,62,62	0
52	MG	CA	1612	1/1	0.88	0.10	77,77,77,77	0
52	MG	DA	3265	1/1	0.88	1.12	79,79,79,79	0
52	MG	CA	1644	1/1	0.88	0.47	74,74,74,74	0
52	MG	DA	3229	1/1	0.88	0.12	45,45,45,45	0
52	MG	BA	3332	1/1	0.88	0.29	61,61,61,61	0
52	MG	DA	3282	1/1	0.88	0.33	62,62,62,62	0
52	MG	BA	3097	1/1	0.88	0.17	70,70,70,70	0
52	MG	DA	3218	1/1	0.88	0.25	78,78,78,78	0
52	MG	DF	301	1/1	0.88	0.38	92,92,92,92	0
52	MG	BA	3162	1/1	0.88	0.16	47,47,47,47	0
52	MG	BA	3348	1/1	0.88	0.12	61,61,61,61	0
52	MG	DA	3307	1/1	0.88	0.31	80,80,80,80	0
52	MG	DA	3228	1/1	0.88	0.10	60,60,60,60	0
52	MG	BF	301	1/1	0.88	0.17	62,62,62,62	0
52	MG	DA	3147	1/1	0.88	0.29	63,63,63,63	0
52	MG	DA	3298	1/1	0.88	0.64	71,71,71,71	0
52	MG	DA	3279	1/1	0.88	0.24	64,64,64,64	0
52	MG	AA	1613	1/1	0.88	0.15	70,70,70,70	0
52	MG	BA	3152	1/1	0.88	0.32	61,61,61,61	0
52	MG	BA	3289	1/1	0.88	0.27	55,55,55,55	0
52	MG	BA	3022	1/1	0.89	0.39	49,49,49,49	0
52	MG	CA	1629	1/1	0.89	0.13	82,82,82,82	0
53	ZN	CN	101	1/1	0.89	0.18	157,157,157,157	0
52	MG	DA	3188	1/1	0.89	0.22	48,48,48,48	0
52	MG	D0	101	1/1	0.89	0.15	62,62,62,62	0
52	MG	DA	3092	1/1	0.89	0.28	61,61,61,61	0
52	MG	DA	3020	1/1	0.89	0.43	64,64,64,64	0
52	MG	DA	3155	1/1	0.89	0.19	62,62,62,62	0
52	MG	DA	3168	1/1	0.89	0.28	53,53,53,53	0
52	MG	CA	1609	1/1	0.89	0.22	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3315	1/1	0.89	0.36	69,69,69,69	0
52	MG	BA	3311	1/1	0.89	0.35	46,46,46,46	0
52	MG	DA	3275	1/1	0.89	0.45	62,62,62,62	0
52	MG	BA	3245	1/1	0.89	0.58	45,45,45,45	0
52	MG	AA	1632	1/1	0.89	0.65	72,72,72,72	0
52	MG	BA	3081	1/1	0.89	0.23	37,37,37,37	0
52	MG	BA	3329	1/1	0.89	0.65	68,68,68,68	0
52	MG	DA	3210	1/1	0.89	0.37	63,63,63,63	0
52	MG	DA	3082	1/1	0.89	0.18	17,17,17,17	0
52	MG	BA	3333	1/1	0.89	0.17	80,80,80,80	0
52	MG	BA	3129	1/1	0.89	0.13	18,18,18,18	0
52	MG	BA	3223	1/1	0.90	0.59	36,36,36,36	0
52	MG	BA	3283	1/1	0.90	0.12	53,53,53,53	0
52	MG	DA	3005	1/1	0.90	0.28	73,73,73,73	0
52	MG	BA	3287	1/1	0.90	0.46	58,58,58,58	0
52	MG	DA	3011	1/1	0.90	0.54	50,50,50,50	0
52	MG	DA	3196	1/1	0.90	0.29	51,51,51,51	0
52	MG	DA	3252	1/1	0.90	0.55	66,66,66,66	0
52	MG	BA	3323	1/1	0.90	0.25	64,64,64,64	0
52	MG	BA	3205	1/1	0.90	0.33	55,55,55,55	0
52	MG	BA	3230	1/1	0.90	0.50	38,38,38,38	0
52	MG	AA	1647	1/1	0.90	0.34	66,66,66,66	0
52	MG	BA	3082	1/1	0.90	0.53	49,49,49,49	0
52	MG	CA	1606	1/1	0.90	0.39	72,72,72,72	0
52	MG	DA	3238	1/1	0.90	0.38	73,73,73,73	0
52	MG	DA	3083	1/1	0.90	0.23	47,47,47,47	0
52	MG	AA	1648	1/1	0.90	0.77	62,62,62,62	0
52	MG	CA	1610	1/1	0.90	0.29	61,61,61,61	0
52	MG	DA	3277	1/1	0.90	0.50	68,68,68,68	0
52	MG	DA	3037	1/1	0.90	0.63	74,74,74,74	0
52	MG	BQ	202	1/1	0.90	0.29	59,59,59,59	0
52	MG	DA	3224	1/1	0.90	0.09	68,68,68,68	0
52	MG	AA	1646	1/1	0.90	0.76	82,82,82,82	0
52	MG	BA	3116	1/1	0.90	0.16	51,51,51,51	0
52	MG	DA	3233	1/1	0.90	0.50	68,68,68,68	0
52	MG	DA	3029	1/1	0.91	0.21	87,87,87,87	0
52	MG	DA	3269	1/1	0.91	0.16	61,61,61,61	0
52	MG	BA	3197	1/1	0.91	0.30	52,52,52,52	0
52	MG	DA	3220	1/1	0.91	0.18	62,62,62,62	0
52	MG	AA	1645	1/1	0.91	0.33	81,81,81,81	0
52	MG	DA	3149	1/1	0.91	0.21	55,55,55,55	0
52	MG	BA	3087	1/1	0.91	0.41	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3170	1/1	0.91	0.31	69,69,69,69	0
52	MG	BA	3214	1/1	0.91	0.47	66,66,66,66	0
52	MG	AA	1607	1/1	0.91	0.29	74,74,74,74	0
52	MG	AA	1638	1/1	0.91	0.45	82,82,82,82	0
52	MG	BA	3305	1/1	0.91	0.28	54,54,54,54	0
52	MG	AA	1611	1/1	0.91	0.16	75,75,75,75	0
52	MG	DA	3167	1/1	0.91	0.42	48,48,48,48	0
52	MG	DA	3001	1/1	0.91	0.42	76,76,76,76	0
52	MG	DA	3225	1/1	0.91	0.21	54,54,54,54	0
52	MG	DA	3263	1/1	0.91	0.26	67,67,67,67	0
52	MG	DA	3272	1/1	0.91	0.27	74,74,74,74	0
52	MG	DA	3211	1/1	0.91	0.15	79,79,79,79	0
52	MG	BA	3331	1/1	0.91	0.46	46,46,46,46	0
