



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2024 – 01:01 AM EDT

PDB ID : 2AAZ
Title : *Cryptococcus neoformans* thymidylate synthase complexed with substrate and an antifolate
Authors : Finer-Moore, J.S.; Anderson, A.C.; O'Neil, R.H.; Costi, M.P.; Ferrari, S.; Krucinski, J.; Stroud, R.M.
Deposited on : 2005-07-14
Resolution : 2.08 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

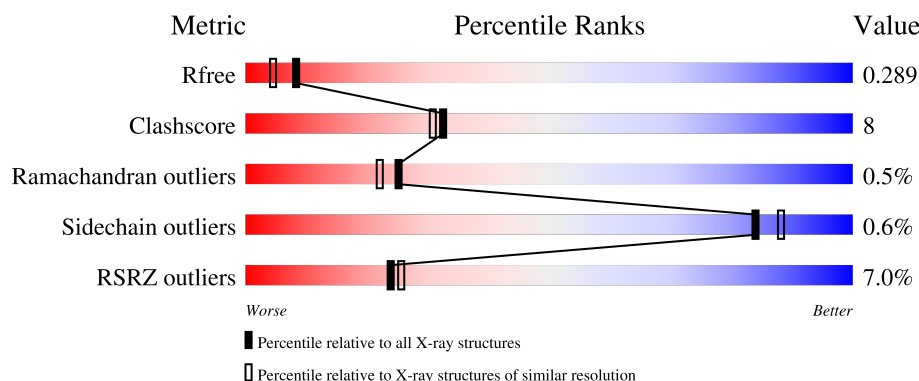
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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}	164625	7574 (2.10-2.06)
Clashscore	180529	8325 (2.10-2.06)
Ramachandran outliers	177936	8271 (2.10-2.06)
Sidechain outliers	177891	8272 (2.10-2.06)
RSRZ outliers	164620	7574 (2.10-2.06)

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

Mol	Chain	Length	Quality of chain
1	1-A	317	<div> <div>2%</div> <div>77%</div> <div>18%</div> <div>• •</div> </div>
1	1-B	317	<div> <div>2%</div> <div>81%</div> <div>15%</div> <div>• •</div> </div>
1	1-C	317	<div> <div>3%</div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	1-D	317	<div> <div>0%</div> <div>79%</div> <div>15%</div> <div>• •</div> </div>


























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Mol	Chain	Length	Quality of chain
1	1-E	317	
1	1-F	317	
1	1-G	317	
1	1-H	317	
1	1-I	317	
1	1-J	317	
1	1-K	317	
1	1-L	317	
1	1-M	317	
1	1-N	317	
1	1-O	317	
1	1-P	317	
1	2-A	317	
1	2-B	317	
1	2-C	317	
1	2-D	317	
1	2-E	317	
1	2-F	317	
1	2-G	317	
1	2-H	317	
1	2-I	317	
1	2-J	317	
1	2-K	317	
1	2-L	317	
1	2-M	317	











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Mol	Chain	Length	Quality of chain
1	2-N	317	
1	2-O	317	
1	2-P	317	
1	3-A	317	
1	3-B	317	
1	3-C	317	
1	3-D	317	
1	3-E	317	
1	3-F	317	
1	3-G	317	
1	3-H	317	
1	3-I	317	
1	3-J	317	
1	3-K	317	
1	3-L	317	
1	3-M	317	
1	3-N	317	
1	3-O	317	
1	3-P	317	
1	4-A	317	
1	4-B	317	
1	4-C	317	
1	4-D	317	
1	4-E	317	
1	4-F	317	

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Mol	Chain	Length	Quality of chain
1	4-G	317	 85% 12% •
1	4-H	317	 80% 16% • •
1	4-I	317	 79% 15% 6%
1	4-J	317	 78% 16% 6%
1	4-K	317	 76% 18% 6%
1	4-L	317	 78% 16% 6%
1	4-M	317	 78% 16% 6%
1	4-N	317	 78% 16% 6%
1	4-O	317	 77% 17% 6%
1	4-P	317	 78% 17% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 161392 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 protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	2-A	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	3-A	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	4-A	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	1-B	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	2-B	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	3-B	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	4-B	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	1-C	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	2-C	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	3-C	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	4-C	305	Total	C	N	O	S	0	305	0
			2427	1553	419	442	13			
1	1-D	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	2-D	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	3-D	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	4-D	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-E	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	2-E	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	3-E	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	4-E	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	1-F	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	2-F	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	3-F	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	4-F	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	1-G	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	2-G	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	3-G	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	4-G	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	1-H	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	2-H	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	3-H	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	4-H	305	Total	C	N	O	S	0	305	0
			2431	1555	419	444	13			
1	1-I	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	2-I	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	3-I	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	4-I	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	1-J	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			

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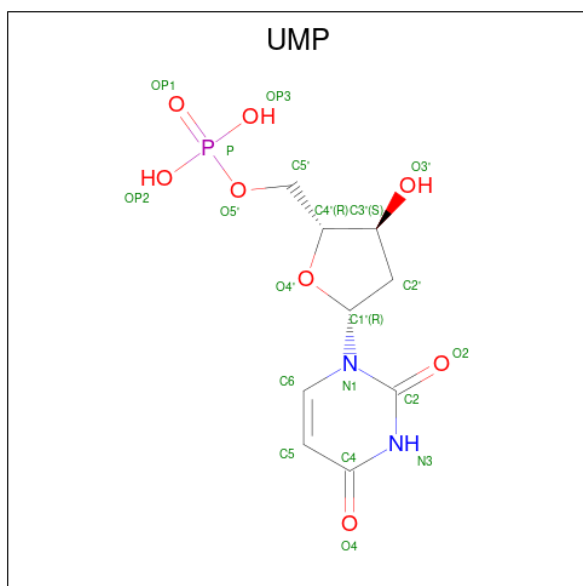
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2-J	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	3-J	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	4-J	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	1-K	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	2-K	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	3-K	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	4-K	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	1-L	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	2-L	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	3-L	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	4-L	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	1-M	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	2-M	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	3-M	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	4-M	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	1-N	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	2-N	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	3-N	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	4-N	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	1-O	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0
1	2-O	299	Total 2387	C 1532	N 409	O 433	S 13	0	299	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	3-O	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	4-O	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	1-P	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	2-P	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	3-P	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			
1	4-P	299	Total	C	N	O	S	0	299	0
			2387	1532	409	433	13			

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-A	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-A	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-A	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-B	1	Total	C	N	O	P	0	1
			20	9	2	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	2-B	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	3-B	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	4-B	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	1-C	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	2-C	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	3-C	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	4-C	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	1-D	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	2-D	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	3-D	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	4-D	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	1-E	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	2-E	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	3-E	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	4-E	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	1-F	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	2-F	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	3-F	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	4-F	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	1-G	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	2-G	1	Total 20	C 9	N 2	O 8	P 1	0	1

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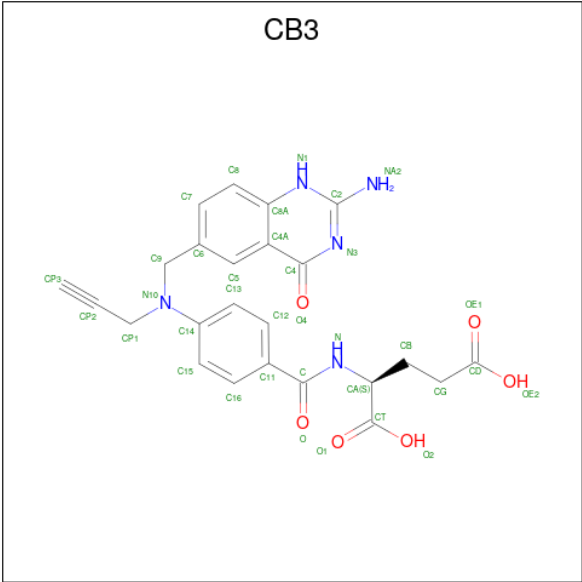
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	3-G	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	4-G	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	1-H	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	2-H	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	3-H	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	4-H	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	1-I	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	2-I	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	3-I	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	4-I	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	1-J	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	2-J	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	3-J	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	4-J	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	1-K	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	2-K	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	3-K	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	4-K	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	1-L	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	2-L	1	Total 20	C 9	N 2	O 8	P 1	0	1
2	3-L	1	Total 20	C 9	N 2	O 8	P 1	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	4-L	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-M	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-M	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-M	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-M	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-N	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-N	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-N	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-N	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-O	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-O	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-O	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-O	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	1-P	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	2-P	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	3-P	1	Total	C	N	O	P	0	1
			20	9	2	8	1		
2	4-P	1	Total	C	N	O	P	0	1
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula: C₂₄H₂₃N₅O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	0	1
			35	24	5	6		
3	2-A	1	Total	C	N	O	0	1
			35	24	5	6		
3	3-A	1	Total	C	N	O	0	1
			35	24	5	6		
3	4-A	1	Total	C	N	O	0	1
			35	24	5	6		
3	1-B	1	Total	C	N	O	0	1
			35	24	5	6		
3	2-B	1	Total	C	N	O	0	1
			35	24	5	6		
3	3-B	1	Total	C	N	O	0	1
			35	24	5	6		
3	4-B	1	Total	C	N	O	0	1
			35	24	5	6		
3	1-C	1	Total	C	N	O	0	1
			35	24	5	6		
3	2-C	1	Total	C	N	O	0	1
			35	24	5	6		
3	3-C	1	Total	C	N	O	0	1
			35	24	5	6		
3	4-C	1	Total	C	N	O	0	1
			35	24	5	6		
3	1-D	1	Total	C	N	O	0	1
			35	24	5	6		
3	2-D	1	Total	C	N	O	0	1
			35	24	5	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	3-D	1	Total	C	N	O	0	1
			35	24	5	6		
3	4-D	1	Total	C	N	O	0	1
			35	24	5	6		
3	1-E	1	Total	C	N	O	0	1
			35	24	5	6		
3	2-E	1	Total	C	N	O	0	1
			35	24	5	6		
3	3-E	1	Total	C	N	O	0	1
			35	24	5	6		
3	4-E	1	Total	C	N	O	0	1
			35	24	5	6		
3	1-F	1	Total	C	N	O	0	1
			35	24	5	6		
3	2-F	1	Total	C	N	O	0	1
			35	24	5	6		
3	3-F	1	Total	C	N	O	0	1
			35	24	5	6		
3	4-F	1	Total	C	N	O	0	1
			35	24	5	6		
3	1-G	1	Total	C	N	O	0	1
			35	24	5	6		
3	2-G	1	Total	C	N	O	0	1
			35	24	5	6		
3	3-G	1	Total	C	N	O	0	1
			35	24	5	6		
3	4-G	1	Total	C	N	O	0	1
			35	24	5	6		
3	1-H	1	Total	C	N	O	0	1
			35	24	5	6		
3	2-H	1	Total	C	N	O	0	1
			35	24	5	6		
3	3-H	1	Total	C	N	O	0	1
			35	24	5	6		
3	4-H	1	Total	C	N	O	0	1
			35	24	5	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	185	Total	O	0	185
			185	185		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	2-A	185	Total 185	O 185	0	185
4	3-A	185	Total 185	O 185	0	185
4	4-A	185	Total 185	O 185	0	185
4	1-B	143	Total 143	O 143	0	143
4	2-B	143	Total 143	O 143	0	143
4	3-B	143	Total 143	O 143	0	143
4	4-B	143	Total 143	O 143	0	143
4	1-C	151	Total 151	O 151	0	151
4	2-C	151	Total 151	O 151	0	151
4	3-C	151	Total 151	O 151	0	151
4	4-C	151	Total 151	O 151	0	151
4	1-D	148	Total 148	O 148	0	148
4	2-D	148	Total 148	O 148	0	148
4	3-D	148	Total 148	O 148	0	148
4	4-D	148	Total 148	O 148	0	148
4	1-E	155	Total 155	O 155	0	155
4	2-E	155	Total 155	O 155	0	155
4	3-E	155	Total 155	O 155	0	155
4	4-E	155	Total 155	O 155	0	155
4	1-F	138	Total 138	O 138	0	138
4	2-F	138	Total 138	O 138	0	138

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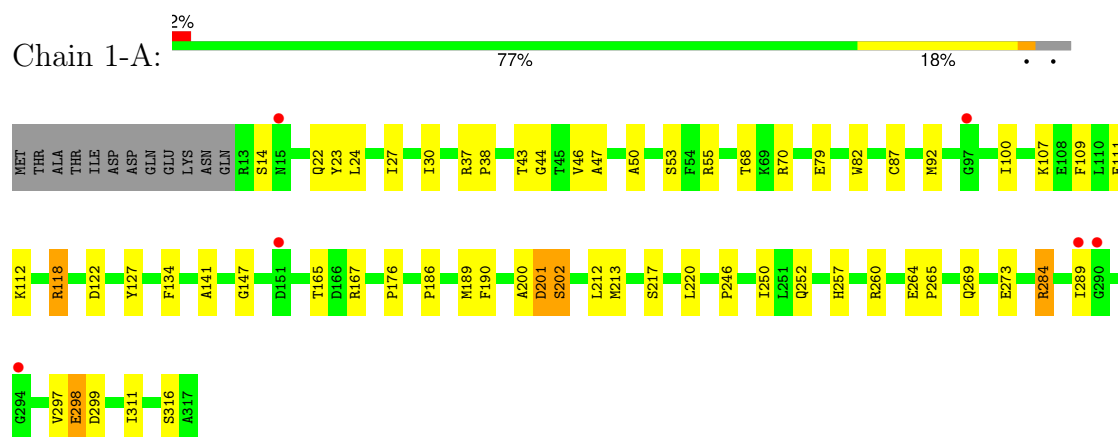
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	3-F	138	Total 138	O 138	0	138
4	4-F	138	Total 138	O 138	0	138
4	1-G	153	Total 153	O 153	0	153
4	2-G	153	Total 153	O 153	0	153
4	3-G	153	Total 153	O 153	0	153
4	4-G	153	Total 153	O 153	0	153
4	1-H	139	Total 139	O 139	0	139
4	2-H	139	Total 139	O 139	0	139
4	3-H	139	Total 139	O 139	0	139
4	4-H	139	Total 139	O 139	0	139

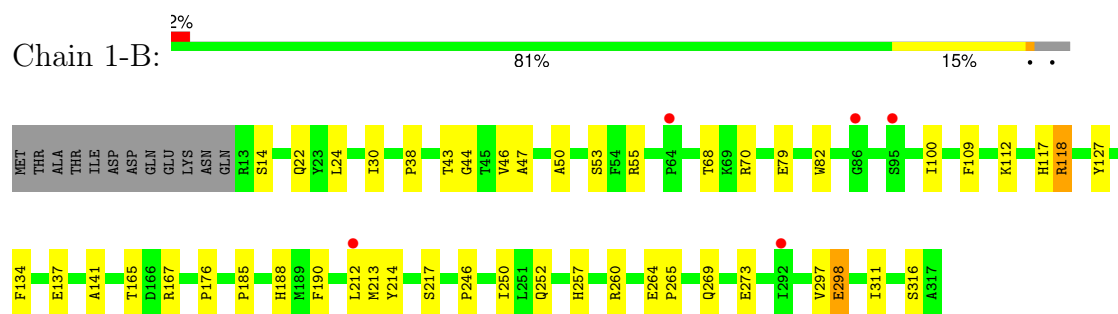
3 Residue-property plots [i](#)

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

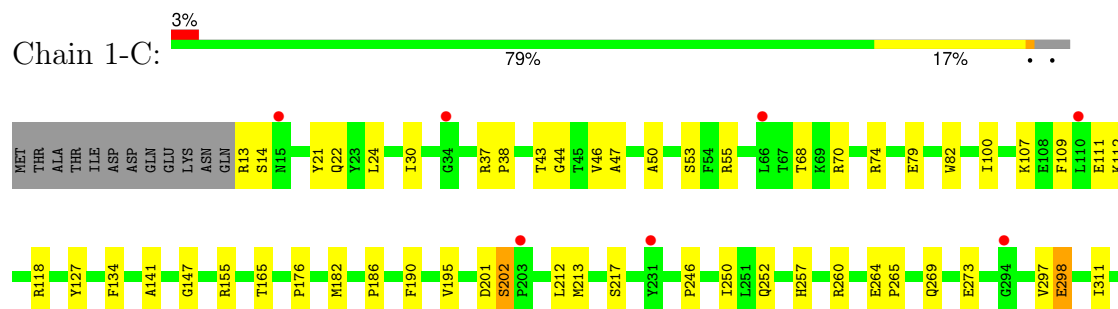
- Molecule 1: Thymidylate synthase



- Molecule 1: Thymidylate synthase

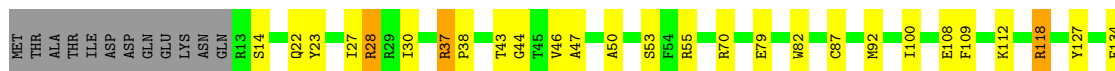
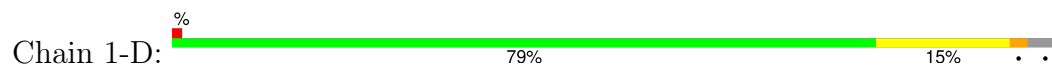


- Molecule 1: Thymidylate synthase

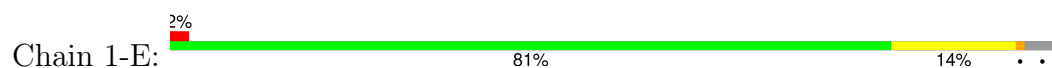




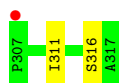
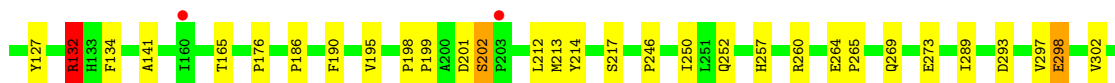
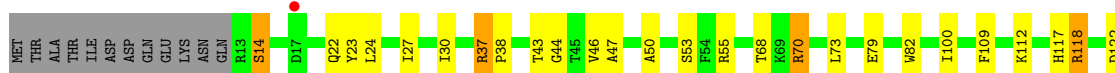
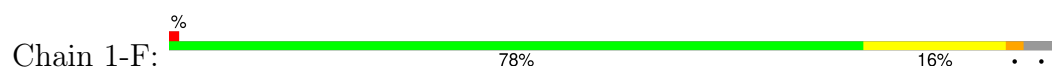
• Molecule 1: Thymidylate synthase



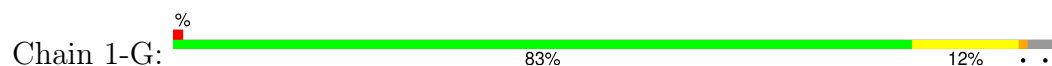
• Molecule 1: Thymidylate synthase



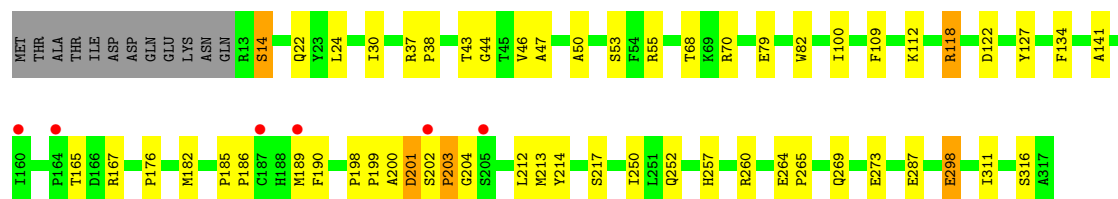
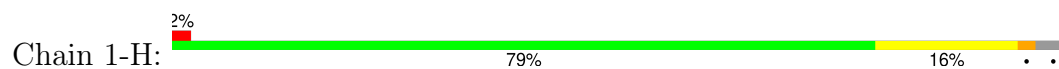
• Molecule 1: Thymidylate synthase



