



Full wwPDB NMR Structure Validation Report ⓘ

Mar 15, 2026 – 03:40 PM UTC

PDB ID : 2V93 / pdb_00002v93
Title : EQUILLIBRIUM MIXTURE OF OPEN AND PARTIALLY-CLOSED SPECIES IN THE APO STATE OF MALTODEXTRIN-BINDING PROTEIN BY PARAMAGNETIC RELAXATION ENHANCEMENT NMR
Authors : Clore, G.M.; Tang, C.
Deposited on : 2007-08-21

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

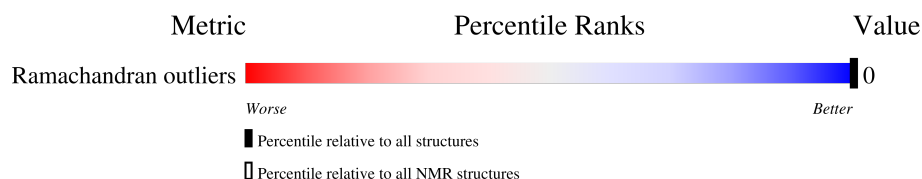
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

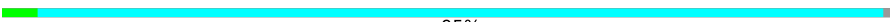
The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Ramachandran outliers	224038	12848

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	370	 95%

2 Ensemble composition and analysis ⓘ

This entry contains 50 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:81-A:87, A:103-A:105, A:266-A:268, A:311-A:313 (16)	0.00	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: No clusters in NmrClust output

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3792 atoms, of which 1003 are hydrogens and 0 are deuteriums.

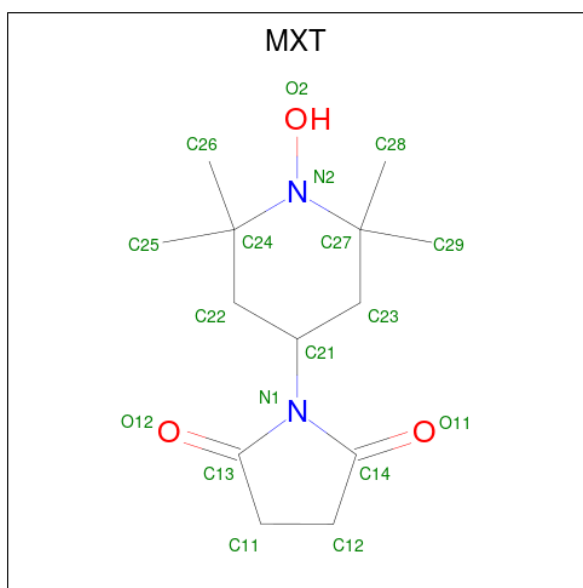
- Molecule 1 is a protein called MALTOSE-BINDING PERIPLASMIC PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	366	Total	C	H	N	O	S	0
			2904	1169	547	583	581	24	

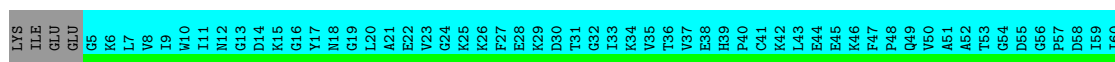
There are 2 discrepancies between the modelled and reference sequences:

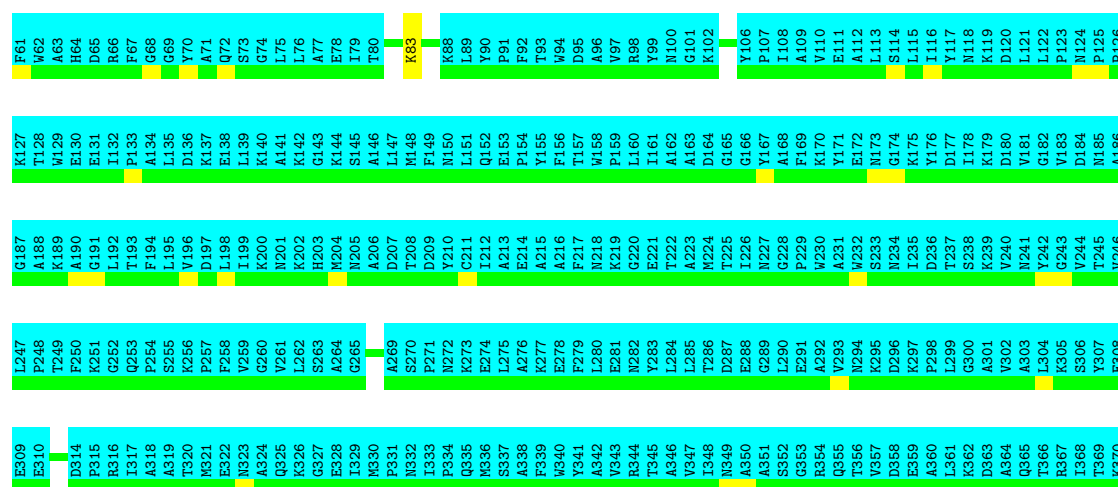
Chain	Residue	Modelled	Actual	Comment	Reference
A	41	CYS	ASP	engineered mutation	UNP P0AEY0
A	211	CYS	SER	engineered mutation	UNP P0AEY0