52	MG	BA	3328	1/1	0.91	0.17	65,65,65,65	0
52	MG	DA	3292	1/1	0.91	0.58	75,75,75,75	0
52	MG	DA	3164	1/1	0.91	0.11	71,71,71,71	0
52	MG	DA	3113	1/1	0.91	0.48	62,62,62,62	0
52	MG	BA	3345	1/1	0.91	0.30	60,60,60,60	0
52	MG	BA	3337	1/1	0.91	0.31	58,58,58,58	0
52	MG	BA	3326	1/1	0.91	0.22	54,54,54,54	0
52	MG	BA	3068	1/1	0.91	0.34	54,54,54,54	0
52	MG	DA	3162	1/1	0.91	0.28	69,69,69,69	0
55	ZIT	BA	3351	52/52	0.91	0.32	100,100,100,100	0
52	MG	BA	3208	1/1	0.91	0.11	23,23,23,23	0
52	MG	CA	1647	1/1	0.91	0.21	84,84,84,84	0
52	MG	DA	3041	1/1	0.91	0.18	37,37,37,37	0
52	MG	BA	3319	1/1	0.91	0.49	40,40,40,40	0
52	MG	CA	1636	1/1	0.91	0.50	79,79,79,79	0
52	MG	DA	3242	1/1	0.91	0.19	69,69,69,69	0
52	MG	BA	3268	1/1	0.91	0.27	40,40,40,40	0
52	MG	DA	3094	1/1	0.91	0.41	56,56,56,56	0
52	MG	DA	3290	1/1	0.92	0.37	52,52,52,52	0
52	MG	AA	1635	1/1	0.92	0.65	63,63,63,63	0
52	MG	DA	3197	1/1	0.92	0.46	75,75,75,75	0
52	MG	DB	201	1/1	0.92	0.39	52,52,52,52	0
52	MG	BA	3236	1/1	0.92	0.35	70,70,70,70	0
52	MG	DA	3161	1/1	0.92	0.70	72,72,72,72	0
52	MG	AA	1626	1/1	0.92	0.49	76,76,76,76	0
52	MG	DA	3200	1/1	0.92	0.36	50,50,50,50	0
52	MG	DA	3170	1/1	0.92	0.51	53,53,53,53	0
52	MG	CA	1618	1/1	0.92	0.40	62,62,62,62	0
52	MG	BA	3202	1/1	0.92	0.31	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3303	1/1	0.92	0.59	49,49,49,49	0
52	MG	CA	1624	1/1	0.92	0.41	65,65,65,65	0
52	MG	BA	3227	1/1	0.92	0.13	39,39,39,39	0
52	MG	BA	3102	1/1	0.92	0.28	24,24,24,24	0
52	MG	DA	3230	1/1	0.92	0.25	56,56,56,56	0
52	MG	DA	3096	1/1	0.92	0.35	45,45,45,45	0
52	MG	DA	3249	1/1	0.92	0.83	79,79,79,79	0
52	MG	DA	3143	1/1	0.92	0.50	57,57,57,57	0
52	MG	DA	3085	1/1	0.92	0.40	54,54,54,54	0
52	MG	AA	1651	1/1	0.92	0.26	75,75,75,75	0
52	MG	BA	3191	1/1	0.92	0.68	64,64,64,64	0
52	MG	AA	1627	1/1	0.92	0.38	66,66,66,66	0
52	MG	CA	1602	1/1	0.92	0.47	70,70,70,70	0
52	MG	BA	3071	1/1	0.92	0.48	47,47,47,47	0
52	MG	BA	3278	1/1	0.92	0.23	41,41,41,41	0
52	MG	DR	201	1/1	0.92	0.34	43,43,43,43	0
52	MG	DA	3217	1/1	0.92	0.64	62,62,62,62	0
52	MG	BA	3128	1/1	0.92	0.28	54,54,54,54	0
52	MG	DA	3171	1/1	0.92	0.34	43,43,43,43	0
52	MG	DA	3024	1/1	0.92	0.45	61,61,61,61	0
52	MG	BA	3195	1/1	0.92	0.63	58,58,58,58	0
52	MG	BA	3125	1/1	0.92	0.18	46,46,46,46	0
52	MG	CA	1635	1/1	0.92	0.20	86,86,86,86	0
52	MG	DA	3069	1/1	0.92	0.52	51,51,51,51	0
52	MG	BA	3112	1/1	0.92	0.14	43,43,43,43	0
52	MG	BA	3140	1/1	0.92	0.62	40,40,40,40	0
52	MG	BA	3180	1/1	0.92	0.57	64,64,64,64	0
52	MG	DA	3259	1/1	0.92	0.63	74,74,74,74	0
55	ZIT	DA	3311	52/52	0.92	0.31	100,100,100,100	0
52	MG	BA	3330	1/1	0.92	0.82	71,71,71,71	0
52	MG	BA	3151	1/1	0.92	0.30	74,74,74,74	0
52	MG	BA	3040	1/1	0.92	0.74	51,51,51,51	0
52	MG	DE	301	1/1	0.92	0.36	40,40,40,40	0
52	MG	CA	1604	1/1	0.92	0.28	86,86,86,86	0
53	ZN	AN	101	1/1	0.92	0.15	159,159,159,159	0
52	MG	AA	1614	1/1	0.92	0.12	77,77,77,77	0
52	MG	BA	3156	1/1	0.92	0.46	53,53,53,53	0
52	MG	DA	3079	1/1	0.92	0.33	59,59,59,59	0
52	MG	BA	3335	1/1	0.92	0.19	52,52,52,52	0
52	MG	DA	3304	1/1	0.92	0.36	52,52,52,52	0
52	MG	DA	3254	1/1	0.92	0.19	65,65,65,65	0
52	MG	BA	3074	1/1	0.92	0.46	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3111	1/1	0.92	0.13	19,19,19,19	0
52	MG	DA	3202	1/1	0.92	0.21	40,40,40,40	0
52	MG	DA	3308	1/1	0.92	0.12	81,81,81,81	0
52	MG	BA	3277	1/1	0.92	0.47	62,62,62,62	0
52	MG	BA	3136	1/1	0.93	0.52	32,32,32,32	0
52	MG	AA	1628	1/1	0.93	0.51	66,66,66,66	0
52	MG	CA	1619	1/1	0.93	0.35	75,75,75,75	0
52	MG	BA	3338	1/1	0.93	0.28	73,73,73,73	0
52	MG	BA	3297	1/1	0.93	0.29	61,61,61,61	0
52	MG	DA	3152	1/1	0.93	0.54	43,43,43,43	0
52	MG	DA	3158	1/1	0.93	0.12	61,61,61,61	0
52	MG	BA	3288	1/1	0.93	0.45	72,72,72,72	0
52	MG	BA	3182	1/1	0.93	0.51	68,68,68,68	0
52	MG	DB	203	1/1	0.93	0.46	56,56,56,56	0