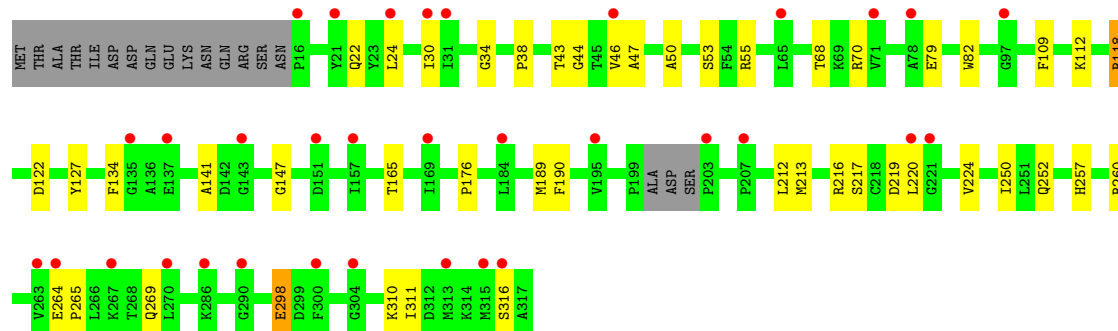
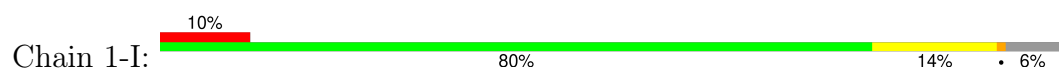
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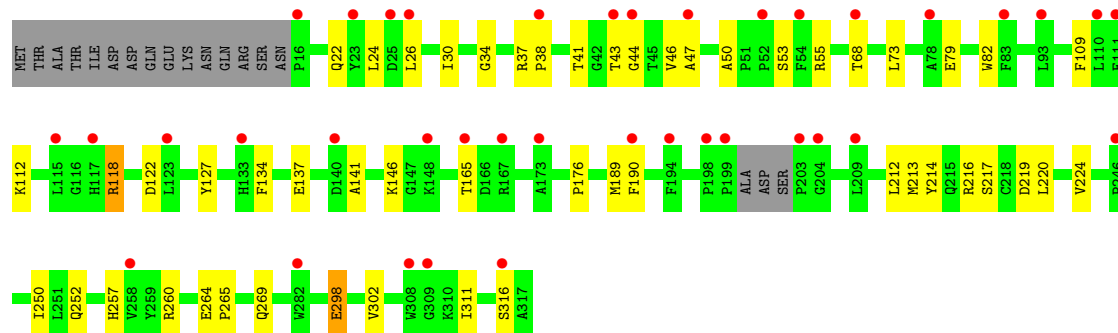
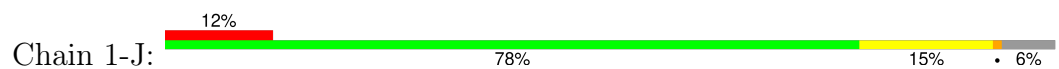
- Molecule 1: Thymidylate synthase



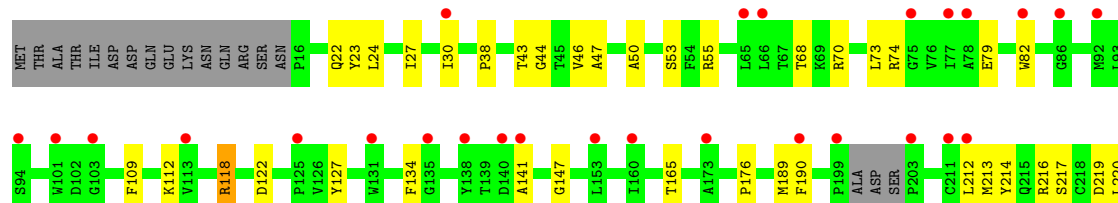
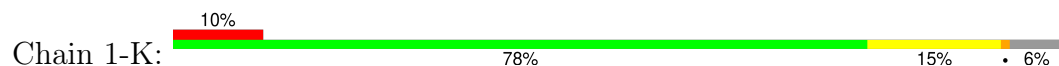
- Molecule 1: Thymidylate synthase

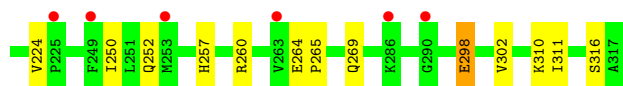


- Molecule 1: Thymidylate synthase

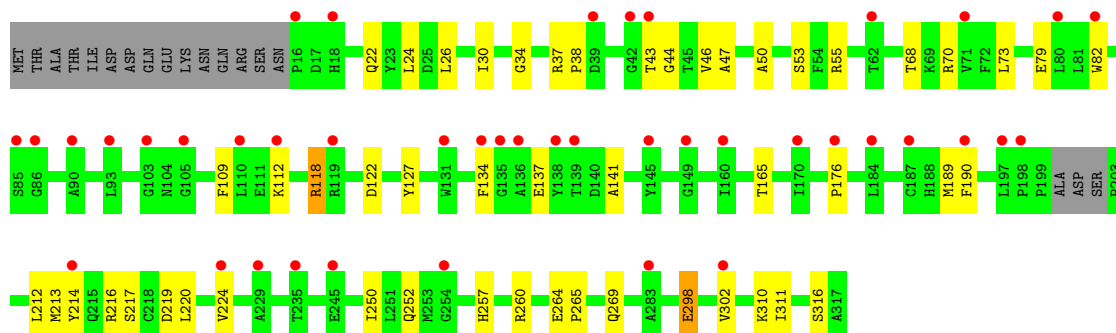
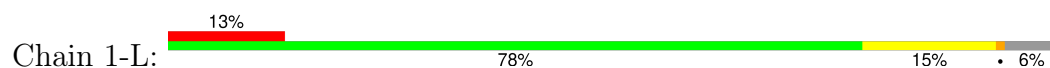


- Molecule 1: Thymidylate synthase

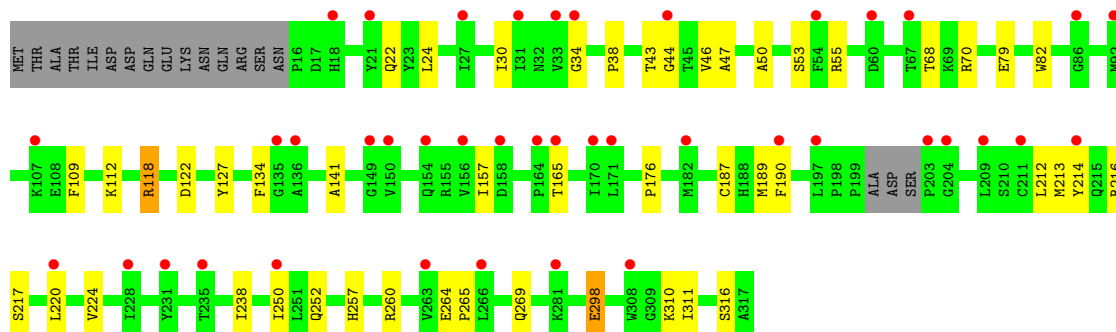
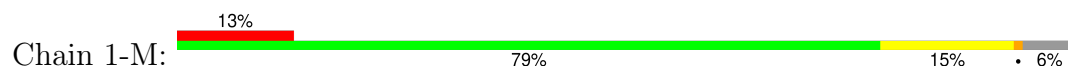




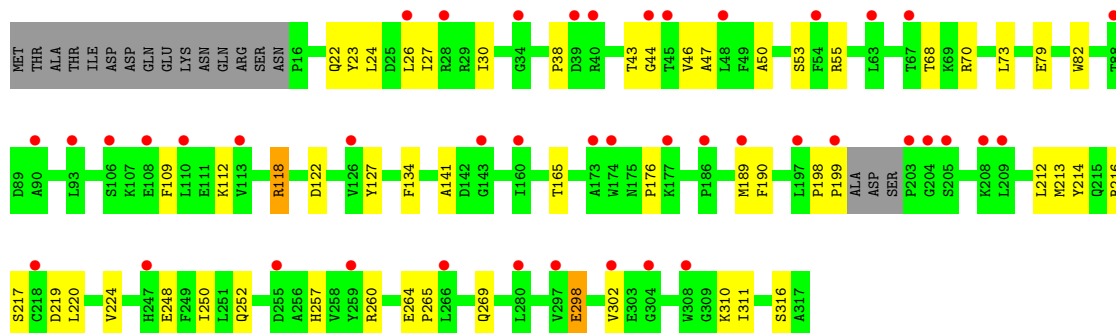
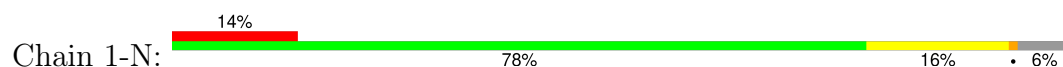
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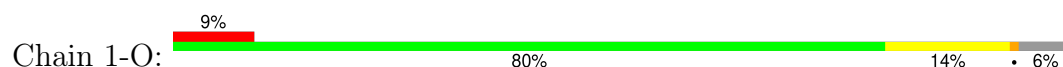
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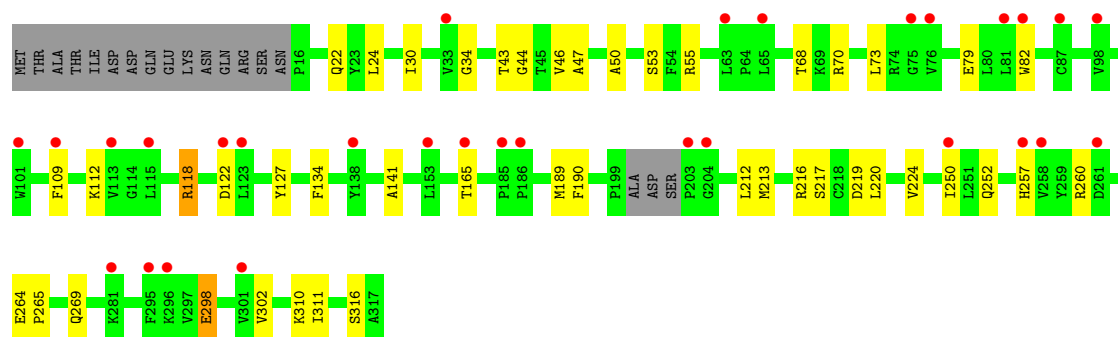


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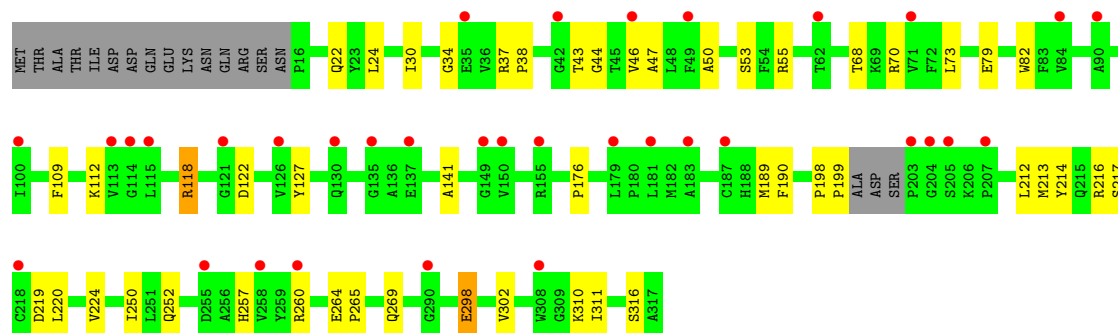
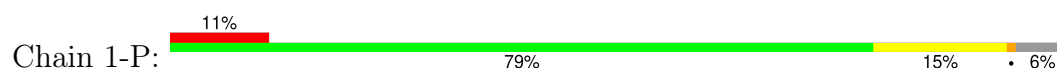


• Molecule 1: Thymidylate synthase

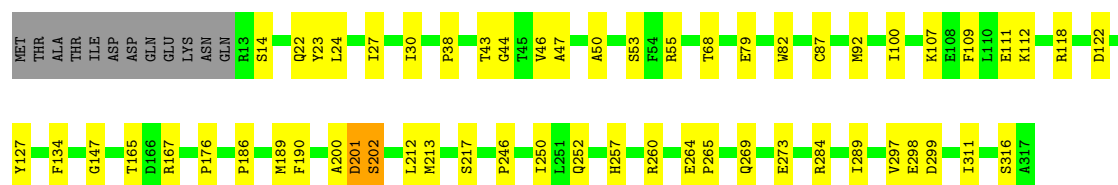
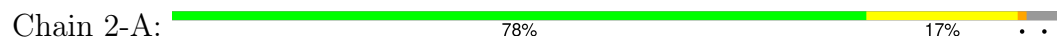




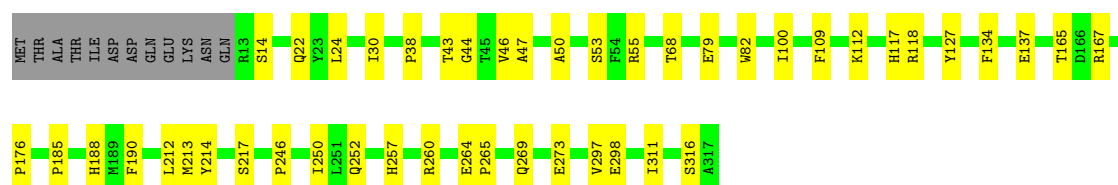
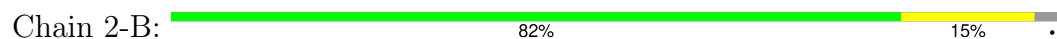
- Molecule 1: Thymidylate synthase



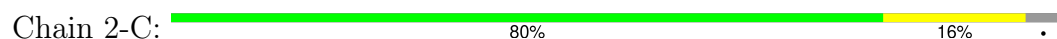
- Molecule 1: Thymidylate synthase

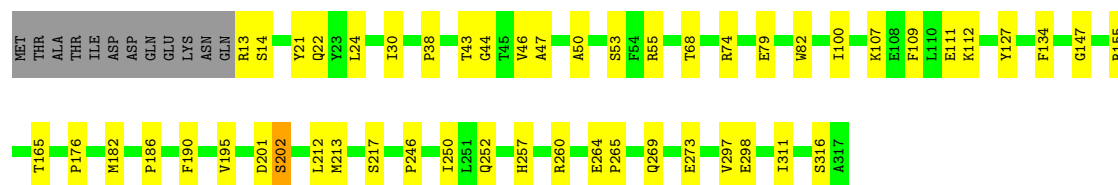


- Molecule 1: Thymidylate synthase



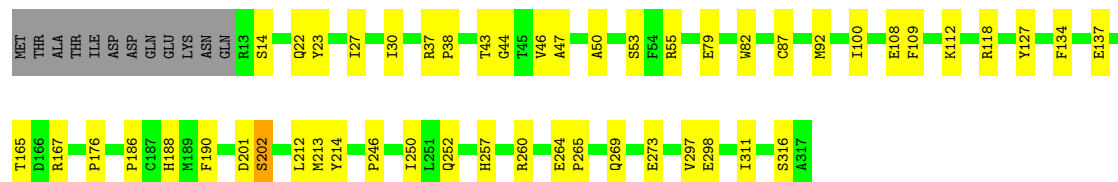
- Molecule 1: Thymidylate synthase





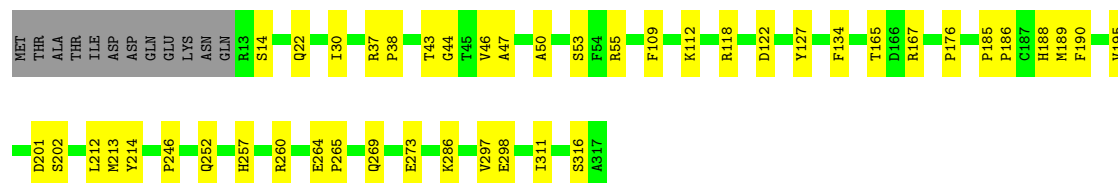
- Molecule 1: Thymidylate synthase

Chain 2-D: 80% 15% •



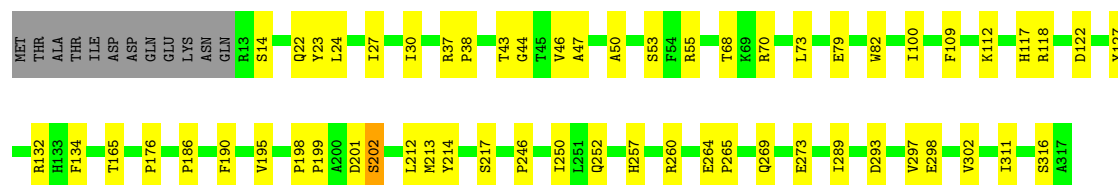
- Molecule 1: Thymidylate synthase

Chain 2-E: 82% 14% •



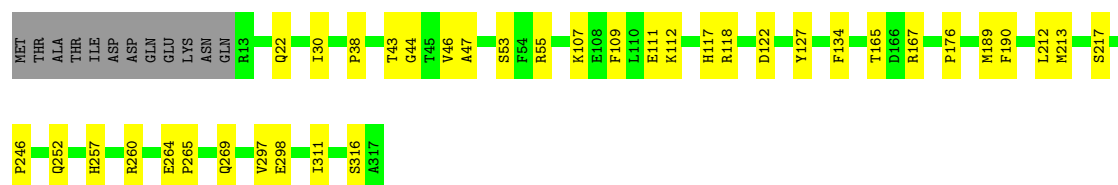
- Molecule 1: Thymidylate synthase

Chain 2-F: 78% 18% •



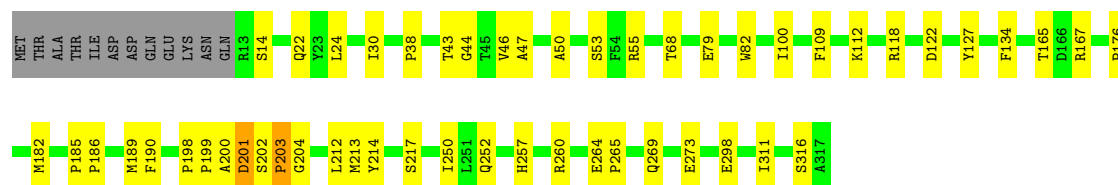
- Molecule 1: Thymidylate synthase

Chain 2-G: 85% 12% •



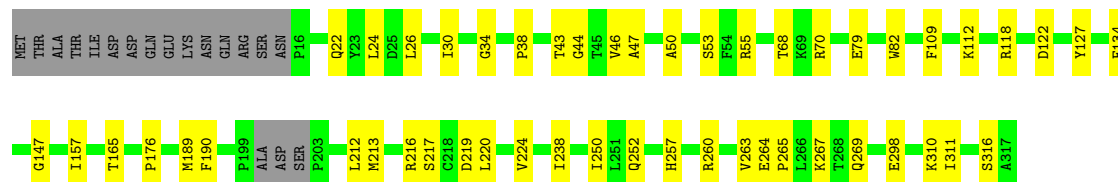
- Molecule 1: Thymidylate synthase

Chain 2-H: 80% 16% • •



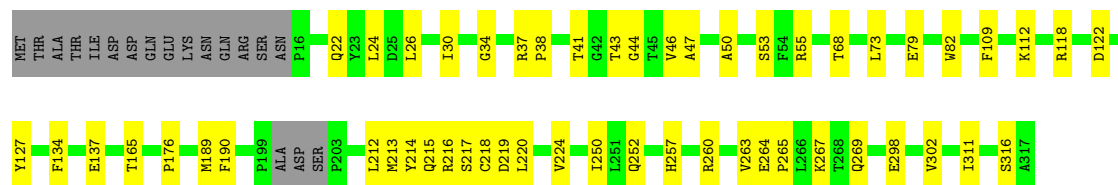
- Molecule 1: Thymidylate synthase

Chain 2-I: 79% 16% 6%



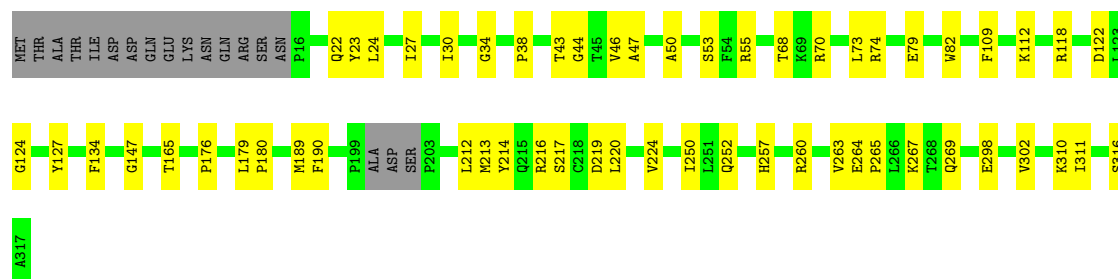
- Molecule 1: Thymidylate synthase

Chain 2-J: 78% 17% 6%



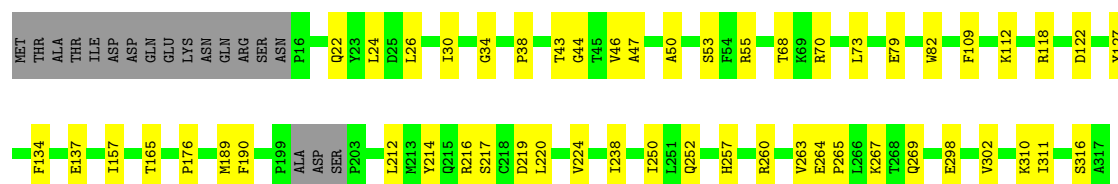
- Molecule 1: Thymidylate synthase

Chain 2-K: 77% 18% 6%




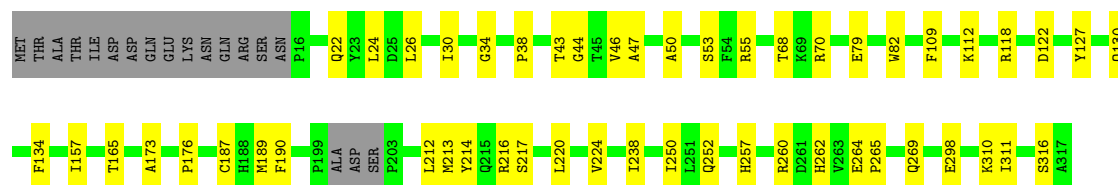
- Molecule 1: Thymidylate synthase

Chain 2-L: 78% 16% 6%




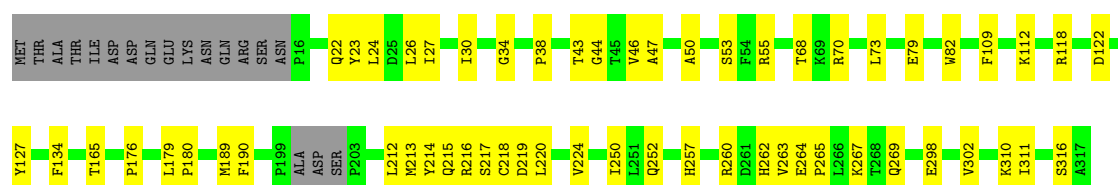
- Molecule 1: Thymidylate synthase

Chain 2-M: 