52	MG	BA	3340	1/1	0.93	0.46	62,62,62,62	0
52	MG	BA	3228	1/1	0.93	0.65	69,69,69,69	0
52	MG	BA	3255	1/1	0.93	0.33	45,45,45,45	0
52	MG	BA	3009	1/1	0.93	0.38	38,38,38,38	0
52	MG	DA	3192	1/1	0.93	0.54	55,55,55,55	0
52	MG	BA	3088	1/1	0.93	0.25	10,10,10,10	0
52	MG	BA	3235	1/1	0.93	0.41	72,72,72,72	0
52	MG	AA	1622	1/1	0.93	0.54	75,75,75,75	0
52	MG	CA	1607	1/1	0.93	0.48	82,82,82,82	0
52	MG	BA	3049	1/1	0.93	0.58	41,41,41,41	0
52	MG	DA	3146	1/1	0.93	0.34	69,69,69,69	0
52	MG	BX	101	1/1	0.93	0.26	61,61,61,61	0
52	MG	DA	3112	1/1	0.93	0.33	68,68,68,68	0
52	MG	DB	202	1/1	0.93	0.36	63,63,63,63	0
52	MG	AA	1608	1/1	0.93	0.33	54,54,54,54	0
52	MG	DA	3165	1/1	0.93	0.32	52,52,52,52	0
52	MG	DA	3241	1/1	0.93	0.29	60,60,60,60	0
52	MG	DA	3256	1/1	0.93	0.18	57,57,57,57	0
52	MG	BP	202	1/1	0.93	0.32	58,58,58,58	0
52	MG	DA	3072	1/1	0.93	0.37	46,46,46,46	0
52	MG	BA	3163	1/1	0.93	0.41	47,47,47,47	0
52	MG	DA	3266	1/1	0.93	0.28	75,75,75,75	0
52	MG	BA	3145	1/1	0.93	0.55	40,40,40,40	0
52	MG	BA	3293	1/1	0.93	0.26	55,55,55,55	0
52	MG	DA	3058	1/1	0.93	0.21	58,58,58,58	0
52	MG	BA	3253	1/1	0.93	0.15	51,51,51,51	0
52	MG	CA	1630	1/1	0.93	0.35	77,77,77,77	0
52	MG	BA	3183	1/1	0.93	0.16	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3110	1/1	0.93	0.39	73,73,73,73	0
52	MG	DA	3177	1/1	0.93	0.31	61,61,61,61	0
52	MG	BA	3259	1/1	0.94	0.51	46,46,46,46	0
52	MG	BA	3221	1/1	0.94	0.47	40,40,40,40	0
52	MG	BA	3001	1/1	0.94	0.36	49,49,49,49	0
52	MG	BD	301	1/1	0.94	0.20	43,43,43,43	0
52	MG	DA	3016	1/1	0.94	0.45	56,56,56,56	0
52	MG	AA	1612	1/1	0.94	0.30	66,66,66,66	0
52	MG	BA	3159	1/1	0.94	0.47	45,45,45,45	0
52	MG	BA	3285	1/1	0.94	0.52	57,57,57,57	0
52	MG	DA	3086	1/1	0.94	0.48	38,38,38,38	0
52	MG	DA	3087	1/1	0.94	0.30	55,55,55,55	0
52	MG	DA	3153	1/1	0.94	0.53	59,59,59,59	0
52	MG	DA	3061	1/1	0.94	0.29	57,57,57,57	0
52	MG	BA	3007	1/1	0.94	0.54	48,48,48,48	0
52	MG	BA	3325	1/1	0.94	0.41	43,43,43,43	0
52	MG	DA	3163	1/1	0.94	0.58	68,68,68,68	0
52	MG	AA	1629	1/1	0.94	0.56	67,67,67,67	0
52	MG	BA	3066	1/1	0.94	0.47	43,43,43,43	0
52	MG	DA	3049	1/1	0.94	0.35	35,35,35,35	0
52	MG	BA	3174	1/1	0.94	0.64	57,57,57,57	0
52	MG	DA	3117	1/1	0.94	0.10	59,59,59,59	0
52	MG	DA	3235	1/1	0.94	0.28	79,79,79,79	0
52	MG	AA	1609	1/1	0.94	0.27	51,51,51,51	0
52	MG	BA	3137	1/1	0.94	0.26	61,61,61,61	0
52	MG	CA	1615	1/1	0.94	0.61	67,67,67,67	0
52	MG	AA	1618	1/1	0.94	0.60	72,72,72,72	0
52	MG	DA	3183	1/1	0.94	0.38	44,44,44,44	0
52	MG	DA	3273	1/1	0.94	0.71	75,75,75,75	0
52	MG	DA	3133	1/1	0.94	0.59	53,53,53,53	0
52	MG	BA	3344	1/1	0.94	0.74	48,48,48,48	0
52	MG	BA	3027	1/1	0.94	0.47	42,42,42,42	0
52	MG	DA	3281	1/1	0.94	0.16	30,30,30,30	0
52	MG	DA	3189	1/1	0.94	0.51	63,63,63,63	0
52	MG	BA	3239	1/1	0.94	0.25	48,48,48,48	0
52	MG	DA	3214	1/1	0.94	0.38	65,65,65,65	0
52	MG	BA	3224	1/1	0.94	0.12	40,40,40,40	0
52	MG	DA	3109	1/1	0.94	0.40	71,71,71,71	0
52	MG	DA	3227	1/1	0.94	0.26	74,74,74,74	0
52	MG	CA	1620	1/1	0.94	0.35	66,66,66,66	0
52	MG	DA	3151	1/1	0.94	0.42	72,72,72,72	0
52	MG	AA	1625	1/1	0.94	0.18	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	AA	1624	1/1	0.94	0.38	56,56,56,56	0
52	MG	DA	3105	1/1	0.94	0.39	47,47,47,47	0
52	MG	BA	3003	1/1	0.94	0.42	43,43,43,43	0
52	MG	DA	3138	1/1	0.94	0.33	50,50,50,50	0
52	MG	BA	3118	1/1	0.94	0.31	59,59,59,59	0
52	MG	BA	3226	1/1	0.94	0.15	32,32,32,32	0
52	MG	DA	3084	1/1	0.94	0.18	54,54,54,54	0
52	MG	BA	3243	1/1	0.94	0.10	58,58,58,58	0
52	MG	DA	3174	1/1	0.94	0.56	63,63,63,63	0
52	MG	BA	3101	1/1	0.94	0.42	39,39,39,39	0
52	MG	DA	3289	1/1	0.94	0.34	92,92,92,92	0
52	MG	CA	1614	1/1	0.94	0.57	76,76,76,76	0
52	MG	CA	1642	1/1	0.94	0.27	62,62,62,62	0
52	MG	CA	1638	1/1	0.94	0.30	71,71,71,71	0
52	MG	AA	1601	1/1	0.94	0.19	58,58,58,58	0
52	MG	BA	3308	1/1	0.94	0.47	64,64,64,64	0
52	MG	DA	3121	1/1	0.94	0.17	37,37,37,37	0
52	MG	BA	3006	1/1	0.94	0.39	29,29,29,29	0
52	MG	DA	3209	1/1	0.95	0.56	59,59,59,59	0
52	MG	BA	3313	1/1	0.95	0.42	54,54,54,54	0
52	MG	BA	3094	1/1	0.95	0.39	52,52,52,52	0
52	MG	BA	3282	1/1	0.95	0.14	67,67,67,67	0
52	MG	DA	3090	1/1	0.95	0.41	76,76,76,76	0
52	MG	DA	3103	1/1	0.95	0.83	70,70,70,70	0
52	MG	DA	3286	1/1	0.95	0.50	58,58,58,58	0
52	MG	BA	3321	1/1	0.95	0.50	75,75,75,75	0
52	MG	DA	3205	1/1	0.95	0.51	54,54,54,54	0
52	MG	BA	3126	1/1	0.95	0.54	50,50,50,50	0
52	MG	DA	3118	1/1	0.95	0.16	66,66,66,66	0
52	MG	BA	3327	1/1	0.95	0.29	47,47,47,47	0
52	MG	DA	3098	1/1	0.95	0.18	49,49,49,49	0
52	MG	CA	1643	1/1	0.95	0.75	62,62,62,62	0
52	MG	DA	3142	1/1	0.95	0.45	41,41,41,41	0
52	MG	BA	3317	1/1	0.95	0.17	41,41,41,41	0
52	MG	BA	3263	1/1	0.95	0.58	62,62,62,62	0
52	MG	DA	3054	1/1	0.95	0.30	36,36,36,36	0
52	MG	BA	3324	1/1	0.95	0.42	59,59,59,59	0
52	MG	DA	3301	1/1	0.95	0.28	57,57,57,57	0
52	MG	BA	3166	1/1	0.95	0.61	39,39,39,39	0
52	MG	BA	3320	1/1	0.95	0.35	54,54,54,54	0
52	MG	BA	3120	1/1	0.95	0.46	52,52,52,52	0
52	MG	DA	3004	1/1	0.95	0.25	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3063	1/1	0.95	0.43	48,48,48,48	0
52	MG	DU	201	1/1	0.95	0.26	60,60,60,60	0
52	MG	CA	1640	1/1	0.95	0.25	68,68,68,68	0
52	MG	DA	3186	1/1	0.95	0.54	63,63,63,63	0
52	MG	BA	3272	1/1	0.95	0.31	51,51,51,51	0
52	MG	DA	3140	1/1	0.95	0.21	49,49,49,49	0
52	MG	BA	3262	1/1	0.95	0.14	75,75,75,75	0
52	MG	BA	3186	1/1	0.95	0.49	66,66,66,66	0
52	MG	BA	3346	1/1	0.95	0.43	80,80,80,80	0
52	MG	CA	1608	1/1	0.95	0.25	51,51,51,51	0
52	MG	DA	3123	1/1	0.95	0.13	61,61,61,61	0
52	MG	BA	3122	1/1	0.95	0.30	40,40,40,40	0
52	MG	BA	3104	1/1	0.95	0.42	37,37,37,37	0
52	MG	AA	1620	1/1	0.95	0.42	73,73,73,73	0
52	MG	CA	1603	1/1	0.95	0.52	63,63,63,63	0
52	MG	DA	3285	1/1	0.95	0.55	66,66,66,66	0
52	MG	BA	3012	1/1	0.95	0.30	22,22,22,22	0
52	MG	DA	3125	1/1	0.95	0.63	58,58,58,58	0
52	MG	BP	201	1/1	0.95	0.26	13,13,13,13	0
52	MG	D5	101	1/1	0.95	0.44	47,47,47,47	0
52	MG	BA	3133	1/1	0.95	0.49	35,35,35,35	0
52	MG	BA	3290	1/1	0.95	0.33	47,47,47,47	0
52	MG	DA	3015	1/1	0.95	0.36	23,23,23,23	0
52	MG	AA	1615	1/1	0.95	0.51	76,76,76,76	0
52	MG	BA	3117	1/1	0.95	0.40	39,39,39,39	0
52	MG	DA	3025	1/1	0.95	0.57	50,50,50,50	0
52	MG	BA	3284	1/1	0.95	0.32	71,71,71,71	0
52	MG	DA	3297	1/1	0.95	0.36	74,74,74,74	0
52	MG	CA	1641	1/1	0.95	0.81	87,87,87,87	0
52	MG	CA	1601	1/1	0.95	0.23	83,83,83,83	0
52	MG	DA	3180	1/1	0.95	0.49	52,52,52,52	0
52	MG	DA	3199	1/1	0.95	0.21	47,47,47,47	0
52	MG	BA	3339	1/1	0.95	0.16	41,41,41,41	0
52	MG	DA	3206	1/1	0.95	0.10	48,48,48,48	0
52	MG	CA	1637	1/1	0.95	0.91	80,80,80,80	0
52	MG	DA	3250	1/1	0.95	0.18	75,75,75,75	0
52	MG	BA	3172	1/1	0.95	0.20	64,64,64,64	0
52	MG	CA	1625	1/1	0.95	0.70	74,74,74,74	0
52	MG	BA	3209	1/1	0.95	0.56	56,56,56,56	0
52	MG	BA	3167	1/1	0.95	0.59	52,52,52,52	0
52	MG	DD	301	1/1	0.95	0.13	35,35,35,35	0
52	MG	AA	1606	1/1	0.95	0.74	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3184	1/1	0.95	0.45	50,50,50,50	0
52	MG	BA	3121	1/1	0.96	0.40	57,57,57,57	0
52	MG	DA	3045	1/1	0.96	0.48	39,39,39,39	0
52	MG	DA	3239	1/1	0.96	0.22	59,59,59,59	0
52	MG	DA	3053	1/1	0.96	0.60	51,51,51,51	0
52	MG	BA	3217	1/1	0.96	0.43	50,50,50,50	0
52	MG	BA	3108	1/1	0.96	0.39	56,56,56,56	0
52	MG	CA	1631	1/1	0.96	0.86	70,70,70,70	0
52	MG	DA	3237	1/1	0.96	0.17	53,53,53,53	0
52	MG	BA	3250	1/1	0.96	0.29	54,54,54,54	0
52	MG	B7	101	1/1	0.96	0.12	37,37,37,37	0
52	MG	BA	3131	1/1	0.96	0.21	45,45,45,45	0
52	MG	DA	3135	1/1	0.96	0.22	71,71,71,71	0
52	MG	AA	1649	1/1	0.96	0.47	86,86,86,86	0
52	MG	DA	3154	1/1	0.96	0.69	62,62,62,62	0
52	MG	DA	3204	1/1	0.96	0.45	45,45,45,45	0
52	MG	DA	3044	1/1	0.96	0.41	46,46,46,46	0