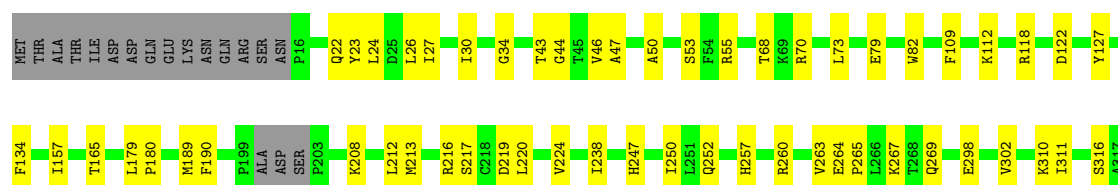
- Molecule 1: Thymidylate synthase

Chain 2-N: 




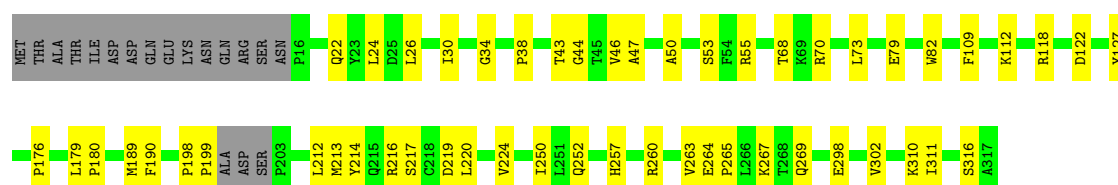
- Molecule 1: Thymidylate synthase

Chain 2-O: 




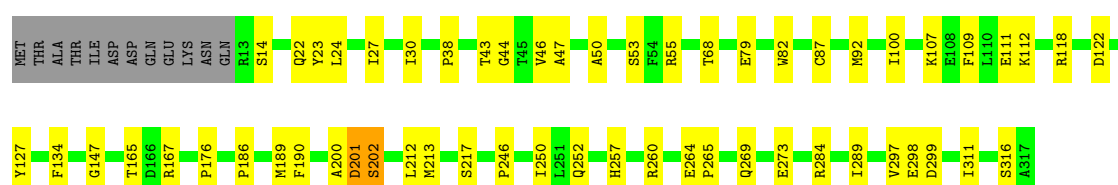
- Molecule 1: Thymidylate synthase

Chain 2-P: 

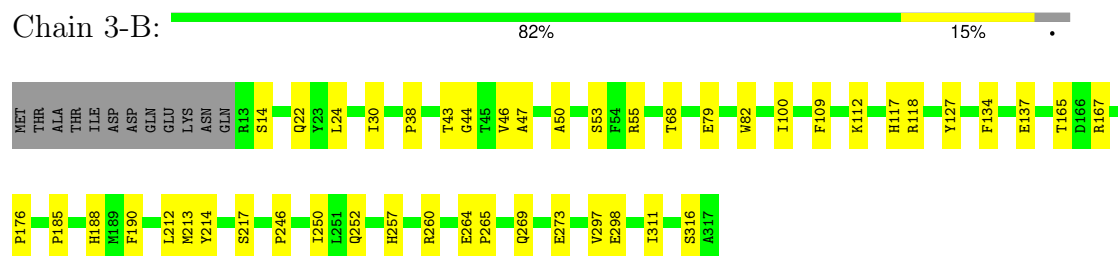


- Molecule 1: Thymidylate synthase

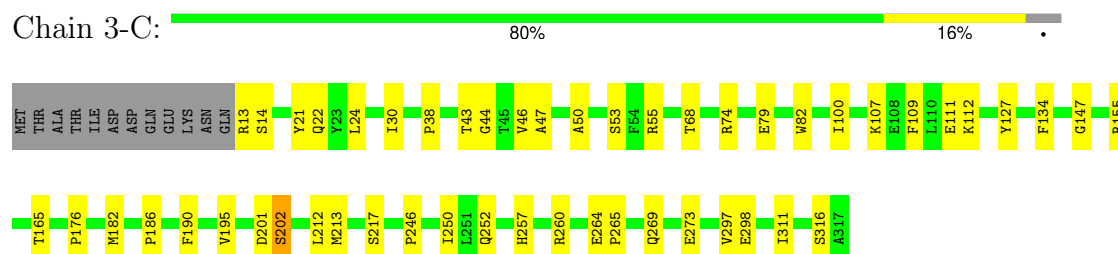
Chain 3-A: 



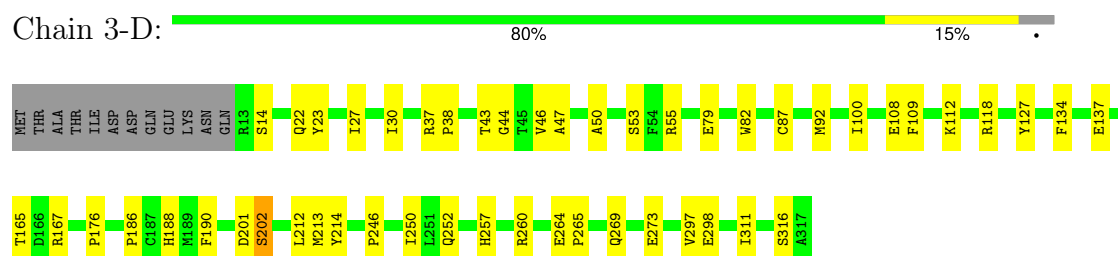
- Molecule 1: Thymidylate synthase



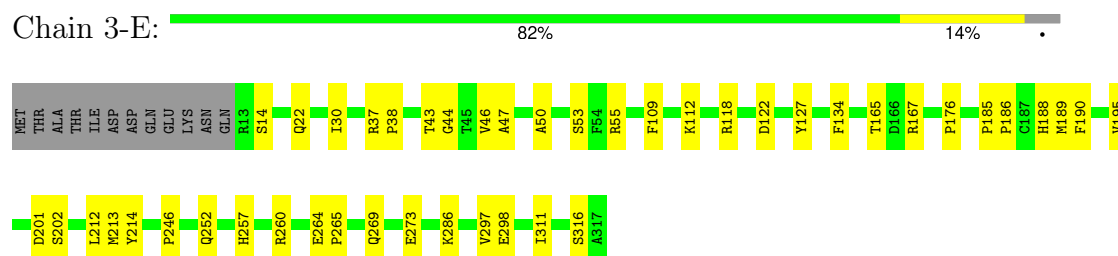
- Molecule 1: Thymidylate synthase



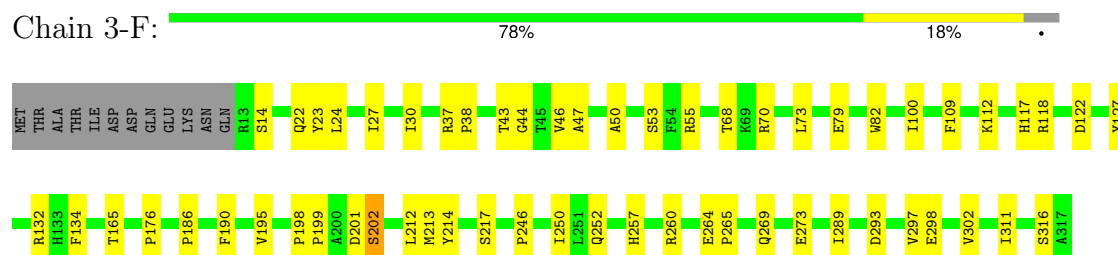
- Molecule 1: Thymidylate synthase



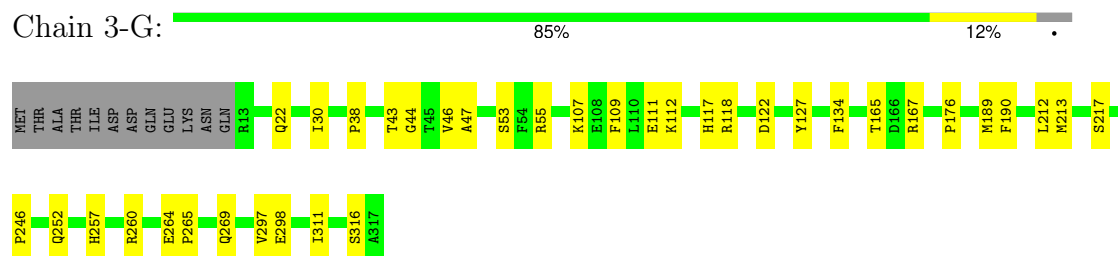
- Molecule 1: Thymidylate synthase



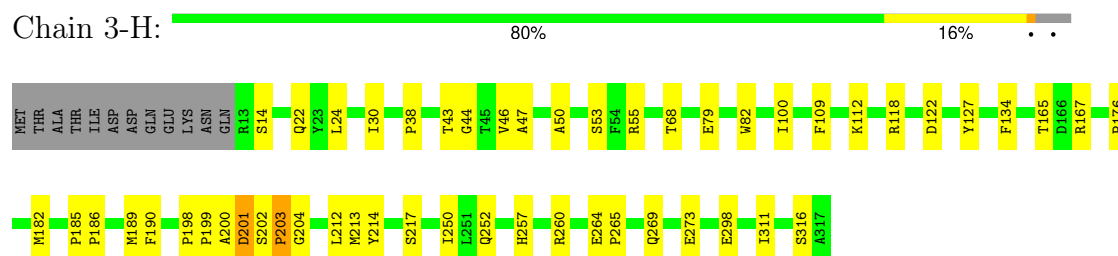
- Molecule 1: Thymidylate synthase



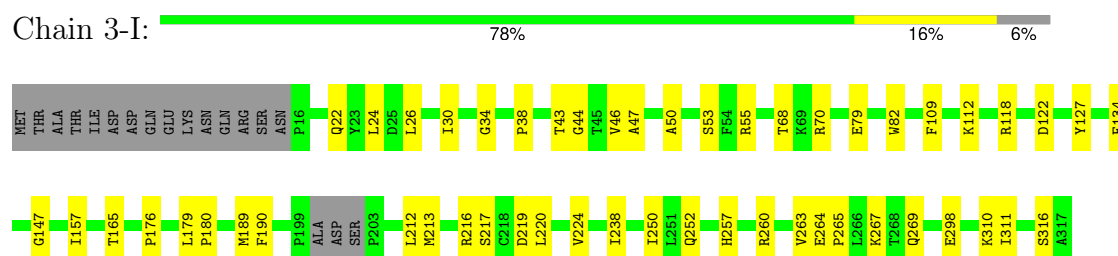
• Molecule 1: Thymidylate synthase



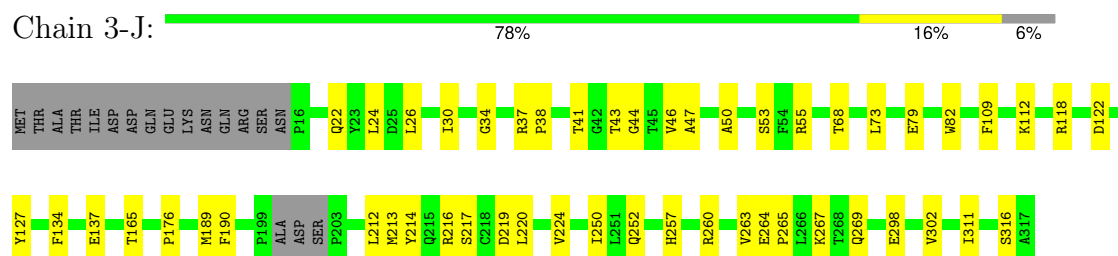
• Molecule 1: Thymidylate synthase



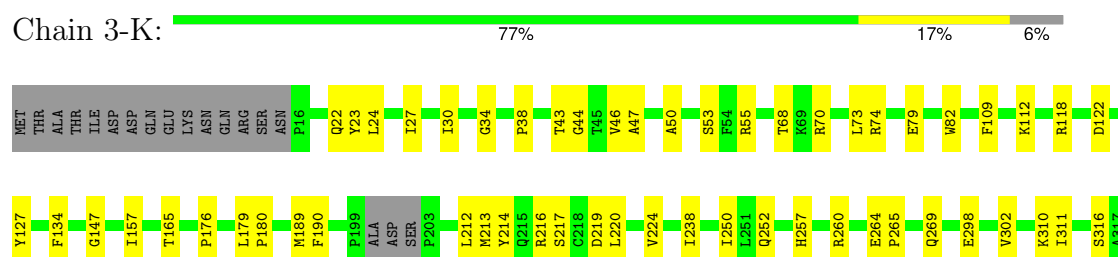
• Molecule 1: Thymidylate synthase



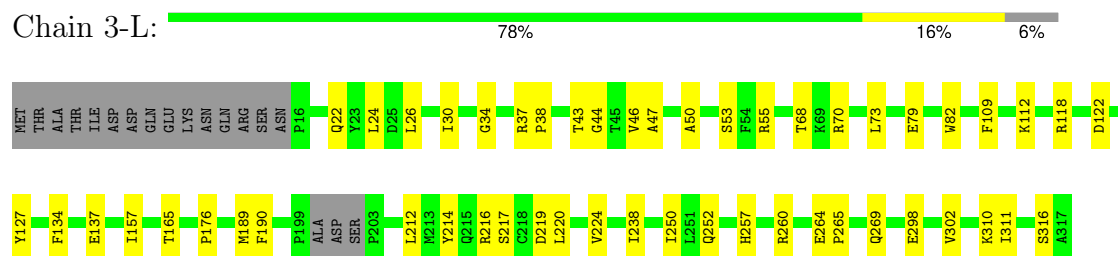
• Molecule 1: Thymidylate synthase



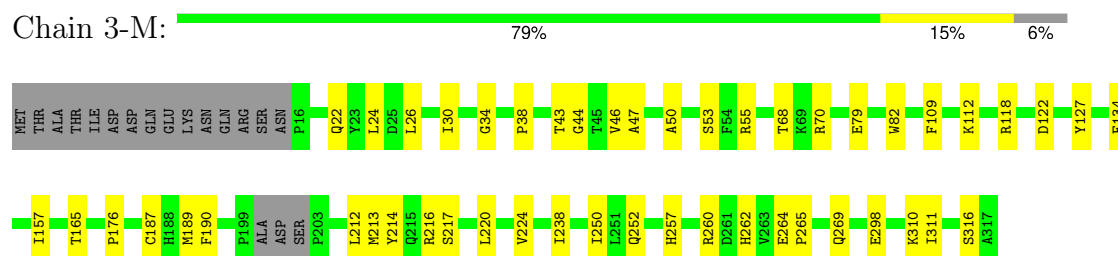
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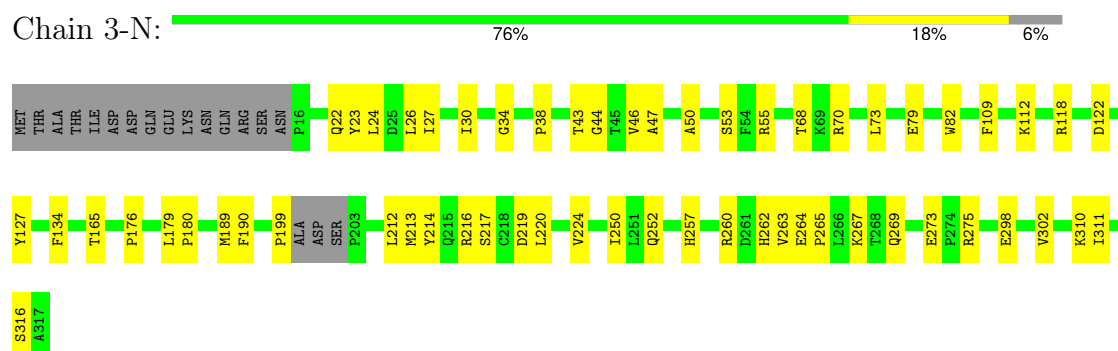
- Molecule 1: Thymidylate synthase



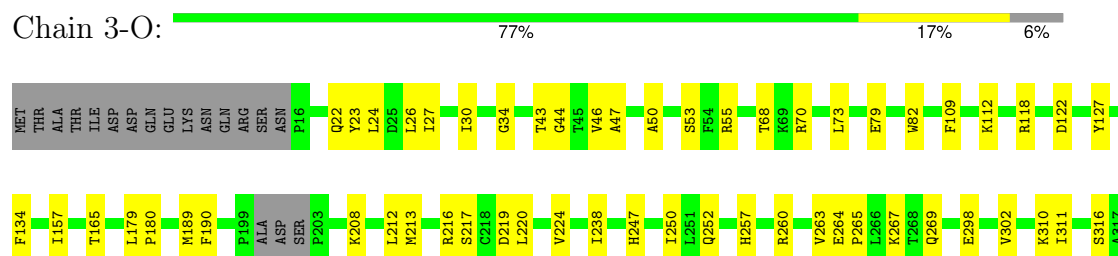
- Molecule 1: Thymidylate synthase



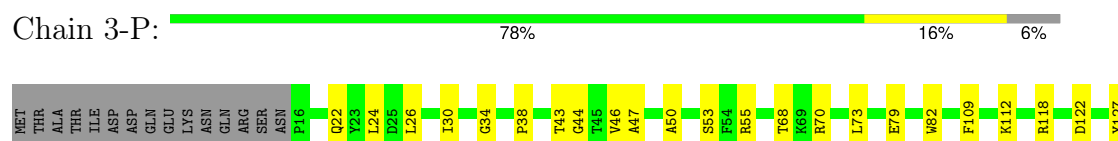
- Molecule 1: Thymidylate synthase



- Molecule 1: Thymidylate synthase



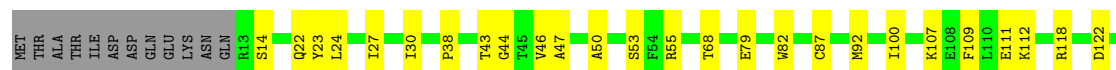
- Molecule 1: Thymidylate synthase





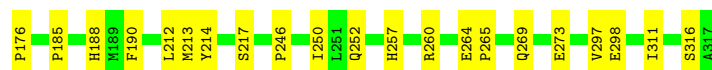
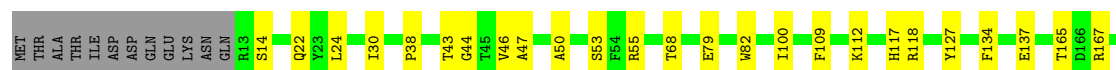
- Molecule 1: Thymidylate synthase

Chain 4-A: 78% 17% • •



- Molecule 1: Thymidylate synthase

Chain 4-B: 82% 15% •



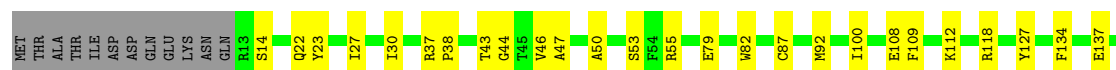
- Molecule 1: Thymidylate synthase

Chain 4-C: 80% 16% •



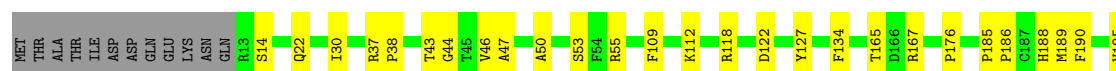
- Molecule 1: Thymidylate synthase

Chain 4-D: 80% 15% •



- Molecule 1: Thymidylate synthase

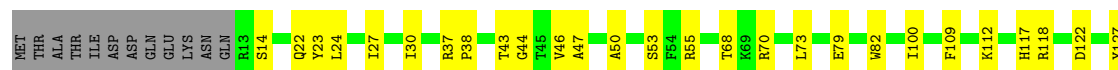
Chain 4-E: 82% 14% •





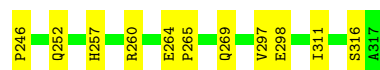
- Molecule 1: Thymidylate synthase

Chain 4-F: 78% 18% •



- Molecule 1: Thymidylate synthase

Chain 4-G: 85% 12% •



- Molecule 1: Thymidylate synthase

Chain 4-H: 80% 16% • •



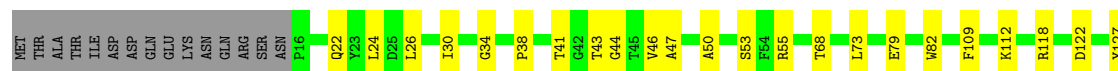
- Molecule 1: Thymidylate synthase

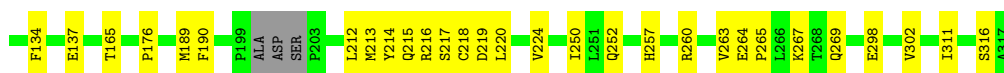
Chain 4-I: 79% 15% 6%



- Molecule 1: Thymidylate synthase

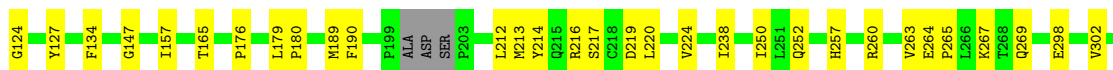
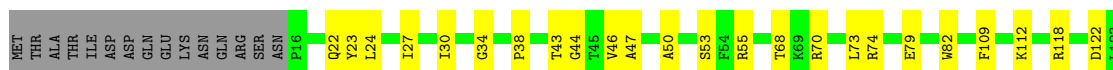
Chain 4-J: 78% 16% 6%