52	MG	DA	3122	1/1	0.96	0.23	61,61,61,61	0
52	MG	DA	3080	1/1	0.96	0.46	40,40,40,40	0
52	MG	CA	1613	1/1	0.96	0.20	80,80,80,80	0
52	MG	DA	3251	1/1	0.96	0.40	63,63,63,63	0
52	MG	BB	205	1/1	0.96	0.26	78,78,78,78	0
52	MG	DA	3190	1/1	0.96	0.39	63,63,63,63	0
52	MG	BA	3310	1/1	0.96	0.19	47,47,47,47	0
52	MG	BA	3165	1/1	0.96	0.56	50,50,50,50	0
52	MG	DA	3173	1/1	0.96	0.41	65,65,65,65	0
52	MG	DA	3022	1/1	0.96	0.39	47,47,47,47	0
52	MG	DA	3276	1/1	0.96	0.13	70,70,70,70	0
52	MG	BA	3073	1/1	0.96	0.33	53,53,53,53	0
52	MG	B0	101	1/1	0.96	0.16	34,34,34,34	0
52	MG	BA	3314	1/1	0.96	0.27	56,56,56,56	0
52	MG	BA	3065	1/1	0.96	0.31	32,32,32,32	0
52	MG	BA	3347	1/1	0.96	0.26	66,66,66,66	0
52	MG	BA	3299	1/1	0.96	0.46	58,58,58,58	0
52	MG	AA	1630	1/1	0.96	0.54	59,59,59,59	0
52	MG	BA	3275	1/1	0.96	0.23	47,47,47,47	0
52	MG	BA	3132	1/1	0.96	0.22	55,55,55,55	0
52	MG	AA	1634	1/1	0.96	0.33	58,58,58,58	0
52	MG	BA	3269	1/1	0.96	0.14	55,55,55,55	0
52	MG	BA	3115	1/1	0.96	0.24	49,49,49,49	0
52	MG	CA	1627	1/1	0.96	0.09	66,66,66,66	0
52	MG	DA	3160	1/1	0.96	0.29	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3207	1/1	0.96	0.19	23,23,23,23	0
52	MG	BA	3215	1/1	0.96	0.42	36,36,36,36	0
52	MG	B5	101	1/1	0.96	0.23	27,27,27,27	0
52	MG	BA	3105	1/1	0.96	0.48	46,46,46,46	0
52	MG	BA	3084	1/1	0.96	0.09	14,14,14,14	0
52	MG	BA	3124	1/1	0.96	0.16	42,42,42,42	0
52	MG	BA	3086	1/1	0.96	0.19	18,18,18,18	0
52	MG	BA	3164	1/1	0.96	0.27	47,47,47,47	0
52	MG	BA	3176	1/1	0.96	0.51	48,48,48,48	0
52	MG	DA	3047	1/1	0.96	0.51	45,45,45,45	0
52	MG	BA	3281	1/1	0.96	0.35	46,46,46,46	0
52	MG	BA	3158	1/1	0.96	0.41	49,49,49,49	0
52	MG	BA	3019	1/1	0.96	0.42	24,24,24,24	0
52	MG	DA	3144	1/1	0.96	0.39	47,47,47,47	0
52	MG	DA	3002	1/1	0.96	0.40	38,38,38,38	0
52	MG	DA	3074	1/1	0.96	0.23	53,53,53,53	0
52	MG	AA	1603	1/1	0.96	0.38	62,62,62,62	0
52	MG	BA	3092	1/1	0.96	0.65	52,52,52,52	0
52	MG	AA	1610	1/1	0.96	0.62	65,65,65,65	0
52	MG	DA	3093	1/1	0.96	0.31	64,64,64,64	0
52	MG	BA	3256	1/1	0.96	0.37	63,63,63,63	0
52	MG	BA	3198	1/1	0.96	0.48	44,44,44,44	0
52	MG	BA	3036	1/1	0.96	0.21	0,0,0,0	0
52	MG	BA	3231	1/1	0.96	0.65	52,52,52,52	0
52	MG	BA	3147	1/1	0.96	0.13	12,12,12,12	0
52	MG	AA	1643	1/1	0.96	0.10	78,78,78,78	0
52	MG	BA	3041	1/1	0.96	0.33	29,29,29,29	0
52	MG	BA	3042	1/1	0.96	0.27	15,15,15,15	0
52	MG	DA	3062	1/1	0.96	0.60	65,65,65,65	0
52	MG	DA	3064	1/1	0.96	0.36	68,68,68,68	0
52	MG	BA	3026	1/1	0.96	0.15	49,49,49,49	0
52	MG	DA	3046	1/1	0.96	0.34	28,28,28,28	0
52	MG	BA	3064	1/1	0.96	0.23	28,28,28,28	0
52	MG	BA	3015	1/1	0.96	0.33	48,48,48,48	0
52	MG	BA	3251	1/1	0.96	0.16	35,35,35,35	0
52	MG	CA	1645	1/1	0.96	0.46	97,97,97,97	0
52	MG	BA	3270	1/1	0.96	0.23	50,50,50,50	0
52	MG	BA	3085	1/1	0.96	0.22	40,40,40,40	0
52	MG	BA	3039	1/1	0.96	0.74	60,60,60,60	0
52	MG	BB	204	1/1	0.96	0.54	56,56,56,56	0
52	MG	DA	3003	1/1	0.96	0.70	56,56,56,56	0
52	MG	BA	3181	1/1	0.96	0.39	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3089	1/1	0.96	0.44	26,26,26,26	0
52	MG	DA	3040	1/1	0.96	0.24	43,43,43,43	0
52	MG	DP	201	1/1	0.96	0.18	50,50,50,50	0
52	MG	BA	3273	1/1	0.96	0.51	58,58,58,58	0
52	MG	BA	3119	1/1	0.96	0.24	52,52,52,52	0
52	MG	AA	1642	1/1	0.96	0.32	51,51,51,51	0
52	MG	DA	3114	1/1	0.96	0.35	65,65,65,65	0
52	MG	BA	3113	1/1	0.96	0.35	26,26,26,26	0
52	MG	DA	3166	1/1	0.96	0.40	46,46,46,46	0
52	MG	AA	1631	1/1	0.97	0.11	60,60,60,60	0
52	MG	DA	3130	1/1	0.97	0.33	43,43,43,43	0
52	MG	DA	3271	1/1	0.97	0.16	46,46,46,46	0
52	MG	DA	3027	1/1	0.97	0.41	61,61,61,61	0
52	MG	BA	3248	1/1	0.97	0.16	47,47,47,47	0
52	MG	DA	3078	1/1	0.97	0.65	46,46,46,46	0
52	MG	BA	3014	1/1	0.97	0.41	32,32,32,32	0
52	MG	BA	3171	1/1	0.97	0.33	62,62,62,62	0
52	MG	BA	3080	1/1	0.97	0.52	34,34,34,34	0
52	MG	BA	3258	1/1	0.97	0.33	61,61,61,61	0
52	MG	BA	3025	1/1	0.97	0.33	54,54,54,54	0
52	MG	DA	3019	1/1	0.97	0.34	42,42,42,42	0
52	MG	BA	3038	1/1	0.97	0.47	25,25,25,25	0
52	MG	BA	3254	1/1	0.97	0.21	53,53,53,53	0
52	MG	AA	1616	1/1	0.97	0.19	77,77,77,77	0
52	MG	BA	3264	1/1	0.97	0.22	35,35,35,35	0
52	MG	BA	3060	1/1	0.97	0.38	40,40,40,40	0
52	MG	BA	3146	1/1	0.97	0.52	42,42,42,42	0
52	MG	DA	3212	1/1	0.97	0.10	68,68,68,68	0
52	MG	BA	3062	1/1	0.97	0.39	44,44,44,44	0
52	MG	BP	203	1/1	0.97	0.11	0,0,0,0	0
52	MG	DA	3052	1/1	0.97	0.39	63,63,63,63	0
52	MG	DA	3128	1/1	0.97	0.65	51,51,51,51	0
52	MG	BA	3107	1/1	0.97	0.10	34,34,34,34	0
52	MG	CA	1639	1/1	0.97	0.20	64,64,64,64	0
52	MG	DA	3131	1/1	0.97	0.59	47,47,47,47	0
52	MG	BA	3109	1/1	0.97	0.42	34,34,34,34	0
52	MG	AA	1621	1/1	0.97	0.37	46,46,46,46	0
52	MG	DA	3028	1/1	0.97	0.25	39,39,39,39	0
52	MG	AA	1617	1/1	0.97	0.40	64,64,64,64	0
52	MG	BA	3078	1/1	0.97	0.22	34,34,34,34	0
52	MG	BA	3292	1/1	0.97	0.79	60,60,60,60	0
52	MG	BA	3179	1/1	0.97	0.18	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3161	1/1	0.97	0.35	42,42,42,42	0
52	MG	BA	3155	1/1	0.97	0.41	41,41,41,41	0
52	MG	BA	3034	1/1	0.97	0.34	62,62,62,62	0
52	MG	DA	3169	1/1	0.97	0.79	51,51,51,51	0
52	MG	BA	3077	1/1	0.97	0.41	28,28,28,28	0
52	MG	B5	102	1/1	0.97	0.42	56,56,56,56	0
52	MG	DA	3068	1/1	0.97	0.41	49,49,49,49	0
52	MG	DA	3081	1/1	0.97	0.40	43,43,43,43	0
52	MG	BB	202	1/1	0.97	0.27	30,30,30,30	0
52	MG	BA	3052	1/1	0.97	0.29	15,15,15,15	0
52	MG	BA	3058	1/1	0.97	0.39	39,39,39,39	0
52	MG	AA	1636	1/1	0.97	0.18	63,63,63,63	0
52	MG	BA	3286	1/1	0.97	0.06	45,45,45,45	0
52	MG	BA	3234	1/1	0.97	0.42	45,45,45,45	0
52	MG	DA	3031	1/1	0.97	0.34	47,47,47,47	0
52	MG	DA	3035	1/1	0.97	0.80	54,54,54,54	0
52	MG	DA	3178	1/1	0.97	0.41	65,65,65,65	0
52	MG	DA	3048	1/1	0.97	0.25	40,40,40,40	0
52	MG	DA	3139	1/1	0.97	0.38	68,68,68,68	0
52	MG	BA	3316	1/1	0.97	0.16	56,56,56,56	0
52	MG	BA	3204	1/1	0.97	0.26	46,46,46,46	0
52	MG	BA	3008	1/1	0.97	0.49	34,34,34,34	0
52	MG	DA	3132	1/1	0.97	0.42	43,43,43,43	0
52	MG	DA	3221	1/1	0.97	0.44	53,53,53,53	0
52	MG	BA	3173	1/1	0.97	0.37	24,24,24,24	0
52	MG	BA	3093	1/1	0.97	0.59	43,43,43,43	0
52	MG	BA	3160	1/1	0.97	0.36	39,39,39,39	0
52	MG	CA	1648	1/1	0.97	0.16	79,79,79,79	0
52	MG	DA	3185	1/1	0.97	0.38	61,61,61,61	0
52	MG	DA	3299	1/1	0.97	0.30	66,66,66,66	0
52	MG	BA	3018	1/1	0.97	0.20	26,26,26,26	0
52	MG	DA	3056	1/1	0.97	0.32	60,60,60,60	0
52	MG	BA	3211	1/1	0.97	0.16	39,39,39,39	0
52	MG	BA	3300	1/1	0.97	0.50	59,59,59,59	0
52	MG	BA	3070	1/1	0.97	0.35	35,35,35,35	0
52	MG	BA	3020	1/1	0.97	0.44	38,38,38,38	0
52	MG	DA	3051	1/1	0.97	0.38	26,26,26,26	0
52	MG	DA	3134	1/1	0.97	0.55	47,47,47,47	0
52	MG	DA	3065	1/1	0.97	0.23	49,49,49,49	0
52	MG	DA	3234	1/1	0.97	0.63	60,60,60,60	0
52	MG	BA	3301	1/1	0.97	0.16	57,57,57,57	0
52	MG	BA	3090	1/1	0.97	0.16	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3088	1/1	0.97	0.52	34,34,34,34	0
52	MG	DA	3156	1/1	0.97	0.41	44,44,44,44	0
52	MG	BA	3154	1/1	0.97	0.25	32,32,32,32	0
52	MG	DA	3159	1/1	0.97	0.47	61,61,61,61	0
52	MG	DA	3101	1/1	0.97	0.35	43,43,43,43	0
52	MG	DA	3012	1/1	0.97	0.35	23,23,23,23	0
52	MG	BA	3031	1/1	0.97	0.33	77,77,77,77	0
52	MG	BA	3110	1/1	0.97	0.45	45,45,45,45	0
52	MG	BA	3067	1/1	0.97	0.58	37,37,37,37	0
52	MG	BA	3076	1/1	0.97	0.28	43,43,43,43	0
52	MG	BA	3142	1/1	0.97	0.62	39,39,39,39	0
52	MG	BA	3141	1/1	0.97	0.43	27,27,27,27	0
52	MG	AA	1623	1/1	0.97	0.42	54,54,54,54	0
52	MG	BA	3216	1/1	0.97	0.41	43,43,43,43	0
52	MG	BA	3175	1/1	0.97	0.08	49,49,49,49	0
52	MG	BA	3028	1/1	0.97	0.35	28,28,28,28	0
52	MG	BA	3123	1/1	0.97	0.45	22,22,22,22	0
52	MG	BA	3098	1/1	0.97	0.27	46,46,46,46	0
52	MG	DA	3124	1/1	0.97	0.32	83,83,83,83	0
52	MG	BA	3046	1/1	0.97	0.25	37,37,37,37	0