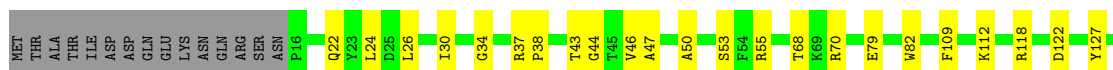
- Molecule 1: Thymidylate synthase

Chain 4-K: 76% 18% 6%



- Molecule 1: Thymidylate synthase

Chain 4-L: 78% 16% 6%



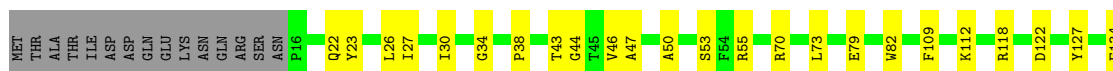
- Molecule 1: Thymidylate synthase

Chain 4-M: 78% 16% 6%



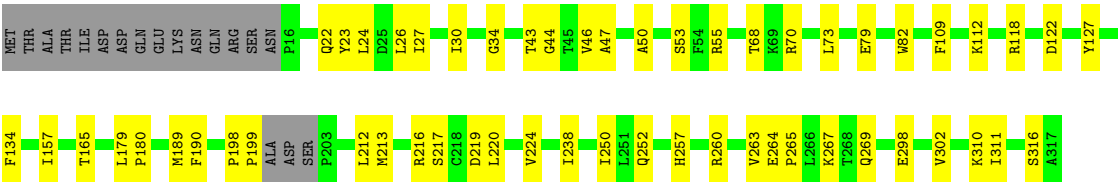
- Molecule 1: Thymidylate synthase

Chain 4-N: 78% 16% 6%

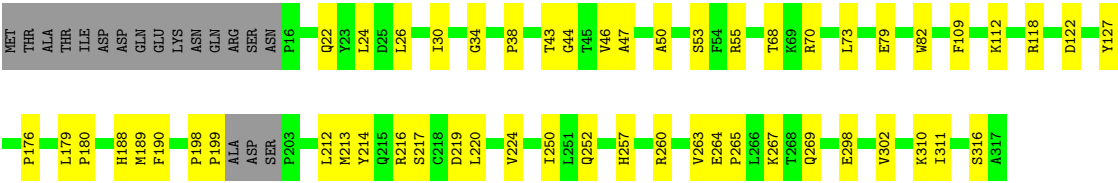
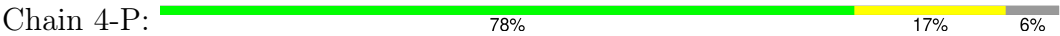


- Molecule 1: Thymidylate synthase

Chain 4-O: 77% 17% 6%



● Molecule 1: Thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.40Å 179.50Å 209.10Å 90.00° 89.80° 90.00°	Depositor
Resolution (Å)	49.91 – 2.08 49.91 – 2.08	Depositor EDS
% Data completeness (in resolution range)	88.1 (49.91-2.08) 87.2 (49.91-2.08)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.07Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.290 , 0.305 0.273 , 0.289	Depositor DCC
R_{free} test set	34851 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.08 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.206 for k,h,-l 0.198 for -k,-h,-l 0.349 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	161392	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.29% 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: CB3, UMP

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	1-A	0.50	0/2492	1.21	11/3375 (0.3%)
1	1-B	0.47	0/2496	0.71	4/3380 (0.1%)
1	1-C	0.48	0/2492	1.03	8/3375 (0.2%)
1	1-D	0.51	0/2496	1.39	13/3380 (0.4%)
1	1-E	0.49	0/2496	1.01	8/3380 (0.2%)
1	1-F	0.50	1/2496 (0.0%)	1.28	12/3380 (0.4%)
1	1-G	0.49	0/2496	0.86	8/3380 (0.2%)
1	1-H	0.49	0/2496	0.85	7/3380 (0.2%)
1	1-I	0.28	0/2451	0.59	2/3316 (0.1%)
1	1-J	0.28	0/2451	0.59	3/3316 (0.1%)
1	1-K	0.28	0/2451	0.59	3/3316 (0.1%)
1	1-L	0.28	0/2451	0.59	2/3316 (0.1%)
1	1-M	0.28	0/2451	0.59	2/3316 (0.1%)
1	1-N	0.28	0/2451	0.59	2/3316 (0.1%)
1	1-O	0.28	0/2451	0.59	2/3316 (0.1%)
1	1-P	0.28	0/2451	0.59	3/3316 (0.1%)
All	All	0.40	1/39568 (0.0%)	0.86	90/53558 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-F	132[A]	ARG	CD-NE	-5.44	1.37	1.46

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-D	37[A]	ARG	NE-CZ-NH1	-31.12	104.74	120.30
1	1-F	132[A]	ARG	NE-CZ-NH1	-30.91	104.84	120.30
1	1-F	132[A]	ARG	NE-CZ-NH2	30.10	135.35	120.30
1	1-E	37[A]	ARG	NE-CZ-NH1	-29.08	105.76	120.30
1	1-F	37[A]	ARG	NE-CZ-NH1	-28.95	105.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	2427	0	2393	50	0
1	1-B	2431	0	2397	45	0
1	1-C	2427	0	2393	49	0
1	1-D	2431	0	2397	48	0
1	1-E	2431	0	2397	43	0
1	1-F	2431	0	2397	53	0
1	1-G	2431	0	2397	35	0
1	1-H	2431	0	2397	51	0
1	1-I	2387	0	2360	40	0
1	1-J	2387	0	2360	47	0
1	1-K	2387	0	2360	47	0
1	1-L	2387	0	2360	46	0
1	1-M	2387	0	2360	41	0
1	1-N	2387	0	2360	46	0
1	1-O	2387	0	2360	37	0
1	1-P	2387	0	2360	38	0
1	2-A	2427	0	2393	50	0
1	2-B	2431	0	2397	45	0
1	2-C	2427	0	2393	49	0
1	2-D	2431	0	2397	48	0
1	2-E	2431	0	2397	43	0
1	2-F	2431	0	2397	53	0
1	2-G	2431	0	2397	35	0
1	2-H	2431	0	2397	47	0
1	2-I	2387	0	2360	45	0
1	2-J	2387	0	2360	46	0
1	2-K	2387	0	2360	51	0
1	2-L	2387	0	2360	46	0
1	2-M	2387	0	2360	46	0
1	2-N	2387	0	2360	49	0
1	2-O	2387	0	2360	45	0
1	2-P	2387	0	2360	45	0
1	3-A	2427	0	2393	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3-B	2431	0	2397	45	0
1	3-C	2427	0	2393	49	0
1	3-D	2431	0	2397	48	0
1	3-E	2431	0	2397	43	0
1	3-F	2431	0	2397	53	0
1	3-G	2431	0	2397	35	0
1	3-H	2431	0	2397	61	0
1	3-I	2387	0	2360	46	0
1	3-J	2387	0	2360	45	0
1	3-K	2387	0	2360	49	0
1	3-L	2387	0	2360	45	0
1	3-M	2387	0	2360	44	0
1	3-N	2387	0	2360	62	0
1	3-O	2387	0	2360	46	0
1	3-P	2387	0	2360	45	0
1	4-A	2427	0	2393	50	0
1	4-B	2431	0	2397	45	0
1	4-C	2427	0	2393	49	0
1	4-D	2431	0	2397	48	0
1	4-E	2431	0	2397	43	0
1	4-F	2431	0	2397	53	0
1	4-G	2431	0	2397	35	0
1	4-H	2431	0	2397	47	0
1	4-I	2387	0	2360	45	0
1	4-J	2387	0	2360	44	0
1	4-K	2387	0	2360	52	0
1	4-L	2387	0	2360	46	0
1	4-M	2387	0	2360	44	0
1	4-N	2387	0	2360	46	0
1	4-O	2387	0	2360	45	0
1	4-P	2387	0	2360	45	0
2	1-A	20	0	10	0	0
2	1-B	20	0	10	0	0
2	1-C	20	0	10	0	0
2	1-D	20	0	10	0	0
2	1-E	20	0	10	0	0
2	1-F	20	0	10	0	0
2	1-G	20	0	10	0	0
2	1-H	20	0	10	0	0
2	1-I	20	0	10	1	0
2	1-J	20	0	10	1	0
2	1-K	20	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1-L	20	0	10	1	0
2	1-M	20	0	10	1	0
2	1-N	20	0	10	1	0
2	1-O	20	0	10	1	0
2	1-P	20	0	10	1	0
2	2-A	20	0	10	0	0
2	2-B	20	0	10	0	0
2	2-C	20	0	10	0	0
2	2-D	20	0	10	0	0
2	2-E	20	0	10	0	0
2	2-F	20	0	10	0	0
2	2-G	20	0	10	0	0
2	2-H	20	0	10	0	0
2	2-I	20	0	10	1	0
2	2-J	20	0	10	1	0
2	2-K	20	0	10	1	0
2	2-L	20	0	10	1	0
2	2-M	20	0	10	1	0
2	2-N	20	0	10	1	0
2	2-O	20	0	10	1	0
2	2-P	20	0	10	1	0
2	3-A	20	0	10	0	0
2	3-B	20	0	10	0	0
2	3-C	20	0	10	0	0
2	3-D	20	0	10	0	0
2	3-E	20	0	10	0	0
2	3-F	20	0	10	0	0
2	3-G	20	0	10	0	0
2	3-H	20	0	10	0	0
2	3-I	20	0	10	1	0
2	3-J	20	0	10	1	0
2	3-K	20	0	10	1	0
2	3-L	20	0	10	1	0
2	3-M	20	0	10	1	0
2	3-N	20	0	10	1	0
2	3-O	20	0	10	1	0
2	3-P	20	0	10	1	0
2	4-A	20	0	10	0	0
2	4-B	20	0	10	0	0
2	4-C	20	0	10	0	0
2	4-D	20	0	10	0	0
2	4-E	20	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	4-F	20	0	10	0	0
2	4-G	20	0	10	0	0
2	4-H	20	0	10	0	0
2	4-I	20	0	10	1	0
2	4-J	20	0	10	1	0
2	4-K	20	0	10	1	0
2	4-L	20	0	10	1	0
2	4-M	20	0	10	1	0
2	4-N	20	0	10	1	0
2	4-O	20	0	10	1	0
2	4-P	20	0	10	1	0
3	1-A	35	0	21	1	0
3	1-B	35	0	21	1	0
3	1-C	35	0	21	1	0
3	1-D	35	0	21	1	0
3	1-E	35	0	21	0	0
3	1-F	35	0	21	1	0
3	1-G	35	0	21	0	0
3	1-H	35	0	21	1	0
3	2-A	35	0	21	1	0
3	2-B	35	0	21	1	0
3	2-C	35	0	21	1	0
3	2-D	35	0	21	1	0
3	2-E	35	0	21	0	0
3	2-F	35	0	21	1	0
3	2-G	35	0	21	0	0
3	2-H	35	0	21	1	0
3	3-A	35	0	21	1	0
3	3-B	35	0	21	1	0
3	3-C	35	0	21	1	0
3	3-D	35	0	21	1	0
3	3-E	35	0	21	0	0
3	3-F	35	0	21	1	0
3	3-G	35	0	21	0	0
3	3-H	35	0	21	1	0
3	4-A	35	0	21	1	0
3	4-B	35	0	21	1	0
3	4-C	35	0	21	1	0
3	4-D	35	0	21	1	0
3	4-E	35	0	21	0	0
3	4-F	35	0	21	1	0
3	4-G	35	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	4-H	35	0	21	1	0
4	1-A	185	0	0	4	0
4	1-B	143	0	0	7	0
4	1-C	151	0	0	4	0
4	1-D	148	0	0	5	0
4	1-E	155	0	0	6	0
4	1-F	138	0	0	6	0
4	1-G	153	0	0	3	0
4	1-H	139	0	0	2	0
4	2-A	185	0	0	4	0
4	2-B	143	0	0	7	0
4	2-C	151	0	0	4	0
4	2-D	148	0	0	5	0
4	2-E	155	0	0	6	0
4	2-F	138	0	0	6	0
4	2-G	153	0	0	3	0
4	2-H	139	0	0	2	0
4	3-A	185	0	0	4	0
4	3-B	143	0	0	7	0
4	3-C	151	0	0	4	0
4	3-D	148	0	0	5	0
4	3-E	155	0	0	6	0
4	3-F	138	0	0	6	0
4	3-G	153	0	0	3	0
4	3-H	139	0	0	2	0
4	4-A	185	0	0	4	0
4	4-B	143	0	0	7	0
4	4-C	151	0	0	4	0
4	4-D	148	0	0	5	0
4	4-E	155	0	0	6	0
4	4-F	138	0	0	6	0
4	4-G	153	0	0	3	0
4	4-H	139	0	0	2	0
All	All	161392	0	153504	2427	0

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 8.

The worst 5 of 2427 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)
1:H:201[C]:ASP:HB3	1:N:273[C]:GLU:CG	1.82	1.08
1:H:287[A]:GLU:HG2	1:J:146[A]:LYS:HZ3	1.25	0.99
1:H:287[A]:GLU:HG2	1:J:146[A]:LYS:NZ	1.78	0.98
1:H:201[C]:ASP:HB3	1:N:273[C]:GLU:HG2	1.45	0.93
1:H:202[C]:SER:HB3	1:N:275[C]:ARG:HG3	1.54	0.89

There are no symmetry-related clashes.

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	
1	1-A	303/317 (96%)	293 (97%)	7 (2%)	3 (1%)	13	8
1	1-B	303/317 (96%)	293 (97%)	9 (3%)	1 (0%)	37	36
1	1-C	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	19	15
1	1-D	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	19	15
1	1-E	303/317 (96%)	292 (96%)	8 (3%)	3 (1%)	13	8
1	1-F	303/317 (96%)	292 (96%)	9 (3%)	2 (1%)	19	15
1	1-G	303/317 (96%)	294 (97%)	8 (3%)	1 (0%)	37	36
1	1-H	303/317 (96%)	291 (96%)	9 (3%)	3 (1%)	13	8
1	1-I	295/317 (93%)	287 (97%)	7 (2%)	1 (0%)	37	36
1	1-J	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	1-K	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	1-L	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	37	36
1	1-M	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	1-N	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	1-O	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	1-P	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2-A	303/317 (96%)	293 (97%)	7 (2%)	3 (1%)	13	8
1	2-B	303/317 (96%)	293 (97%)	9 (3%)	1 (0%)	37	36
1	2-C	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	19	15
1	2-D	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	19	15
1	2-E	303/317 (96%)	292 (96%)	8 (3%)	3 (1%)	13	8
1	2-F	303/317 (96%)	292 (96%)	9 (3%)	2 (1%)	19	15
1	2-G	303/317 (96%)	294 (97%)	8 (3%)	1 (0%)	37	36
1	2-H	303/317 (96%)	291 (96%)	9 (3%)	3 (1%)	13	8
1	2-I	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	2-J	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	2-K	295/317 (93%)	287 (97%)	7 (2%)	1 (0%)	37	36
1	2-L	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	37	36
1	2-M	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	2-N	295/317 (93%)	284 (96%)	10 (3%)	1 (0%)	37	36
1	2-O	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	37	36
1	2-P	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	3-A	303/317 (96%)	293 (97%)	7 (2%)	3 (1%)	13	8
1	3-B	303/317 (96%)	293 (97%)	9 (3%)	1 (0%)	37	36
1	3-C	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	19	15
1	3-D	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	19	15
1	3-E	303/317 (96%)	292 (96%)	8 (3%)	3 (1%)	13	8
1	3-F	303/317 (96%)	292 (96%)	9 (3%)	2 (1%)	19	15
1	3-G	303/317 (96%)	294 (97%)	8 (3%)	1 (0%)	37	36
1	3-H	303/317 (96%)	291 (96%)	9 (3%)	3 (1%)	13	8
1	3-I	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	3-J	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	3-K	295/317 (93%)	287 (97%)	7 (2%)	1 (0%)	37	36
1	3-L	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	37	36
1	3-M	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	3-N	295/317 (93%)	283 (96%)	11 (4%)	1 (0%)	37	36
1	3-O	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-P	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	37	36
1	4-A	303/317 (96%)	293 (97%)	7 (2%)	3 (1%)	13	8
1	4-B	303/317 (96%)	293 (97%)	9 (3%)	1 (0%)	37	36
1	4-C	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	19	15
1	4-D	303/317 (96%)	293 (97%)	8 (3%)	2 (1%)	19	15
1	4-E	303/317 (96%)	292 (96%)	8 (3%)	3 (1%)	13	8
1	4-F	303/317 (96%)	292 (96%)	9 (3%)	2 (1%)	19	15
1	4-G	303/317 (96%)	294 (97%)	8 (3%)	1 (0%)	37	36
1	4-H	303/317 (96%)	291 (96%)	9 (3%)	3 (1%)	13	8
1	4-I	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	4-J	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	4-K	295/317 (93%)	287 (97%)	7 (2%)	1 (0%)	37	36
1	4-L	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	37	36
1	4-M	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
1	4-N	295/317 (93%)	283 (96%)	11 (4%)	1 (0%)	37	36
1	4-O	295/317 (93%)	285 (97%)	9 (3%)	1 (0%)	37	36
1	4-P	295/317 (93%)	286 (97%)	8 (3%)	1 (0%)	37	36
All	All	19136/20288 (94%)	18505 (97%)	531 (3%)	100 (0%)	25	22

5 of 100 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	127[A]	TYR
1	1-B	127[A]	TYR
1	1-C	127[A]	TYR
1	1-C	202[A]	SER
1	1-D	127[A]	TYR

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	
1	1-A	262/274 (96%)	260 (99%)	2 (1%)	79	83
1	1-B	263/274 (96%)	262 (100%)	1 (0%)	89	92
1	1-C	262/274 (96%)	261 (100%)	1 (0%)	89	92
1	1-D	263/274 (96%)	261 (99%)	2 (1%)	79	83
1	1-E	263/274 (96%)	261 (99%)	2 (1%)	79	83
1	1-F	263/274 (96%)	260 (99%)	3 (1%)	70	76
1	1-G	263/274 (96%)	260 (99%)	3 (1%)	70	76
1	1-H	263/274 (96%)	261 (99%)	2 (1%)	79	83
1	1-I	258/274 (94%)	257 (100%)	1 (0%)	89	92
1	1-J	258/274 (94%)	257 (100%)	1 (0%)	89	92
1	1-K	258/274 (94%)	257 (100%)	1 (0%)	89	92
1	1-L	258/274 (94%)	257 (100%)	1 (0%)	89	92
1	1-M	258/274 (94%)	257 (100%)	1 (0%)	89	92
1	1-N	258/274 (94%)	257 (100%)	1 (0%)	89	92
1	1-O	258/274 (94%)	257 (100%)	1 (0%)	89	92
1	1-P	258/274 (94%)	257 (100%)	1 (0%)	89	92
All	All	4166/4384 (95%)	4142 (99%)	24 (1%)	84	88

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-H	14[A]	SER
1	1-J	298[A]	GLU
1	1-I	298[A]	GLU
1	1-K	298[A]	GLU
1	1-E	220[A]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
1	1-J	269[A]	GLN
1	1-M	32[A]	ASN
1	1-K	32[A]	ASN
1	1-L	32[A]	ASN
1	1-M	269[A]	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