52	MG	DA	3057	1/1	0.97	0.48	40,40,40,40	0
52	MG	DA	3215	1/1	0.97	0.42	59,59,59,59	0
52	MG	DA	3193	1/1	0.97	0.49	50,50,50,50	0
52	MG	BA	3103	1/1	0.97	0.21	42,42,42,42	0
52	MG	BA	3185	1/1	0.98	0.30	14,14,14,14	0
52	MG	BA	3169	1/1	0.98	0.37	46,46,46,46	0
52	MG	BA	3244	1/1	0.98	0.34	40,40,40,40	0
52	MG	BA	3222	1/1	0.98	0.24	23,23,23,23	0
52	MG	DA	3300	1/1	0.98	0.05	75,75,75,75	0
52	MG	DA	3095	1/1	0.98	0.52	53,53,53,53	0
52	MG	BA	3139	1/1	0.98	0.28	24,24,24,24	0
52	MG	BA	3057	1/1	0.98	0.36	44,44,44,44	0
52	MG	DA	3181	1/1	0.98	0.34	50,50,50,50	0
52	MG	AA	1605	1/1	0.98	0.27	75,75,75,75	0
52	MG	DA	3071	1/1	0.98	0.36	40,40,40,40	0
52	MG	BA	3048	1/1	0.98	0.48	30,30,30,30	0
52	MG	BA	3075	1/1	0.98	0.19	26,26,26,26	0
52	MG	BA	3342	1/1	0.98	0.21	49,49,49,49	0
52	MG	DA	3073	1/1	0.98	0.23	42,42,42,42	0
52	MG	DA	3148	1/1	0.98	0.35	48,48,48,48	0
52	MG	DA	3050	1/1	0.98	0.34	42,42,42,42	0
52	MG	DA	3066	1/1	0.98	0.51	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	BA	3127	1/1	0.98	0.14	50,50,50,50	0
52	MG	BA	3193	1/1	0.98	0.28	28,28,28,28	0
52	MG	DA	3236	1/1	0.98	0.42	67,67,67,67	0
52	MG	DA	3283	1/1	0.98	0.45	72,72,72,72	0
52	MG	DA	3253	1/1	0.98	0.40	50,50,50,50	0
52	MG	BA	3011	1/1	0.98	0.31	7,7,7,7	0
52	MG	DA	3043	1/1	0.98	0.40	35,35,35,35	0
52	MG	DA	3136	1/1	0.98	0.51	59,59,59,59	0
52	MG	DA	3240	1/1	0.98	0.46	89,89,89,89	0
52	MG	BA	3247	1/1	0.98	0.06	40,40,40,40	0
52	MG	BU	201	1/1	0.98	0.33	26,26,26,26	0
52	MG	DA	3089	1/1	0.98	0.60	47,47,47,47	0
52	MG	DA	3111	1/1	0.98	0.49	71,71,71,71	0
52	MG	DA	3187	1/1	0.98	0.20	52,52,52,52	0
52	MG	BA	3099	1/1	0.98	0.25	26,26,26,26	0
52	MG	BA	3056	1/1	0.98	0.17	20,20,20,20	0
52	MG	DA	3293	1/1	0.98	0.14	53,53,53,53	0
52	MG	BA	3013	1/1	0.98	0.35	21,21,21,21	0
52	MG	DA	3104	1/1	0.98	0.58	48,48,48,48	0
52	MG	DA	3018	1/1	0.98	0.55	32,32,32,32	0
52	MG	DA	3006	1/1	0.98	0.44	39,39,39,39	0
52	MG	DA	3063	1/1	0.98	0.24	47,47,47,47	0
52	MG	BA	3261	1/1	0.98	0.34	38,38,38,38	0
52	MG	BA	3100	1/1	0.98	0.27	21,21,21,21	0
52	MG	BA	3054	1/1	0.98	0.19	68,68,68,68	0
52	MG	D1	101	1/1	0.98	0.25	50,50,50,50	0
52	MG	B1	101	1/1	0.98	0.25	39,39,39,39	0
52	MG	DA	3176	1/1	0.98	0.20	78,78,78,78	0
52	MG	BA	3069	1/1	0.98	0.27	18,18,18,18	0
52	MG	DA	3127	1/1	0.98	0.42	35,35,35,35	0
52	MG	DA	3107	1/1	0.98	0.44	38,38,38,38	0
52	MG	BA	3035	1/1	0.98	0.26	21,21,21,21	0
52	MG	BA	3130	1/1	0.98	0.24	26,26,26,26	0
52	MG	BB	203	1/1	0.98	0.35	41,41,41,41	0
52	MG	BA	3053	1/1	0.98	0.38	15,15,15,15	0
52	MG	BA	3050	1/1	0.98	0.28	38,38,38,38	0
52	MG	BA	3194	1/1	0.98	0.50	44,44,44,44	0
52	MG	DA	3097	1/1	0.98	0.33	44,44,44,44	0
52	MG	BA	3002	1/1	0.98	0.24	20,20,20,20	0
52	MG	BA	3043	1/1	0.98	0.15	36,36,36,36	0
52	MG	BA	3257	1/1	0.98	0.33	48,48,48,48	0
52	MG	DA	3021	1/1	0.98	0.38	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3172	1/1	0.98	0.56	64,64,64,64	0
52	MG	BQ	201	1/1	0.98	0.17	32,32,32,32	0
52	MG	DA	3026	1/1	0.98	0.28	43,43,43,43	0
52	MG	CA	1621	1/1	0.98	0.18	68,68,68,68	0
52	MG	DA	3032	1/1	0.98	0.40	69,69,69,69	0
52	MG	DA	3023	1/1	0.98	0.24	47,47,47,47	0
52	MG	DA	3141	1/1	0.98	0.49	61,61,61,61	0
52	MG	BA	3017	1/1	0.98	0.35	32,32,32,32	0
52	MG	DA	3034	1/1	0.98	0.49	39,39,39,39	0
52	MG	BA	3265	1/1	0.98	0.36	63,63,63,63	0
52	MG	BA	3005	1/1	0.98	0.39	47,47,47,47	0
52	MG	BE	301	1/1	0.98	0.46	29,29,29,29	0
52	MG	BA	3252	1/1	0.98	0.31	50,50,50,50	0
52	MG	BA	3059	1/1	0.98	0.30	39,39,39,39	0
52	MG	BA	3016	1/1	0.98	0.26	21,21,21,21	0
52	MG	BA	3199	1/1	0.98	0.57	49,49,49,49	0
52	MG	BA	3242	1/1	0.98	0.20	48,48,48,48	0
52	MG	BA	3045	1/1	0.98	0.34	26,26,26,26	0
52	MG	BA	3210	1/1	0.98	0.31	37,37,37,37	0
52	MG	BA	3266	1/1	0.98	0.38	35,35,35,35	0
52	MG	BA	3213	1/1	0.98	0.56	32,32,32,32	0
52	MG	BA	3004	1/1	0.98	0.23	23,23,23,23	0