96 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	UMP	3-C	450[C]	-	21,21,21	2.55	4 (19%)	30,31,31	2.61	13 (43%)
2	UMP	4-M	550[D]	-	21,21,21	2.52	5 (23%)	30,31,31	2.38	7 (23%)
3	CB3	1-E	2551[A]	-	36,37,37	2.50	16 (44%)	48,51,51	2.75	15 (31%)
2	UMP	1-A	350[A]	1	21,21,21	2.54	5 (23%)	30,31,31	2.39	8 (26%)
2	UMP	2-E	550[B]	-	21,21,21	2.41	4 (19%)	30,31,31	2.49	11 (36%)
3	CB3	2-C	2451[B]	-	36,37,37	2.30	13 (36%)	48,51,51	2.59	12 (25%)
3	CB3	1-D	2501[A]	-	36,37,37	2.36	14 (38%)	48,51,51	2.39	16 (33%)
2	UMP	4-B	400[D]	-	21,21,21	2.55	5 (23%)	30,31,31	1.87	5 (16%)
2	UMP	1-P	700[A]	1	21,21,21	2.58	5 (23%)	30,31,31	2.39	8 (26%)
3	CB3	2-A	2351[B]	-	36,37,37	2.68	14 (38%)	48,51,51	2.66	14 (29%)
2	UMP	4-O	650[D]	-	21,21,21	2.51	5 (23%)	30,31,31	2.37	7 (23%)
3	CB3	2-G	2651[B]	-	36,37,37	2.52	14 (38%)	48,51,51	2.48	15 (31%)
2	UMP	4-J	400[D]	-	21,21,21	2.55	5 (23%)	30,31,31	2.37	7 (23%)
3	CB3	1-F	2601[A]	-	36,37,37	2.50	15 (41%)	48,51,51	2.50	18 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UMP	1-O	650[A]	1	21,21,21	2.48	5 (23%)	30,31,31	2.40	7 (23%)
2	UMP	4-K	450[D]	-	21,21,21	2.55	5 (23%)	30,31,31	2.42	8 (26%)
2	UMP	2-P	700[B]	-	21,21,21	2.55	5 (23%)	30,31,31	2.38	8 (26%)
2	UMP	4-F	600[D]	-	21,21,21	2.21	3 (14%)	30,31,31	2.10	9 (30%)
2	UMP	3-B	400[C]	-	21,21,21	2.55	5 (23%)	30,31,31	1.87	5 (16%)
2	UMP	1-J	400[A]	1	21,21,21	2.55	5 (23%)	30,31,31	2.43	8 (26%)
3	CB3	2-D	2501[B]	-	36,37,37	2.36	14 (38%)	48,51,51	2.39	16 (33%)
2	UMP	1-H	700[A]	1	21,21,21	3.03	8 (38%)	30,31,31	2.26	10 (33%)
2	UMP	4-C	450[D]	-	21,21,21	2.55	4 (19%)	30,31,31	2.61	13 (43%)
3	CB3	2-F	2601[B]	-	36,37,37	2.50	15 (41%)	48,51,51	2.50	18 (37%)
3	CB3	3-B	2401[C]	-	36,37,37	2.39	16 (44%)	48,51,51	2.60	19 (39%)
3	CB3	4-E	2551[D]	-	36,37,37	2.50	16 (44%)	48,51,51	2.75	15 (31%)
2	UMP	1-E	550[A]	1	21,21,21	2.41	4 (19%)	30,31,31	2.49	11 (36%)
2	UMP	3-K	450[C]	-	21,21,21	2.55	5 (23%)	30,31,31	2.42	8 (26%)
2	UMP	2-O	650[B]	-	21,21,21	2.52	4 (19%)	30,31,31	2.41	7 (23%)
2	UMP	1-I	350[A]	1	21,21,21	2.54	5 (23%)	30,31,31	2.45	7 (23%)
2	UMP	1-F	600[A]	1	21,21,21	2.21	3 (14%)	30,31,31	2.10	9 (30%)
2	UMP	4-N	600[D]	-	21,21,21	2.53	5 (23%)	30,31,31	2.39	6 (20%)
3	CB3	1-A	2351[A]	-	36,37,37	2.68	14 (38%)	48,51,51	2.66	14 (29%)
3	CB3	3-E	2551[C]	-	36,37,37	2.50	16 (44%)	48,51,51	2.75	15 (31%)
2	UMP	2-M	550[B]	-	21,21,21	2.53	5 (23%)	30,31,31	2.38	7 (23%)
3	CB3	4-D	2501[D]	-	36,37,37	2.36	14 (38%)	48,51,51	2.39	16 (33%)
3	CB3	3-F	2601[C]	-	36,37,37	2.50	15 (41%)	48,51,51	2.50	18 (37%)
2	UMP	1-B	400[A]	1	21,21,21	2.55	5 (23%)	30,31,31	1.87	5 (16%)
2	UMP	2-D	500[B]	-	21,21,21	2.44	7 (33%)	30,31,31	2.09	5 (16%)
2	UMP	4-G	650[D]	-	21,21,21	2.34	3 (14%)	30,31,31	2.47	10 (33%)
3	CB3	2-B	2401[B]	-	36,37,37	2.39	16 (44%)	48,51,51	2.60	19 (39%)
2	UMP	1-G	650[A]	1	21,21,21	2.34	3 (14%)	30,31,31	2.47	10 (33%)
2	UMP	1-M	550[A]	1	21,21,21	2.52	5 (23%)	30,31,31	2.36	7 (23%)
2	UMP	3-F	600[C]	-	21,21,21	2.21	3 (14%)	30,31,31	2.10	9 (30%)
2	UMP	3-A	350[C]	-	21,21,21	2.54	5 (23%)	30,31,31	2.39	8 (26%)
2	UMP	1-D	500[A]	1	21,21,21	2.44	7 (33%)	30,31,31	2.09	5 (16%)
2	UMP	3-L	500[C]	-	21,21,21	2.54	5 (23%)	30,31,31	2.41	7 (23%)
2	UMP	3-D	500[C]	-	21,21,21	2.44	7 (33%)	30,31,31	2.09	5 (16%)
2	UMP	4-D	500[D]	-	21,21,21	2.44	7 (33%)	30,31,31	2.09	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UMP	2-H	700[B]	-	21,21,21	3.03	8 (38%)	30,31,31	2.26	10 (33%)
2	UMP	3-I	350[C]	-	21,21,21	2.53	5 (23%)	30,31,31	2.45	7 (23%)
3	CB3	1-H	2701[A]	-	36,37,37	2.04	12 (33%)	48,51,51	2.82	20 (41%)
2	UMP	4-H	700[D]	-	21,21,21	3.03	8 (38%)	30,31,31	2.26	10 (33%)
2	UMP	2-B	400[B]	-	21,21,21	2.55	5 (23%)	30,31,31	1.87	5 (16%)
2	UMP	2-F	600[B]	-	21,21,21	2.21	3 (14%)	30,31,31	2.10	9 (30%)
3	CB3	3-H	2701[C]	-	36,37,37	2.04	12 (33%)	48,51,51	2.82	20 (41%)
3	CB3	4-G	2651[D]	-	36,37,37	2.52	14 (38%)	48,51,51	2.48	15 (31%)
2	UMP	3-M	550[C]	-	21,21,21	2.54	5 (23%)	30,31,31	2.40	7 (23%)
2	UMP	2-C	450[B]	-	21,21,21	2.55	4 (19%)	30,31,31	2.61	13 (43%)
2	UMP	3-J	400[C]	-	21,21,21	2.55	5 (23%)	30,31,31	2.41	8 (26%)
2	UMP	1-C	450[A]	1	21,21,21	2.55	4 (19%)	30,31,31	2.61	13 (43%)
2	UMP	4-E	550[D]	-	21,21,21	2.41	4 (19%)	30,31,31	2.49	11 (36%)
2	UMP	2-G	650[B]	-	21,21,21	2.34	3 (14%)	30,31,31	2.47	10 (33%)
2	UMP	4-L	500[D]	-	21,21,21	2.54	5 (23%)	30,31,31	2.40	7 (23%)
3	CB3	1-G	2651[A]	-	36,37,37	2.52	14 (38%)	48,51,51	2.48	15 (31%)
2	UMP	1-K	450[A]	1	21,21,21	2.55	5 (23%)	30,31,31	2.43	8 (26%)
3	CB3	2-H	2701[B]	-	36,37,37	2.04	12 (33%)	48,51,51	2.82	20 (41%)
3	CB3	4-A	2351[D]	-	36,37,37	2.68	14 (38%)	48,51,51	2.66	14 (29%)
2	UMP	4-I	350[D]	-	21,21,21	2.53	5 (23%)	30,31,31	2.44	7 (23%)
2	UMP	2-K	450[B]	-	21,21,21	2.54	5 (23%)	30,31,31	2.43	8 (26%)
2	UMP	1-L	500[A]	1	21,21,21	2.57	5 (23%)	30,31,31	2.41	7 (23%)
3	CB3	3-D	2501[C]	-	36,37,37	2.36	14 (38%)	48,51,51	2.39	16 (33%)
3	CB3	3-A	2351[C]	-	36,37,37	2.68	14 (38%)	48,51,51	2.66	14 (29%)
3	CB3	1-B	2401[A]	-	36,37,37	2.39	16 (44%)	48,51,51	2.60	19 (39%)
2	UMP	2-I	350[B]	-	21,21,21	2.52	5 (23%)	30,31,31	2.42	7 (23%)
3	CB3	4-F	2601[D]	-	36,37,37	2.50	15 (41%)	48,51,51	2.50	18 (37%)
3	CB3	4-H	2701[D]	-	36,37,37	2.04	12 (33%)	48,51,51	2.82	20 (41%)
2	UMP	1-N	600[A]	1	21,21,21	2.52	5 (23%)	30,31,31	2.39	7 (23%)
3	CB3	3-C	2451[C]	-	36,37,37	2.30	13 (36%)	48,51,51	2.59	12 (25%)
2	UMP	3-H	700[C]	-	21,21,21	3.03	8 (38%)	30,31,31	2.26	10 (33%)
2	UMP	3-P	700[C]	-	21,21,21	2.55	5 (23%)	30,31,31	2.39	8 (26%)
2	UMP	2-A	350[B]	-	21,21,21	2.54	5 (23%)	30,31,31	2.39	8 (26%)
3	CB3	4-C	2451[D]	-	36,37,37	2.30	13 (36%)	48,51,51	2.59	12 (25%)
2	UMP	3-O	650[C]	-	21,21,21	2.53	5 (23%)	30,31,31	2.42	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CB3	1-C	2451[A]	-	36,37,37	2.30	13 (36%)	48,51,51	2.59	12 (25%)
2	UMP	2-L	500[B]	-	21,21,21	2.53	5 (23%)	30,31,31	2.39	7 (23%)
3	CB3	3-G	2651[C]	-	36,37,37	2.52	14 (38%)	48,51,51	2.48	15 (31%)
2	UMP	3-E	550[C]	-	21,21,21	2.41	4 (19%)	30,31,31	2.49	11 (36%)
3	CB3	2-E	2551[B]	-	36,37,37	2.50	16 (44%)	48,51,51	2.75	15 (31%)
2	UMP	2-J	400[B]	-	21,21,21	2.55	5 (23%)	30,31,31	2.40	8 (26%)
2	UMP	4-P	700[D]	-	21,21,21	2.56	5 (23%)	30,31,31	2.39	8 (26%)
2	UMP	4-A	350[D]	-	21,21,21	2.54	5 (23%)	30,31,31	2.39	8 (26%)
3	CB3	4-B	2401[D]	-	36,37,37	2.39	16 (44%)	48,51,51	2.60	19 (39%)
2	UMP	3-N	600[C]	-	21,21,21	2.53	5 (23%)	30,31,31	2.40	7 (23%)
2	UMP	3-G	650[C]	-	21,21,21	2.34	3 (14%)	30,31,31	2.47	10 (33%)
2	UMP	2-N	600[B]	-	21,21,21	2.53	5 (23%)	30,31,31	2.38	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UMP	3-C	450[C]	-	-	1/10/22/22	0/2/2/2
2	UMP	4-M	550[D]	-	-	2/10/22/22	0/2/2/2
3	CB3	1-E	2551[A]	-	-	8/27/28/28	0/3/3/3
2	UMP	1-A	350[A]	1	-	1/10/22/22	0/2/2/2
2	UMP	2-E	550[B]	-	-	1/10/22/22	0/2/2/2
3	CB3	2-C	2451[B]	-	-	2/27/28/28	0/3/3/3
3	CB3	1-D	2501[A]	-	-	2/27/28/28	0/3/3/3
2	UMP	4-B	400[D]	-	-	1/10/22/22	0/2/2/2
2	UMP	1-P	700[A]	1	-	3/10/22/22	0/2/2/2
3	CB3	2-A	2351[B]	-	-	2/27/28/28	0/3/3/3
2	UMP	4-O	650[D]	-	-	3/10/22/22	0/2/2/2
3	CB3	2-G	2651[B]	-	-	2/27/28/28	0/3/3/3
2	UMP	4-J	400[D]	-	-	3/10/22/22	0/2/2/2
3	CB3	1-F	2601[A]	-	-	2/27/28/28	0/3/3/3
2	UMP	1-O	650[A]	1	-	3/10/22/22	0/2/2/2
2	UMP	4-K	450[D]	-	-	3/10/22/22	0/2/2/2
2	UMP	2-P	700[B]	-	-	3/10/22/22	0/2/2/2
2	UMP	4-F	600[D]	-	-	0/10/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UMP	3-B	400[C]	-	-	1/10/22/22	0/2/2/2
2	UMP	1-J	400[A]	1	-	3/10/22/22	0/2/2/2
3	CB3	2-D	2501[B]	-	-	2/27/28/28	0/3/3/3
2	UMP	1-H	700[A]	1	-	0/10/22/22	0/2/2/2
2	UMP	4-C	450[D]	-	-	1/10/22/22	0/2/2/2
3	CB3	2-F	2601[B]	-	-	2/27/28/28	0/3/3/3
3	CB3	3-B	2401[C]	-	-	2/27/28/28	0/3/3/3
3	CB3	4-E	2551[D]	-	-	8/27/28/28	0/3/3/3
2	UMP	1-E	550[A]	1	-	1/10/22/22	0/2/2/2
2	UMP	3-K	450[C]	-	-	3/10/22/22	0/2/2/2
2	UMP	2-O	650[B]	-	-	3/10/22/22	0/2/2/2
2	UMP	1-I	350[A]	1	-	1/10/22/22	0/2/2/2
2	UMP	1-F	600[A]	1	-	0/10/22/22	0/2/2/2
2	UMP	4-N	600[D]	-	-	2/10/22/22	0/2/2/2
3	CB3	1-A	2351[A]	-	-	2/27/28/28	0/3/3/3
3	CB3	3-E	2551[C]	-	-	8/27/28/28	0/3/3/3
2	UMP	2-M	550[B]	-	-	2/10/22/22	0/2/2/2
3	CB3	4-D	2501[D]	-	-	2/27/28/28	0/3/3/3
3	CB3	3-F	2601[C]	-	-	2/27/28/28	0/3/3/3
2	UMP	1-B	400[A]	1	-	1/10/22/22	0/2/2/2
2	UMP	2-D	500[B]	-	-	1/10/22/22	0/2/2/2
2	UMP	4-G	650[D]	-	-	2/10/22/22	0/2/2/2
3	CB3	2-B	2401[B]	-	-	2/27/28/28	0/3/3/3
2	UMP	1-G	650[A]	1	-	2/10/22/22	0/2/2/2
2	UMP	1-M	550[A]	1	-	2/10/22/22	0/2/2/2
2	UMP	3-F	600[C]	-	-	0/10/22/22	0/2/2/2
2	UMP	3-A	350[C]	-	-	1/10/22/22	0/2/2/2
2	UMP	1-D	500[A]	1	-	1/10/22/22	0/2/2/2
2	UMP	3-L	500[C]	-	-	3/10/22/22	0/2/2/2
2	UMP	3-D	500[C]	-	-	1/10/22/22	0/2/2/2
2	UMP	4-D	500[D]	-	-	1/10/22/22	0/2/2/2
2	UMP	2-H	700[B]	-	-	0/10/22/22	0/2/2/2
2	UMP	3-I	350[C]	-	-	1/10/22/22	0/2/2/2
3	CB3	1-H	2701[A]	-	-	2/27/28/28	0/3/3/3
2	UMP	4-H	700[D]	-	-	0/10/22/22	0/2/2/2
2	UMP	2-B	400[B]	-	-	1/10/22/22	0/2/2/2
2	UMP	2-F	600[B]	-	-	0/10/22/22	0/2/2/2
3	CB3	3-H	2701[C]	-	-	2/27/28/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CB3	4-G	2651[D]	-	-	2/27/28/28	0/3/3/3
2	UMP	3-M	550[C]	-	-	2/10/22/22	0/2/2/2
2	UMP	2-C	450[B]	-	-	1/10/22/22	0/2/2/2
2	UMP	3-J	400[C]	-	-	3/10/22/22	0/2/2/2
2	UMP	1-C	450[A]	1	-	1/10/22/22	0/2/2/2
2	UMP	4-E	550[D]	-	-	1/10/22/22	0/2/2/2
2	UMP	2-G	650[B]	-	-	2/10/22/22	0/2/2/2
2	UMP	4-L	500[D]	-	-	3/10/22/22	0/2/2/2
3	CB3	1-G	2651[A]	-	-	2/27/28/28	0/3/3/3
2	UMP	1-K	450[A]	1	-	3/10/22/22	0/2/2/2
3	CB3	2-H	2701[B]	-	-	2/27/28/28	0/3/3/3
3	CB3	4-A	2351[D]	-	-	2/27/28/28	0/3/3/3
2	UMP	4-I	350[D]	-	-	1/10/22/22	0/2/2/2
2	UMP	2-K	450[B]	-	-	3/10/22/22	0/2/2/2
2	UMP	1-L	500[A]	1	-	3/10/22/22	0/2/2/2
3	CB3	3-D	2501[C]	-	-	2/27/28/28	0/3/3/3
3	CB3	3-A	2351[C]	-	-	2/27/28/28	0/3/3/3
3	CB3	1-B	2401[A]	-	-	2/27/28/28	0/3/3/3
2	UMP	2-I	350[B]	-	-	1/10/22/22	0/2/2/2
3	CB3	4-F	2601[D]	-	-	2/27/28/28	0/3/3/3
3	CB3	4-H	2701[D]	-	-	2/27/28/28	0/3/3/3
2	UMP	1-N	600[A]	1	-	2/10/22/22	0/2/2/2
3	CB3	3-C	2451[C]	-	-	2/27/28/28	0/3/3/3
2	UMP	3-H	700[C]	-	-	0/10/22/22	0/2/2/2
2	UMP	3-P	700[C]	-	-	3/10/22/22	0/2/2/2
2	UMP	2-A	350[B]	-	-	1/10/22/22	0/2/2/2
3	CB3	4-C	2451[D]	-	-	2/27/28/28	0/3/3/3
2	UMP	3-O	650[C]	-	-	3/10/22/22	0/2/2/2
3	CB3	1-C	2451[A]	-	-	2/27/28/28	0/3/3/3
2	UMP	2-L	500[B]	-	-	3/10/22/22	0/2/2/2
3	CB3	3-G	2651[C]	-	-	2/27/28/28	0/3/3/3
2	UMP	3-E	550[C]	-	-	1/10/22/22	0/2/2/2
3	CB3	2-E	2551[B]	-	-	8/27/28/28	0/3/3/3
2	UMP	2-J	400[B]	-	-	3/10/22/22	0/2/2/2
2	UMP	4-P	700[D]	-	-	3/10/22/22	0/2/2/2
2	UMP	4-A	350[D]	-	-	1/10/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CB3	4-B	2401[D]	-	-	2/27/28/28	0/3/3/3
2	UMP	3-N	600[C]	-	-	2/10/22/22	0/2/2/2
2	UMP	3-G	650[C]	-	-	2/10/22/22	0/2/2/2
2	UMP	2-N	600[B]	-	-	2/10/22/22	0/2/2/2

The worst 5 of 771 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-L	500[A]	UMP	C6-C5	8.35	1.54	1.35
2	1-P	700[A]	UMP	C6-C5	8.35	1.54	1.35
2	1-I	350[A]	UMP	C6-C5	8.35	1.54	1.35
2	4-K	450[D]	UMP	C6-C5	8.34	1.54	1.35
2	3-J	400[C]	UMP	C6-C5	8.34	1.54	1.35

The worst 5 of 1033 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-A	2351[A]	CB3	C4A-C8A-N1	-9.96	117.76	123.56
3	2-A	2351[B]	CB3	C4A-C8A-N1	-9.96	117.76	123.56
3	3-A	2351[C]	CB3	C4A-C8A-N1	-9.96	117.76	123.56
3	4-A	2351[D]	CB3	C4A-C8A-N1	-9.96	117.76	123.56
3	1-H	2701[A]	CB3	N1-C2-N3	-9.41	115.25	127.21

There are no chirality outliers.

5 of 196 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1-J	400[A]	UMP	C5'-O5'-P-OP1
2	2-J	400[B]	UMP	C5'-O5'-P-OP1
2	3-J	400[C]	UMP	C5'-O5'-P-OP1
2	4-J	400[D]	UMP	C5'-O5'-P-OP1
2	4-J	400[D]	UMP	C5'-O5'-P-OP3

There are no ring outliers.

56 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	4-M	550[D]	UMP	1	0
3	2-C	2451[B]	CB3	1	0
3	1-D	2501[A]	CB3	1	0

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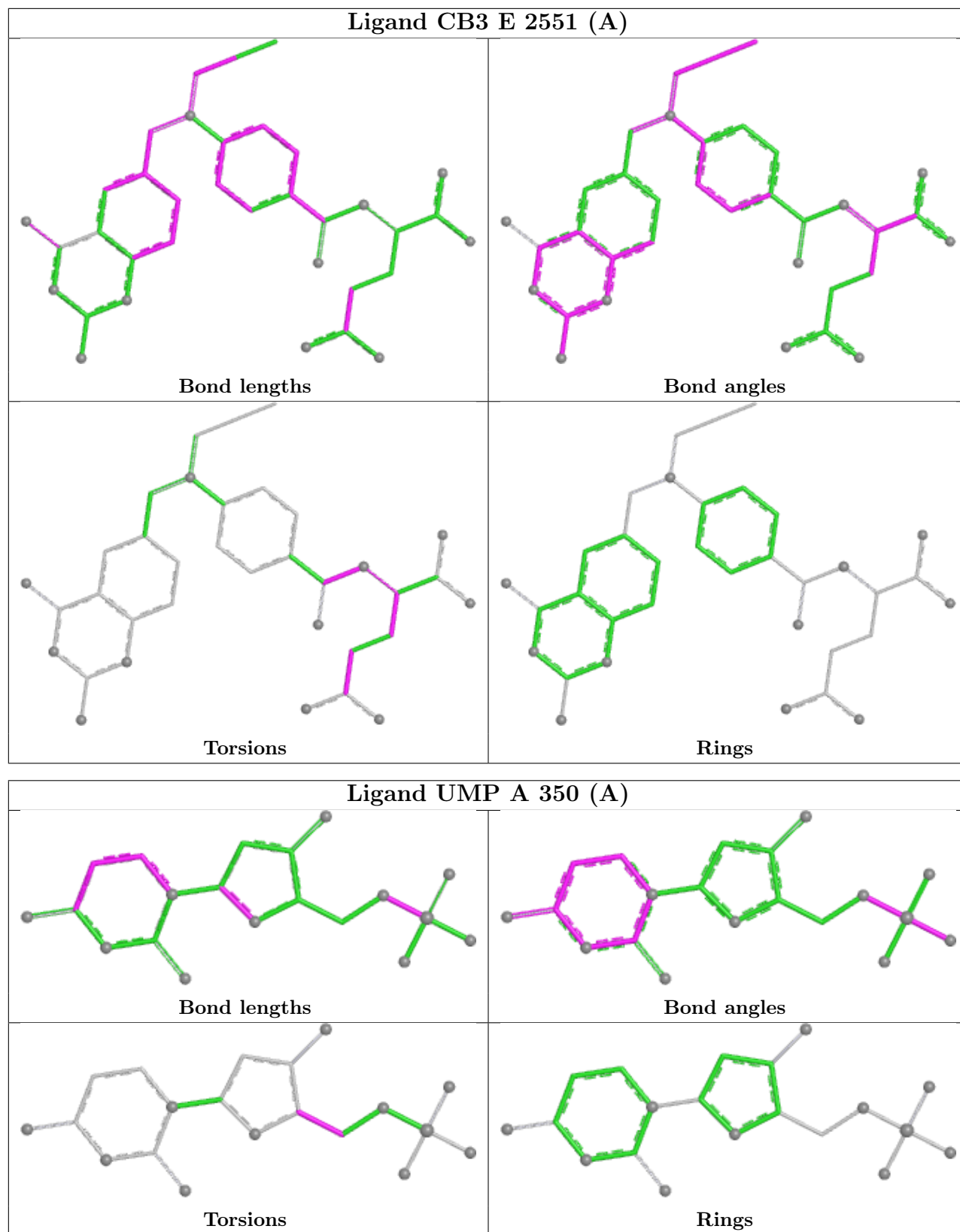
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1-P	700[A]	UMP	1	0
3	2-A	2351[B]	CB3	1	0
2	4-O	650[D]	UMP	1	0
2	4-J	400[D]	UMP	1	0
3	1-F	2601[A]	CB3	1	0
2	1-O	650[A]	UMP	1	0
2	4-K	450[D]	UMP	1	0
2	2-P	700[B]	UMP	1	0
2	1-J	400[A]	UMP	1	0
3	2-D	2501[B]	CB3	1	0
3	2-F	2601[B]	CB3	1	0
3	3-B	2401[C]	CB3	1	0
2	3-K	450[C]	UMP	1	0
2	2-O	650[B]	UMP	1	0
2	1-I	350[A]	UMP	1	0
2	4-N	600[D]	UMP	1	0
3	1-A	2351[A]	CB3	1	0
2	2-M	550[B]	UMP	1	0
3	4-D	2501[D]	CB3	1	0
3	3-F	2601[C]	CB3	1	0
3	2-B	2401[B]	CB3	1	0
2	1-M	550[A]	UMP	1	0
2	3-L	500[C]	UMP	1	0
2	3-I	350[C]	UMP	1	0
3	1-H	2701[A]	CB3	1	0
3	3-H	2701[C]	CB3	1	0
2	3-M	550[C]	UMP	1	0
2	3-J	400[C]	UMP	1	0
2	4-L	500[D]	UMP	1	0
2	1-K	450[A]	UMP	1	0
3	2-H	2701[B]	CB3	1	0
3	4-A	2351[D]	CB3	1	0
2	4-I	350[D]	UMP	1	0
2	2-K	450[B]	UMP	1	0
2	1-L	500[A]	UMP	1	0
3	3-D	2501[C]	CB3	1	0
3	3-A	2351[C]	CB3	1	0
3	1-B	2401[A]	CB3	1	0
2	2-I	350[B]	UMP	1	0
3	4-F	2601[D]	CB3	1	0
3	4-H	2701[D]	CB3	1	0
2	1-N	600[A]	UMP	1	0

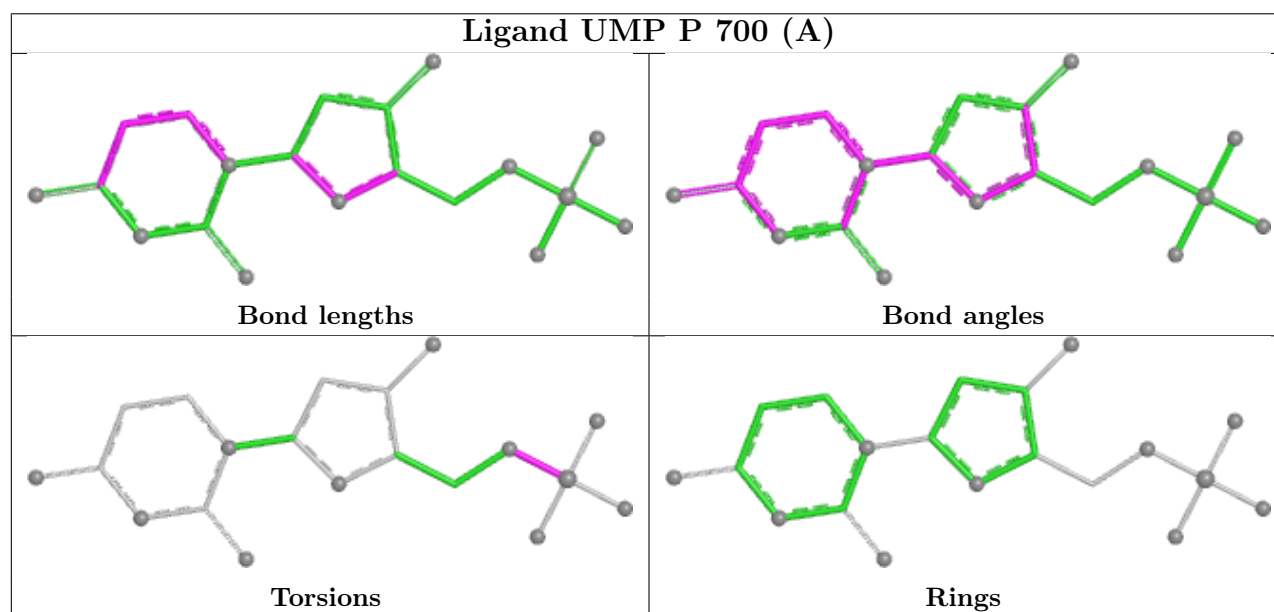
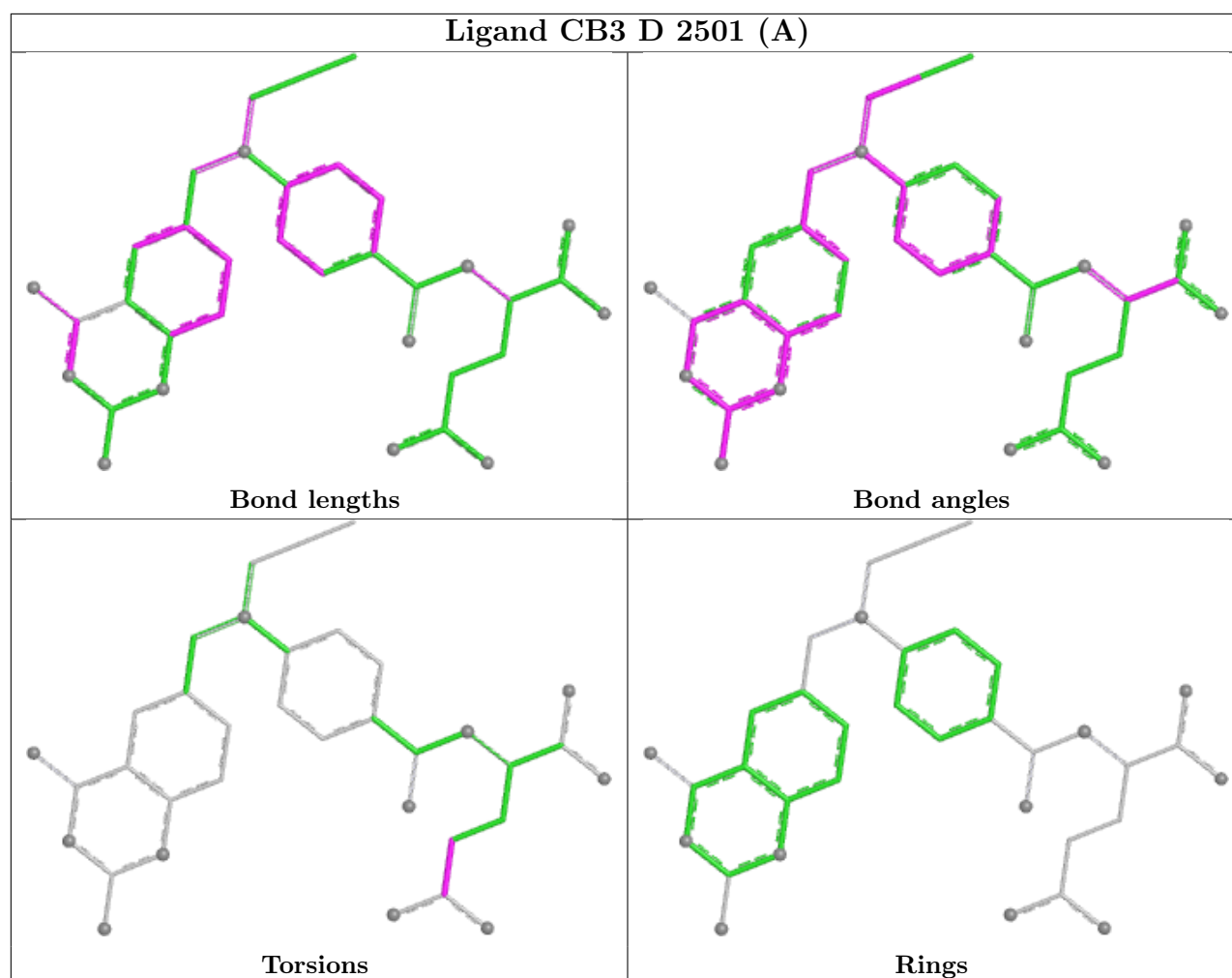
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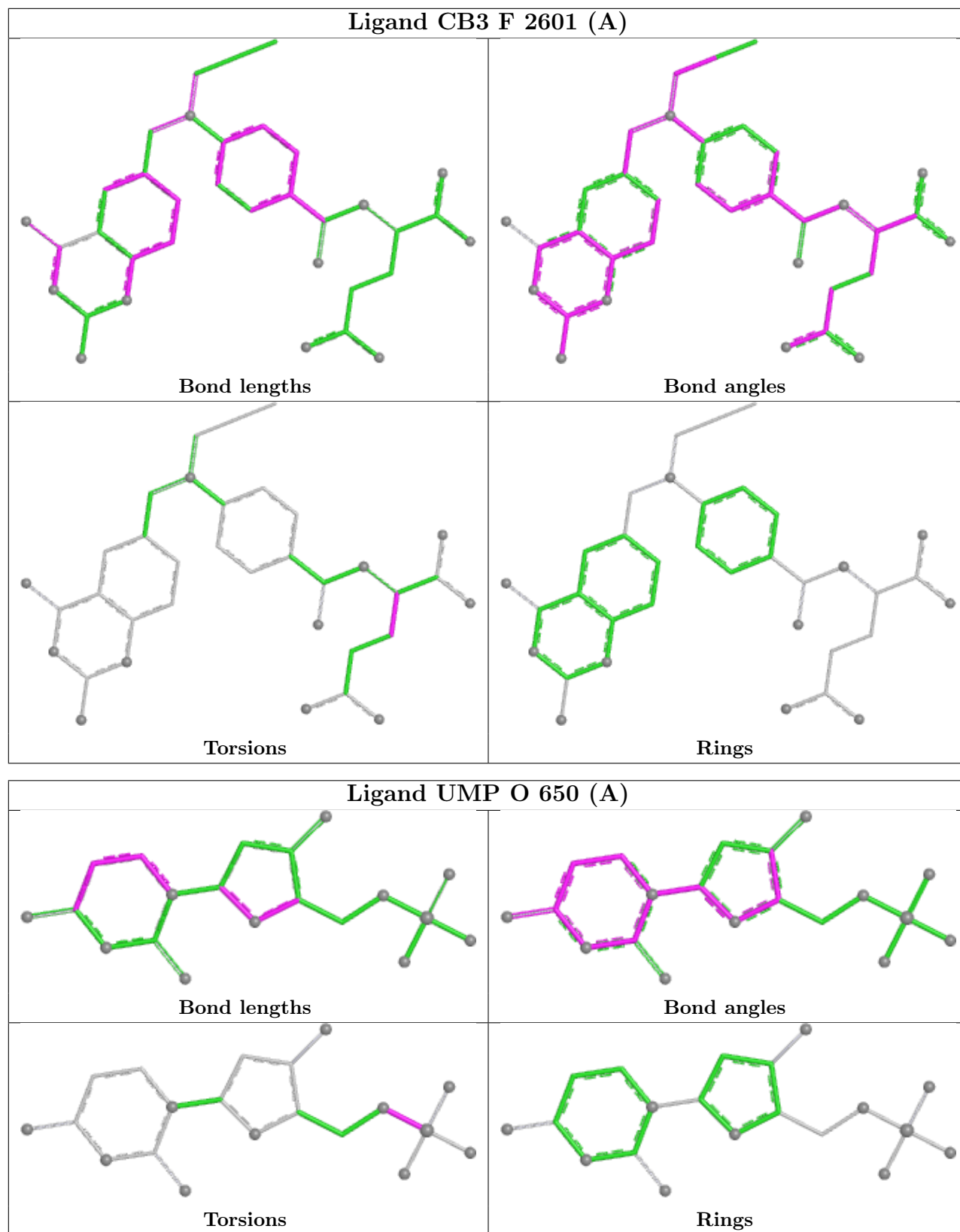
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	3-C	2451[C]	CB3	1	0
2	3-P	700[C]	UMP	1	0
3	4-C	2451[D]	CB3	1	0
2	3-O	650[C]	UMP	1	0
3	1-C	2451[A]	CB3	1	0
2	2-L	500[B]	UMP	1	0
2	2-J	400[B]	UMP	1	0
2	4-P	700[D]	UMP	1	0
3	4-B	2401[D]	CB3	1	0
2	3-N	600[C]	UMP	1	0
2	2-N	600[B]	UMP	1	0

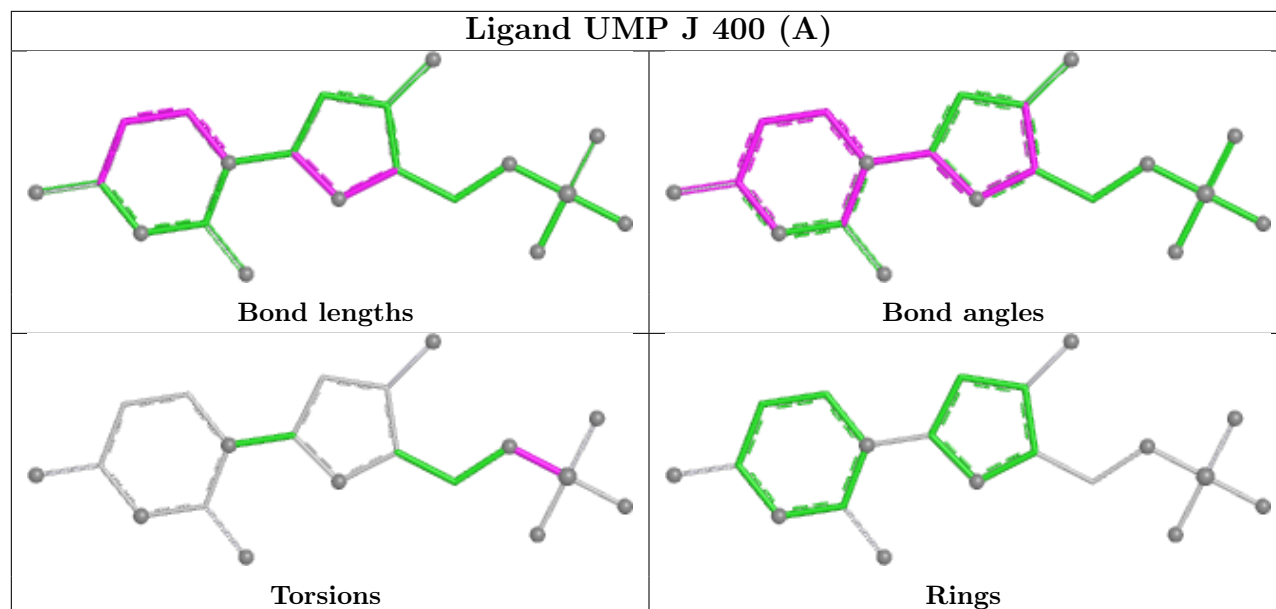
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



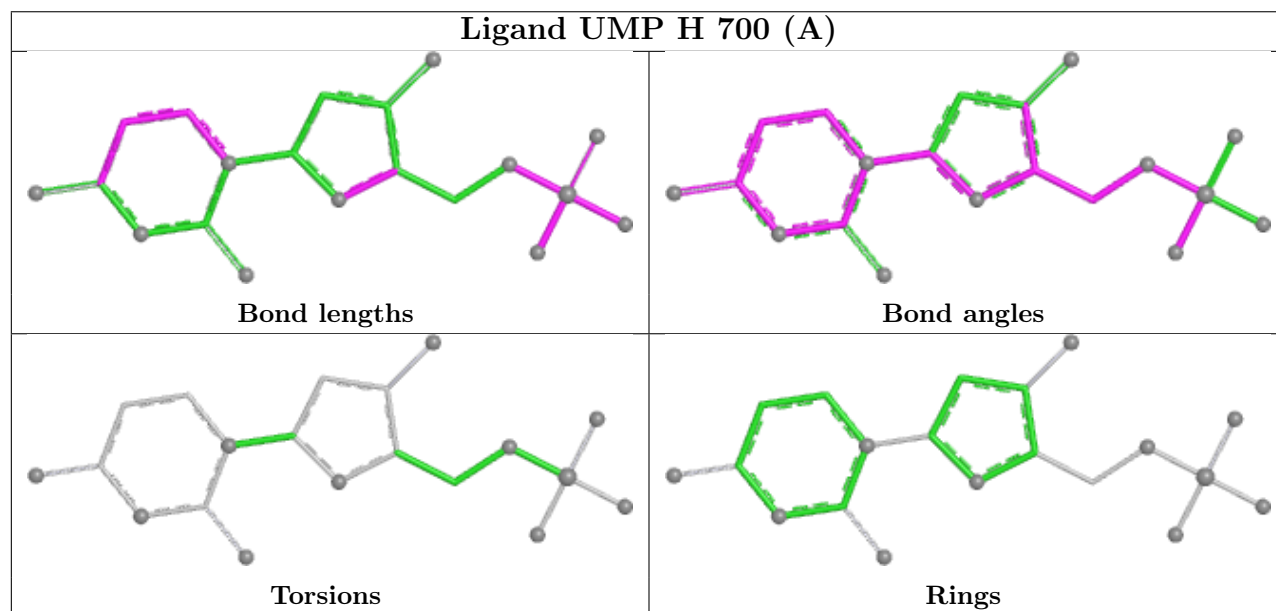


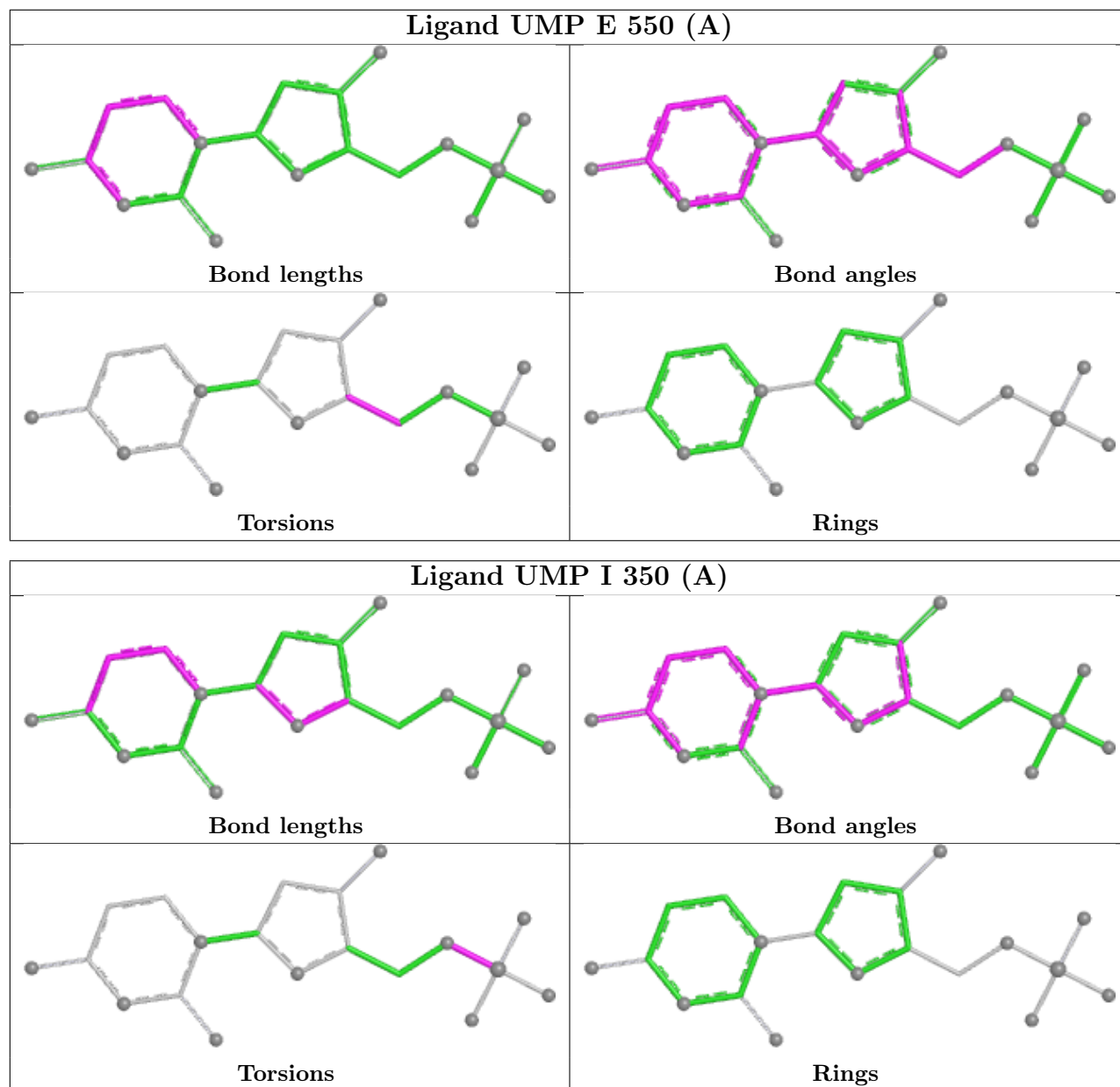


Ligand UMP J 400 (A)