52	MG	DA	3042	1/1	0.98	0.38	47,47,47,47	0
52	MG	DA	3075	1/1	0.98	0.54	55,55,55,55	0
52	MG	DA	3116	1/1	0.98	0.58	41,41,41,41	0
52	MG	DA	3007	1/1	0.98	0.37	39,39,39,39	0
52	MG	BA	3260	1/1	0.98	0.42	42,42,42,42	0
52	MG	BA	3037	1/1	0.98	0.32	14,14,14,14	0
52	MG	DA	3296	1/1	0.98	0.08	60,60,60,60	0
52	MG	BA	3150	1/1	0.98	0.44	50,50,50,50	0
52	MG	BA	3044	1/1	0.98	0.38	26,26,26,26	0
52	MG	BA	3143	1/1	0.98	0.38	30,30,30,30	0
52	MG	DA	3030	1/1	0.98	0.40	42,42,42,42	0
52	MG	BA	3030	1/1	0.98	0.25	17,17,17,17	0
52	MG	DA	3008	1/1	0.98	0.39	52,52,52,52	0
52	MG	DA	3232	1/1	0.98	0.29	72,72,72,72	0
52	MG	DA	3137	1/1	0.98	0.41	38,38,38,38	0
52	MG	BA	3218	1/1	0.98	0.49	33,33,33,33	0
52	MG	DA	3036	1/1	0.98	0.48	39,39,39,39	0
52	MG	BA	3267	1/1	0.98	0.35	38,38,38,38	0
52	MG	BA	3271	1/1	0.98	0.30	46,46,46,46	0
52	MG	BA	3233	1/1	0.98	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3184	1/1	0.98	0.41	63,63,63,63	0
52	MG	BA	3023	1/1	0.98	0.35	34,34,34,34	0
52	MG	AA	1602	1/1	0.98	0.47	37,37,37,37	0
52	MG	BA	3106	1/1	0.98	0.16	12,12,12,12	0
52	MG	BA	3079	1/1	0.99	0.35	0,0,0,0	0
52	MG	BA	3187	1/1	0.99	0.50	42,42,42,42	0
52	MG	DA	3055	1/1	0.99	0.37	42,42,42,42	0
53	ZN	AD	301	1/1	0.99	0.31	108,108,108,108	0
52	MG	BA	3203	1/1	0.99	0.39	35,35,35,35	0
52	MG	BA	3010	1/1	0.99	0.43	38,38,38,38	0
52	MG	DA	3099	1/1	0.99	0.58	46,46,46,46	0
52	MG	BA	3021	1/1	0.99	0.31	16,16,16,16	0
53	ZN	CD	301	1/1	0.99	0.26	93,93,93,93	0
52	MG	BA	3153	1/1	0.99	0.48	25,25,25,25	0
52	MG	BA	3091	1/1	0.99	0.30	9,9,9,9	0
52	MG	DA	3274	1/1	0.99	0.27	63,63,63,63	0
52	MG	BA	3095	1/1	0.99	0.51	38,38,38,38	0
52	MG	BA	3276	1/1	0.99	0.44	55,55,55,55	0
52	MG	BA	3225	1/1	0.99	0.29	33,33,33,33	0
52	MG	DA	3014	1/1	0.99	0.40	68,68,68,68	0
52	MG	DA	3009	1/1	0.99	0.49	54,54,54,54	0
52	MG	DA	3287	1/1	0.99	0.17	51,51,51,51	0
52	MG	BA	3033	1/1	0.99	0.17	20,20,20,20	0
52	MG	DA	3091	1/1	0.99	0.53	41,41,41,41	0
52	MG	DA	3076	1/1	0.99	0.33	55,55,55,55	0
52	MG	BR	201	1/1	0.99	0.34	20,20,20,20	0
52	MG	BA	3083	1/1	0.99	0.21	5,5,5,5	0
52	MG	BA	3061	1/1	0.99	0.15	23,23,23,23	0
52	MG	BA	3291	1/1	0.99	0.60	54,54,54,54	0
52	MG	DA	3010	1/1	0.99	0.39	31,31,31,31	0
52	MG	BA	3212	1/1	0.99	0.45	30,30,30,30	0
52	MG	BA	3135	1/1	0.99	0.29	8,8,8,8	0
52	MG	BA	3029	1/1	0.99	0.23	26,26,26,26	0
52	MG	BA	3047	1/1	0.99	0.45	21,21,21,21	0
52	MG	BA	3168	1/1	0.99	0.09	43,43,43,43	0
52	MG	BA	3322	1/1	0.99	0.22	20,20,20,20	0
52	MG	BA	3032	1/1	0.99	0.32	15,15,15,15	0
52	MG	CA	1616	1/1	0.99	0.52	73,73,73,73	0
52	MG	BA	3072	1/1	0.99	0.30	24,24,24,24	0
52	MG	BA	3134	1/1	0.99	0.17	46,46,46,46	0
52	MG	BA	3177	1/1	0.99	0.42	52,52,52,52	0
52	MG	BA	3206	1/1	0.99	0.51	29,29,29,29	0

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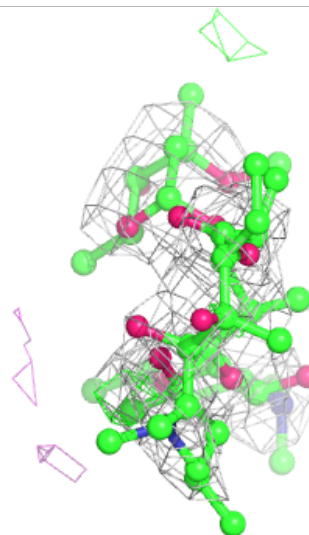
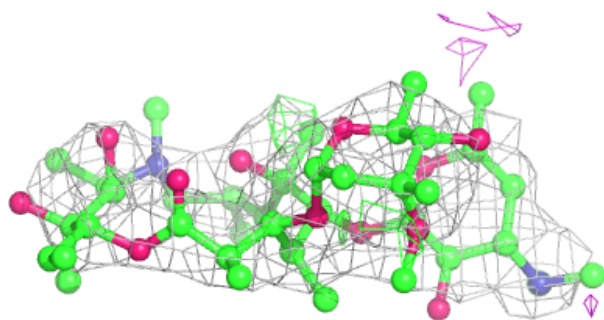
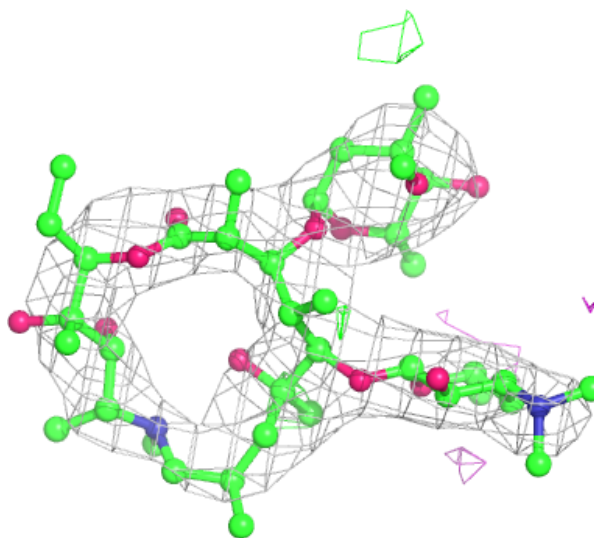
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
52	MG	DA	3213	1/1	0.99	0.46	36,36,36,36	0
52	MG	BA	3024	1/1	0.99	0.20	2,2,2,2	0
52	MG	DA	3060	1/1	0.99	0.10	34,34,34,34	0
52	MG	DA	3039	1/1	0.99	0.33	43,43,43,43	0
52	MG	DA	3033	1/1	0.99	0.41	44,44,44,44	0
52	MG	BA	3220	1/1	0.99	0.46	27,27,27,27	0
52	MG	BA	3055	1/1	0.99	0.28	19,19,19,19	0
52	MG	BA	3201	1/1	0.99	0.34	29,29,29,29	0
52	MG	BA	3051	1/1	0.99	0.31	14,14,14,14	0
52	MG	DA	3077	1/1	0.99	0.69	49,49,49,49	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.

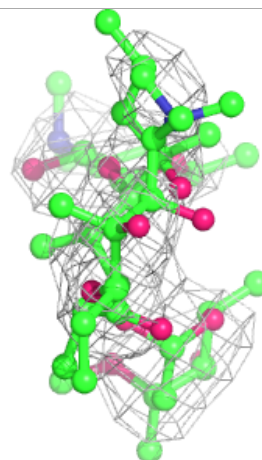
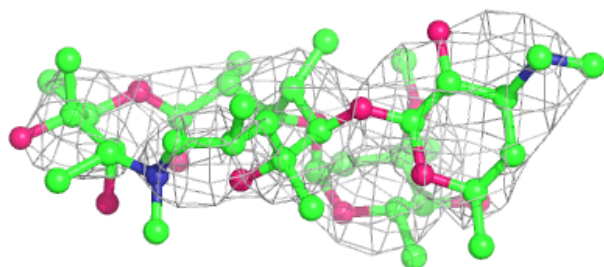
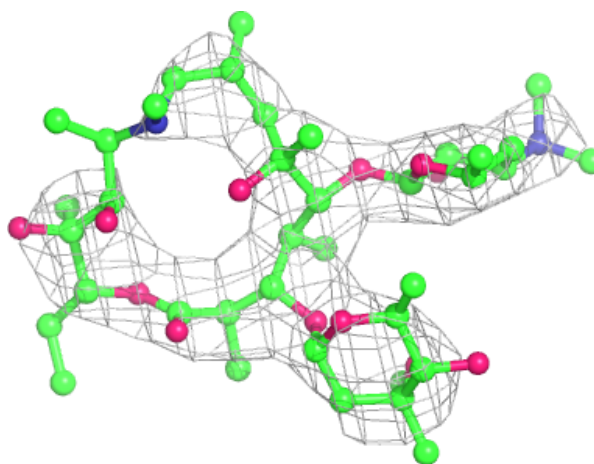
Electron density around ZIT BA 3351:

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



Electron density around ZIT DA 3311:

$2mF_o-DF_c$ (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.