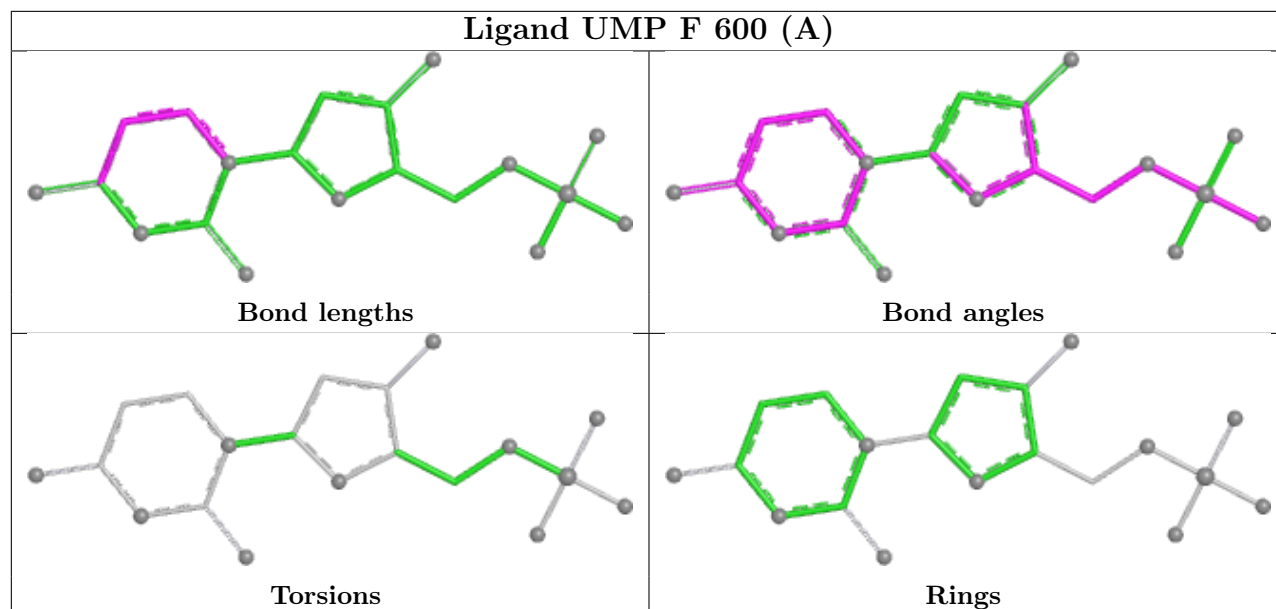


Ligand UMP H 700 (A)

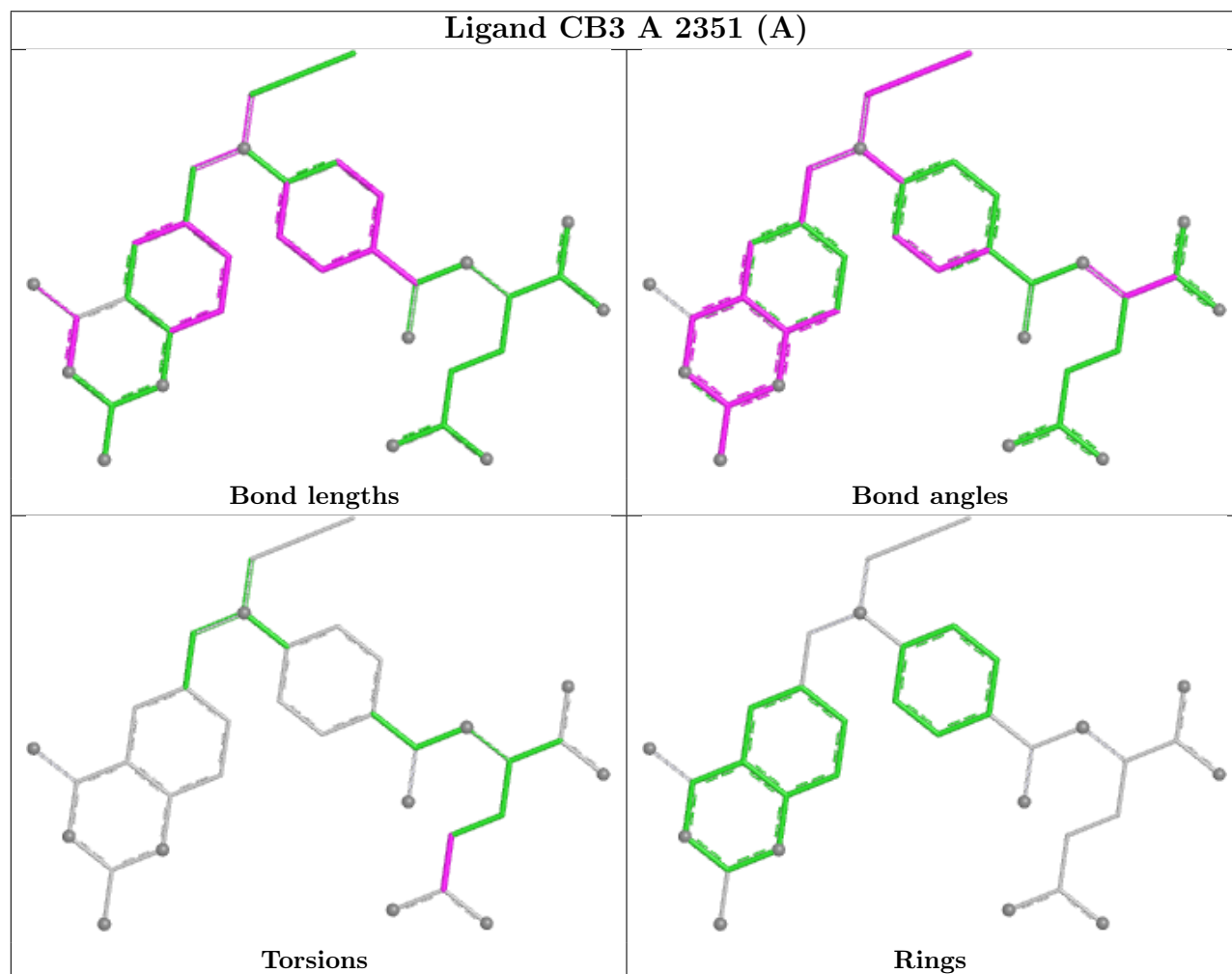


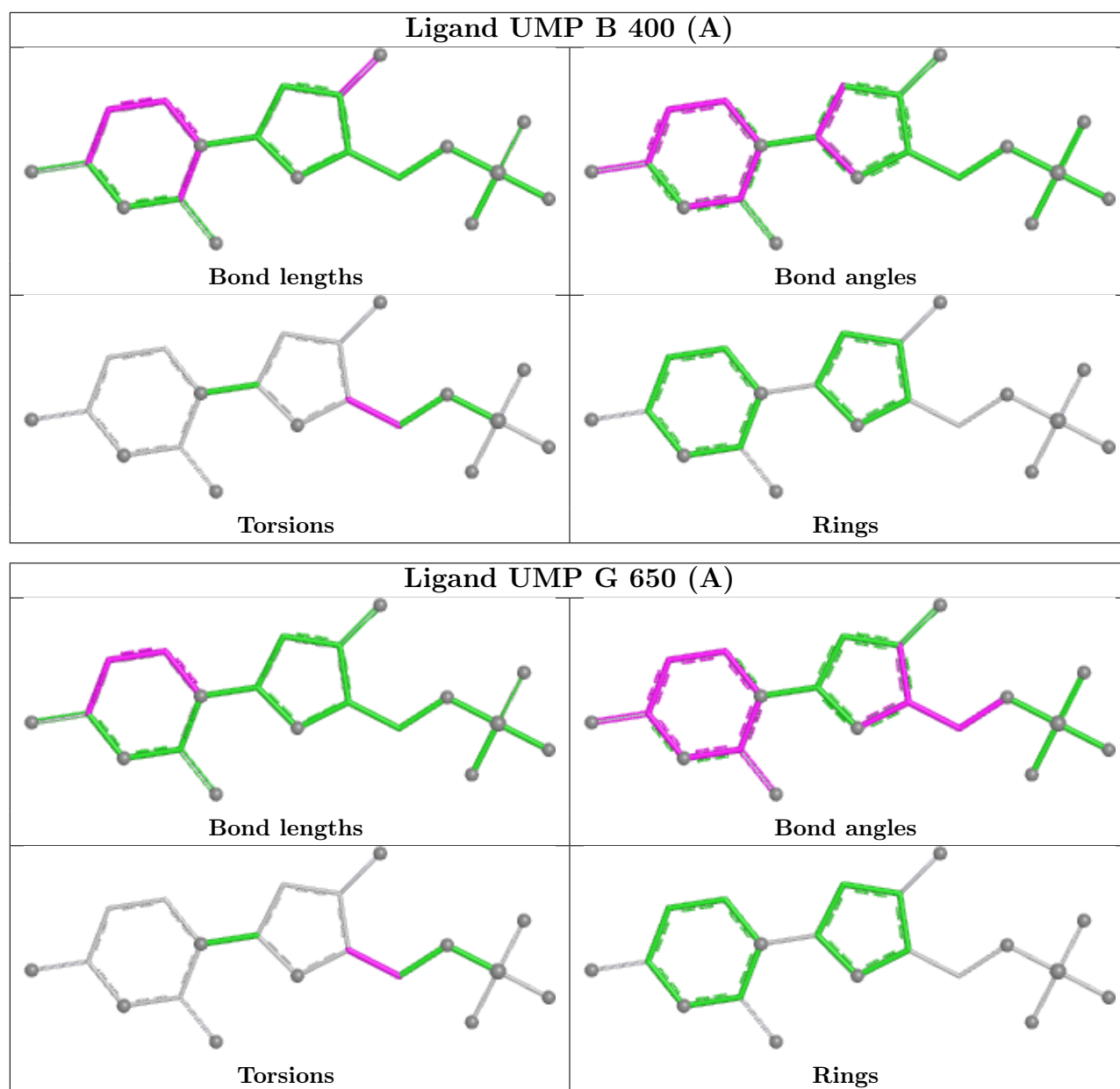


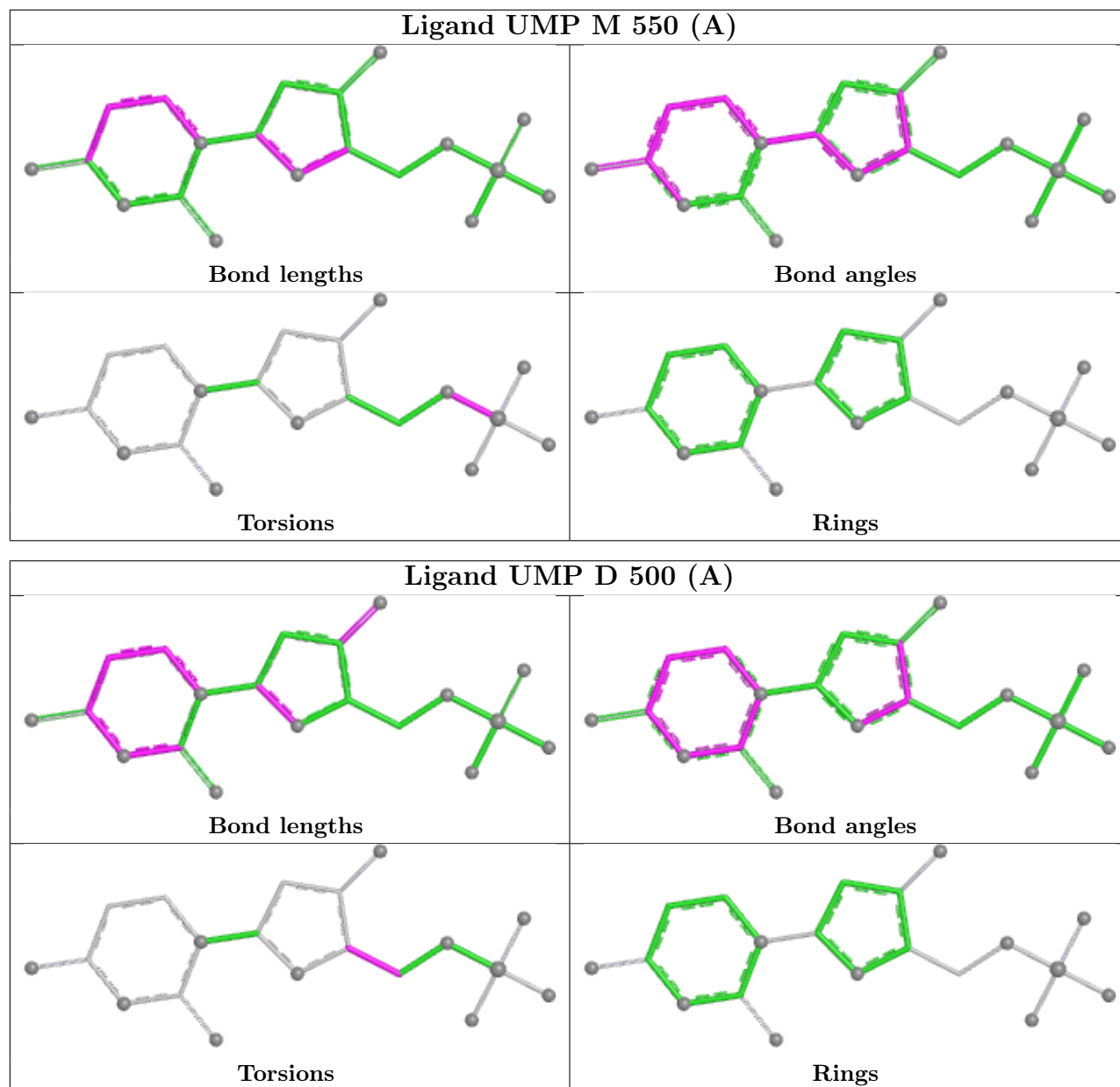
Ligand UMP F 600 (A)

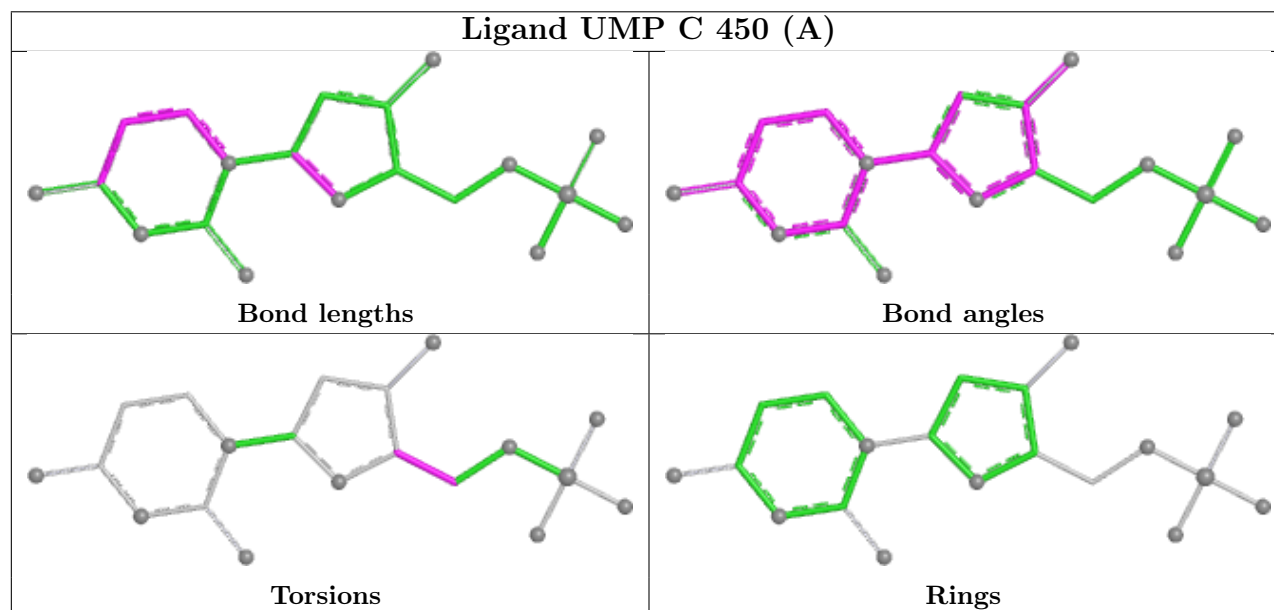
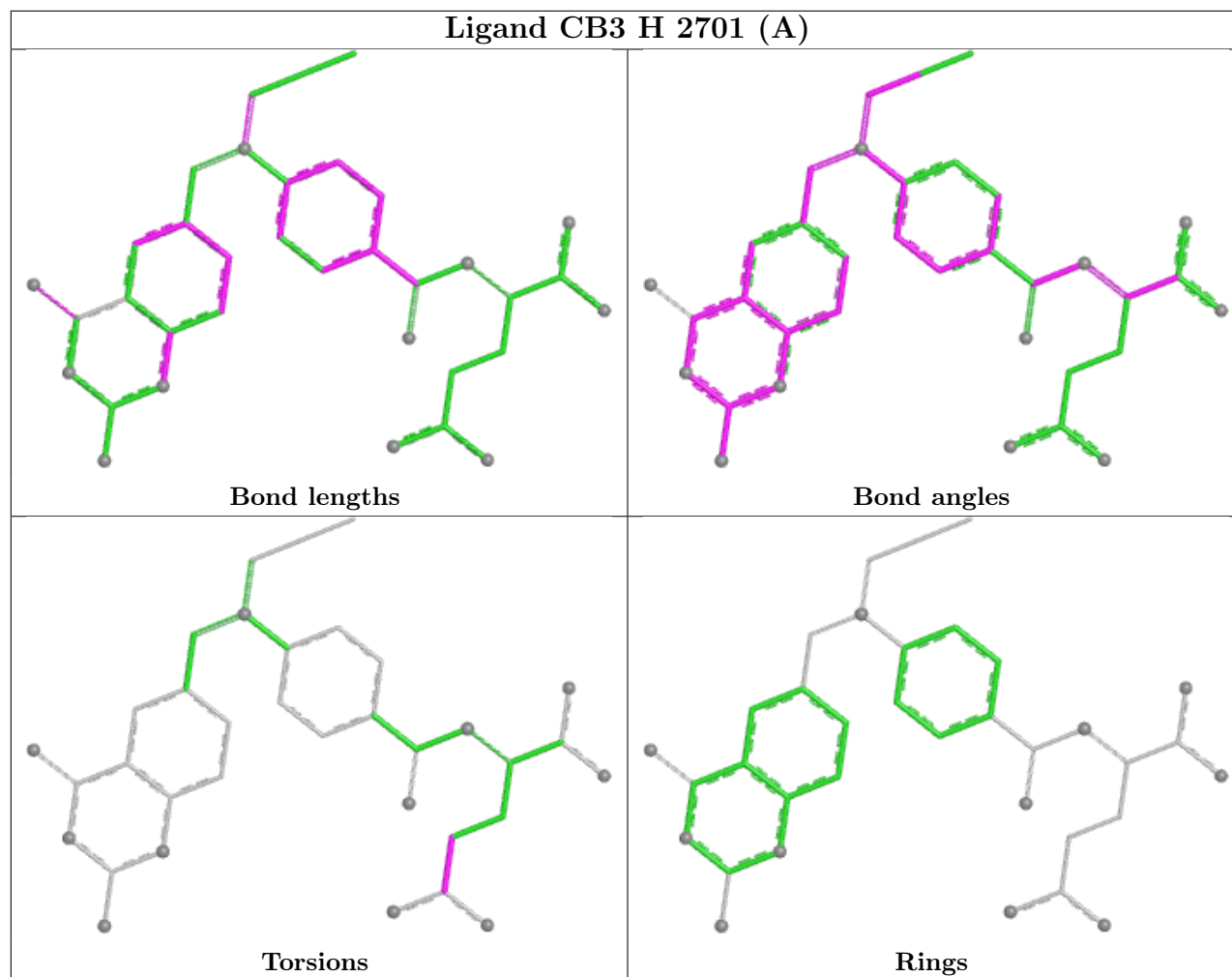


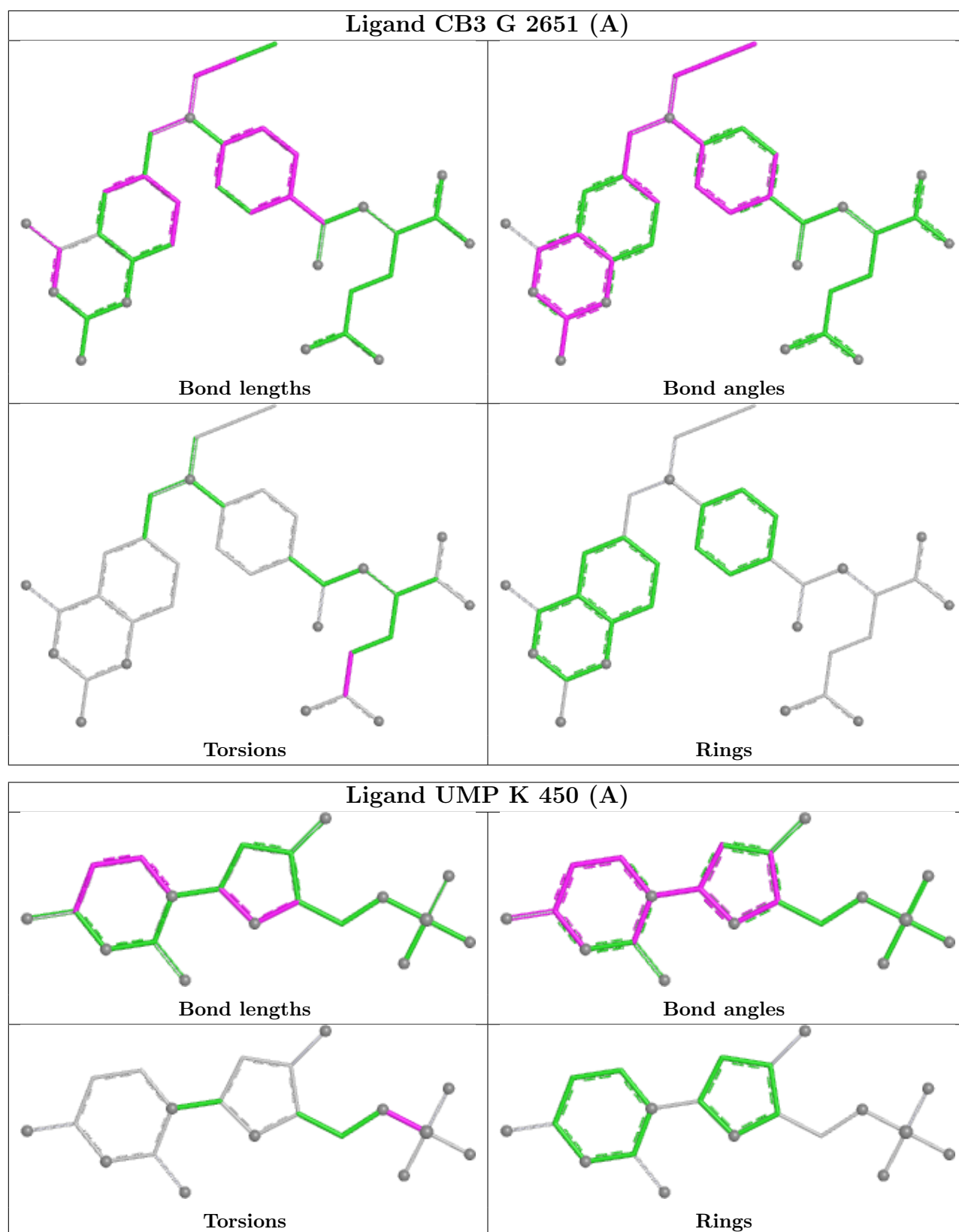
Ligand CB3 A 2351 (A)



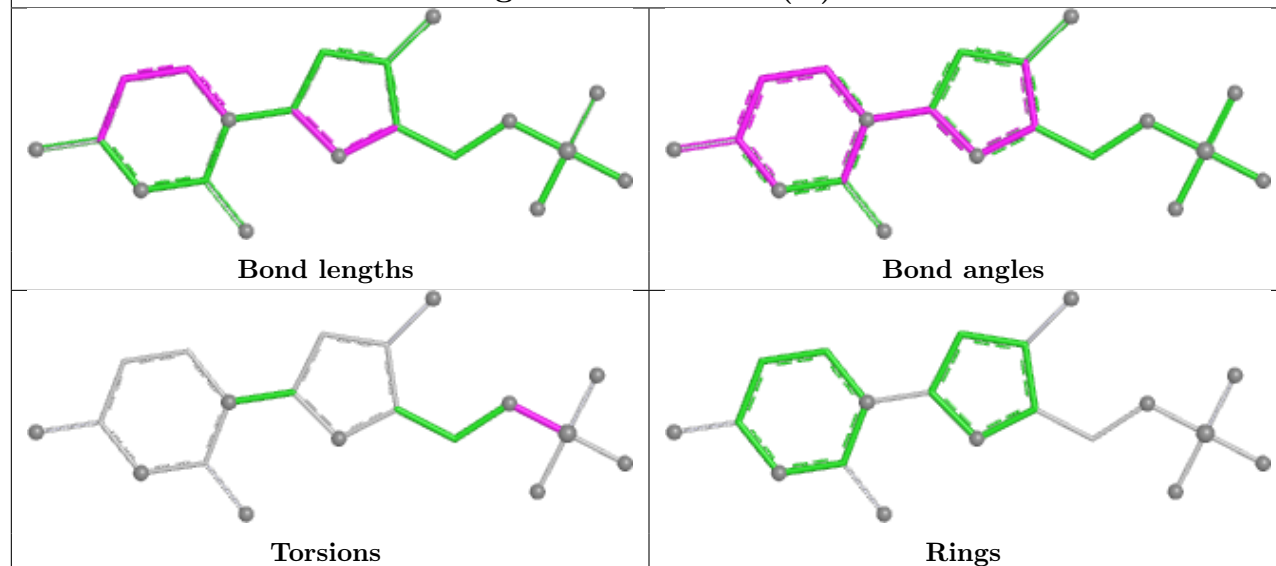




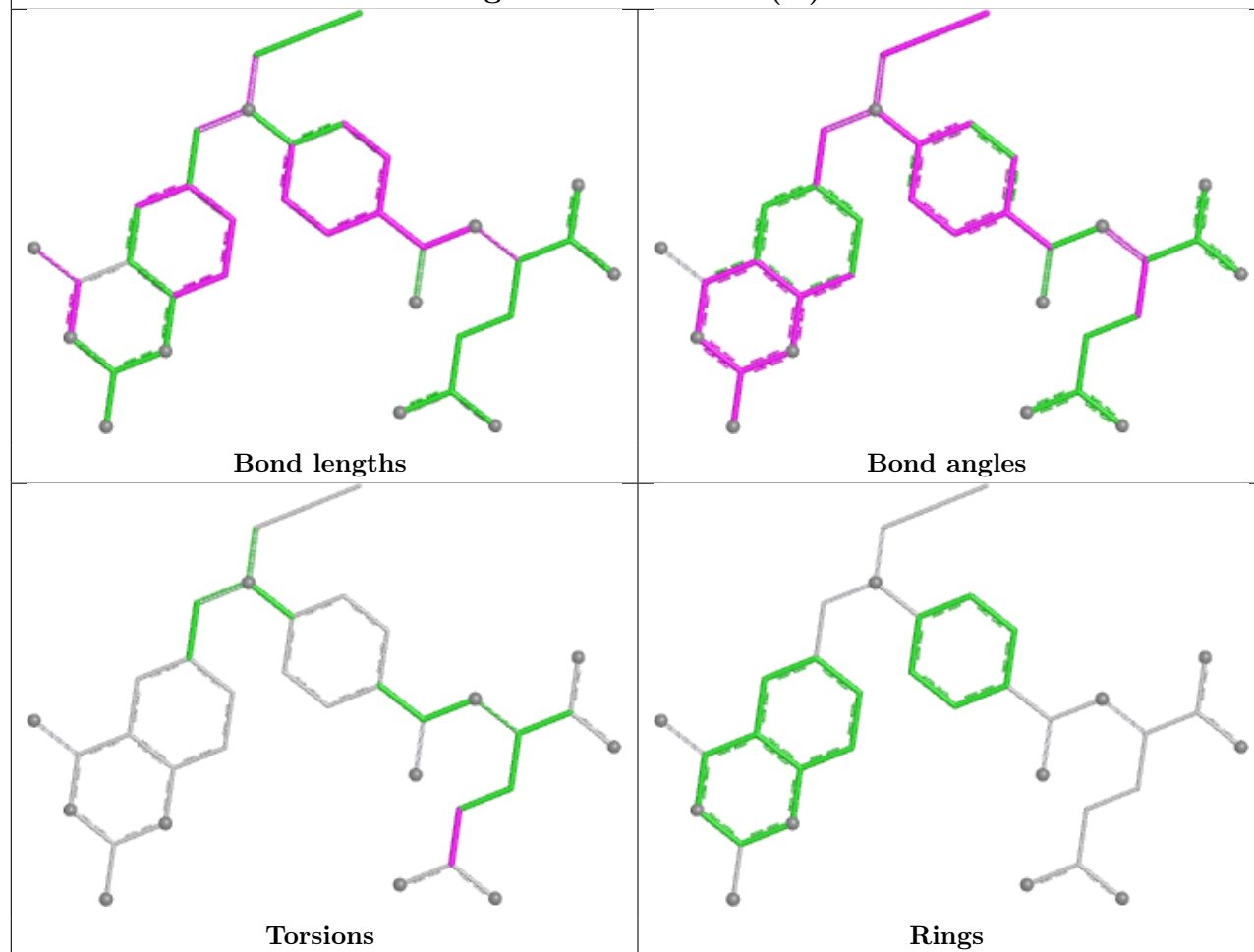




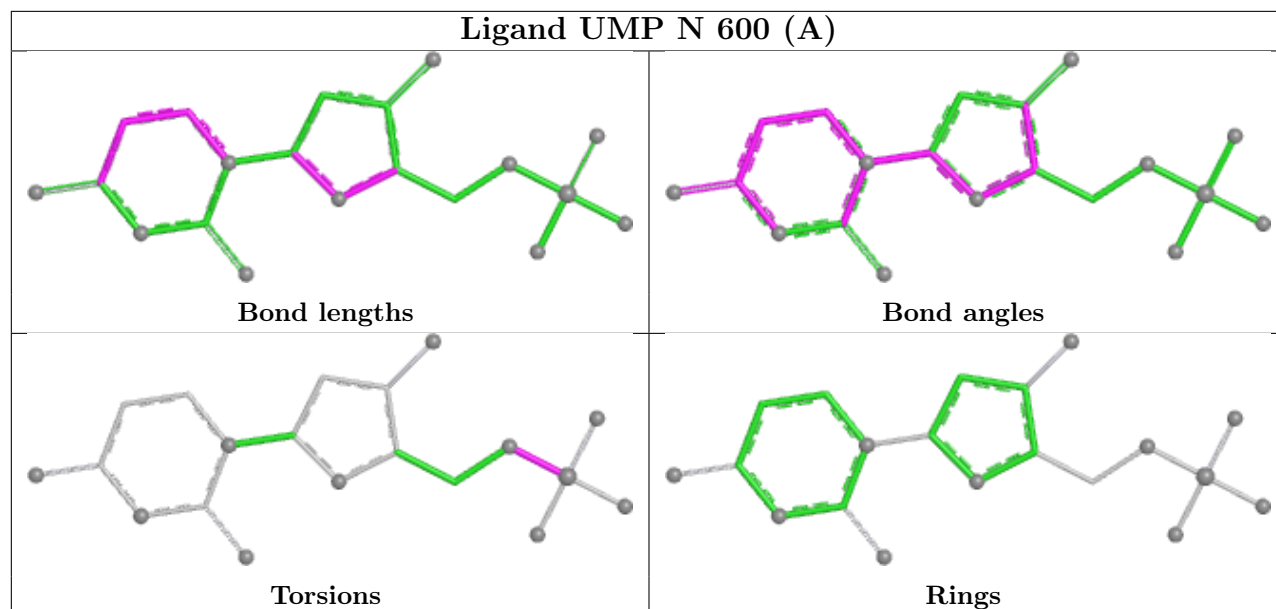
Ligand UMP L 500 (A)



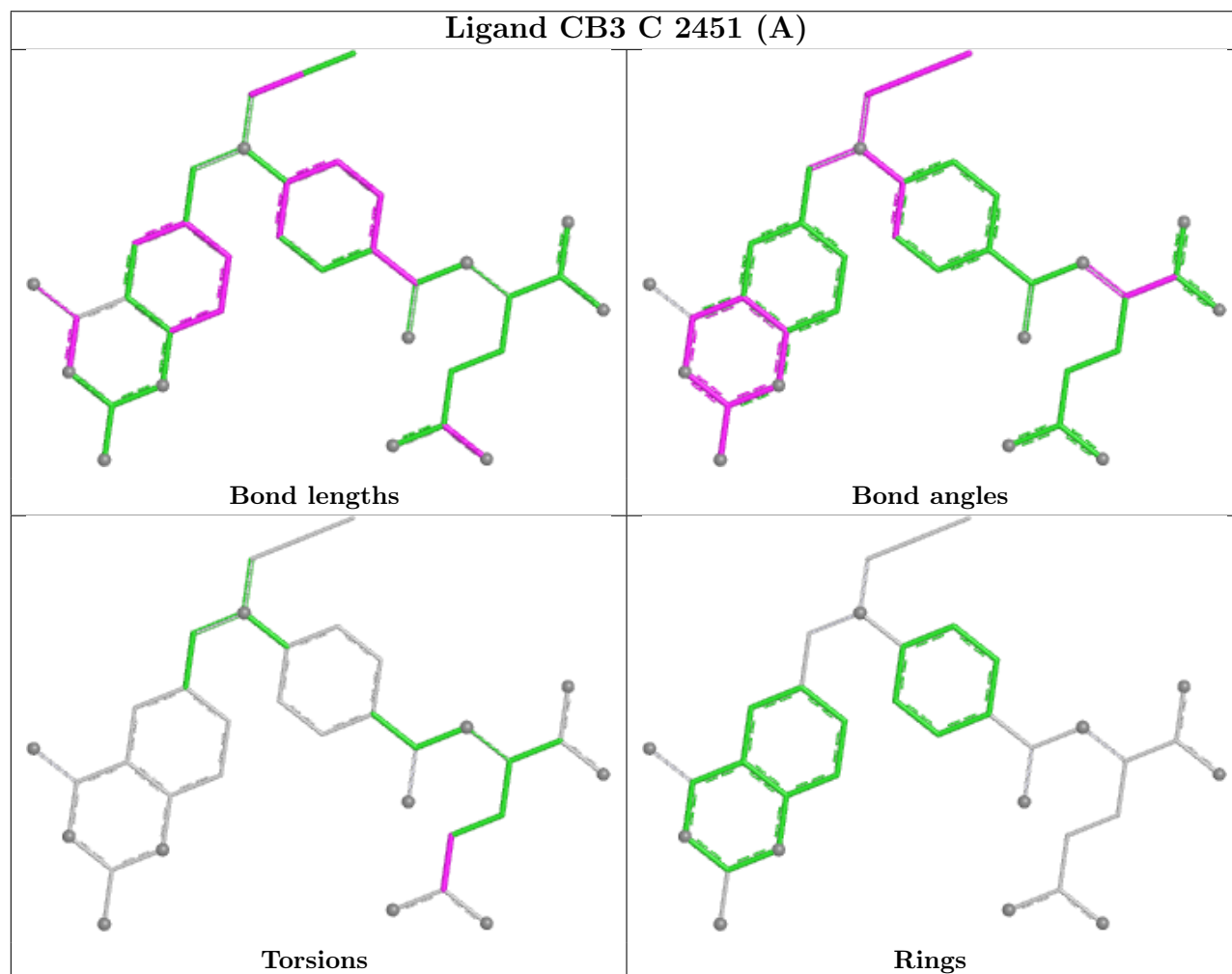
Ligand CB3 B 2401 (A)



Ligand UMP N 600 (A)



Ligand CB3 C 2451 (A)



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	305/317 (96%)	0.15	6 (1%) 64 66	4, 7, 10, 15	305 (100%)
1	1-B	305/317 (96%)	0.15	5 (1%) 70 72	5, 7, 11, 16	305 (100%)
1	1-C	305/317 (96%)	0.13	8 (2%) 57 59	4, 6, 10, 15	305 (100%)
1	1-D	305/317 (96%)	0.14	3 (0%) 79 80	5, 7, 10, 16	305 (100%)
1	1-E	305/317 (96%)	0.17	7 (2%) 61 62	4, 7, 11, 16	305 (100%)
1	1-F	305/317 (96%)	0.23	4 (1%) 74 76	4, 7, 10, 16	305 (100%)
1	1-G	305/317 (96%)	0.12	3 (0%) 79 80	5, 7, 10, 16	305 (100%)
1	1-H	305/317 (96%)	0.24	6 (1%) 64 66	4, 7, 10, 16	305 (100%)
1	1-I	299/317 (94%)	1.05	33 (11%) 12 13	3, 5, 7, 10	299 (100%)
1	1-J	299/317 (94%)	1.07	38 (12%) 9 10	3, 5, 7, 10	299 (100%)
1	1-K	299/317 (94%)	1.00	33 (11%) 12 13	3, 5, 7, 10	299 (100%)
1	1-L	299/317 (94%)	1.02	42 (14%) 7 8	3, 5, 7, 10	299 (100%)
1	1-M	299/317 (94%)	1.09	41 (13%) 8 8	3, 5, 7, 10	299 (100%)
1	1-N	299/317 (94%)	1.11	43 (14%) 7 8	3, 5, 7, 10	299 (100%)
1	1-O	299/317 (94%)	0.94	30 (10%) 14 15	3, 5, 7, 10	299 (100%)
1	1-P	299/317 (94%)	1.00	34 (11%) 11 12	3, 5, 7, 10	299 (100%)
1	2-A	0/317	-	-	-	-
1	2-B	0/317	-	-	-	-
1	2-C	0/317	-	-	-	-
1	2-D	0/317	-	-	-	-
1	2-E	0/317	-	-	-	-
1	2-F	0/317	-	-	-	-
1	2-G	0/317	-	-	-	-
1	2-H	0/317	-	-	-	-
1	2-I	0/317	-	-	-	-
1	2-J	0/317	-	-	-	-
1	2-K	0/317	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2-L	0/317	-	-	-	-
1	2-M	0/317	-	-	-	-
1	2-N	0/317	-	-	-	-
1	2-O	0/317	-	-	-	-
1	2-P	0/317	-	-	-	-
1	3-A	0/317	-	-	-	-
1	3-B	0/317	-	-	-	-
1	3-C	0/317	-	-	-	-
1	3-D	0/317	-	-	-	-
1	3-E	0/317	-	-	-	-
1	3-F	0/317	-	-	-	-
1	3-G	0/317	-	-	-	-
1	3-H	0/317	-	-	-	-
1	3-I	0/317	-	-	-	-
1	3-J	0/317	-	-	-	-
1	3-K	0/317	-	-	-	-
1	3-L	0/317	-	-	-	-
1	3-M	0/317	-	-	-	-
1	3-N	0/317	-	-	-	-
1	3-O	0/317	-	-	-	-
1	3-P	0/317	-	-	-	-
1	4-A	0/317	-	-	-	-
1	4-B	0/317	-	-	-	-
1	4-C	0/317	-	-	-	-
1	4-D	0/317	-	-	-	-
1	4-E	0/317	-	-	-	-
1	4-F	0/317	-	-	-	-
1	4-G	0/317	-	-	-	-
1	4-H	0/317	-	-	-	-
1	4-I	0/317	-	-	-	-
1	4-J	0/317	-	-	-	-
1	4-K	0/317	-	-	-	-
1	4-L	0/317	-	-	-	-
1	4-M	0/317	-	-	-	-
1	4-N	0/317	-	-	-	-
1	4-O	0/317	-	-	-	-
1	4-P	0/317	-	-	-	-
All	All	4832/20288 (23%)	0.60	336 (6%) 24 25	3, 6, 9, 16	4832 (100%)

The worst 5 of 336 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-L	105[A]	GLY	16.6
1	1-M	44[A]	GLY	8.1
1	1-O	76[A]	VAL	7.4
1	1-K	86[A]	GLY	6.7
1	1-K	75[A]	GLY	6.6

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.