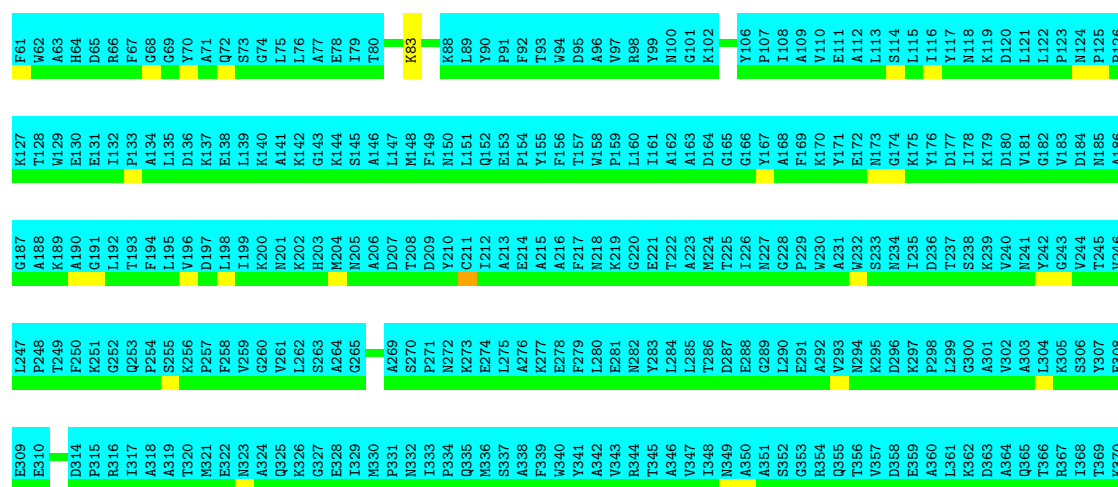
- Molecule 2 is 1-(1-HYDROXY-2,2,6,6-TETRAMETHYLPYRROLIDIN-4-YL)PYRROLIDIN E-2,5-DIONE (CCD ID: MXT) (formula: $C_{13}H_{22}N_2O_3$).



Mol	Chain	Residues	Atoms				
2	A	1	Total	C	H	N	O
			444	156	228	24	36
2	A	1	Total	C	H	N	O
			444	156	228	24	36



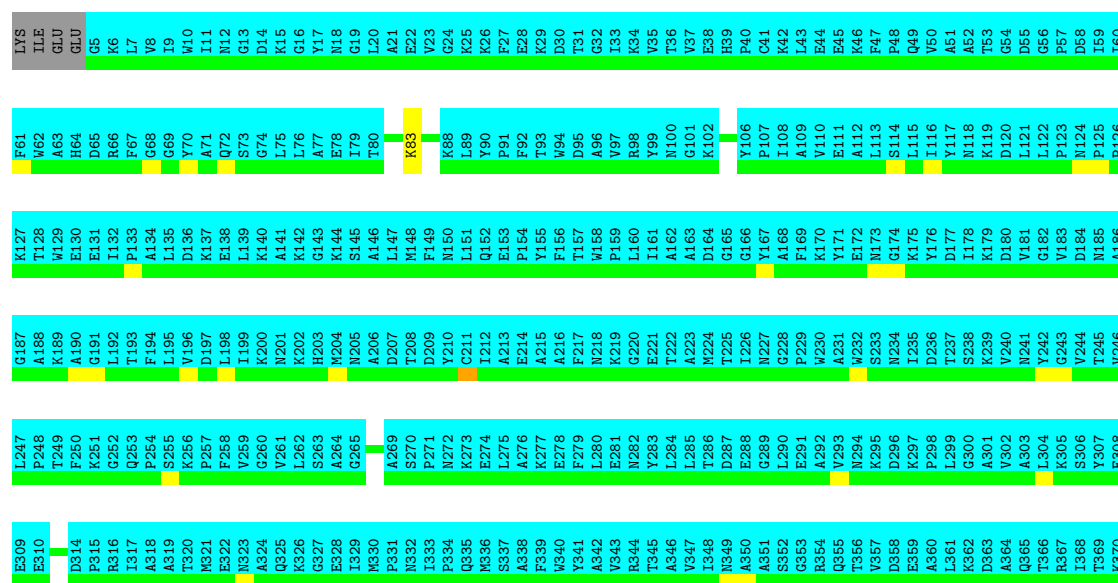




4.2.6 Score per residue for model 6

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

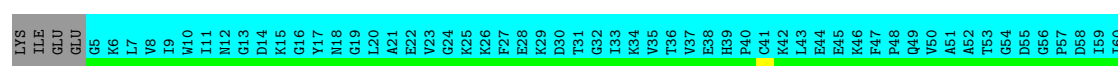
Chain A: . 95%

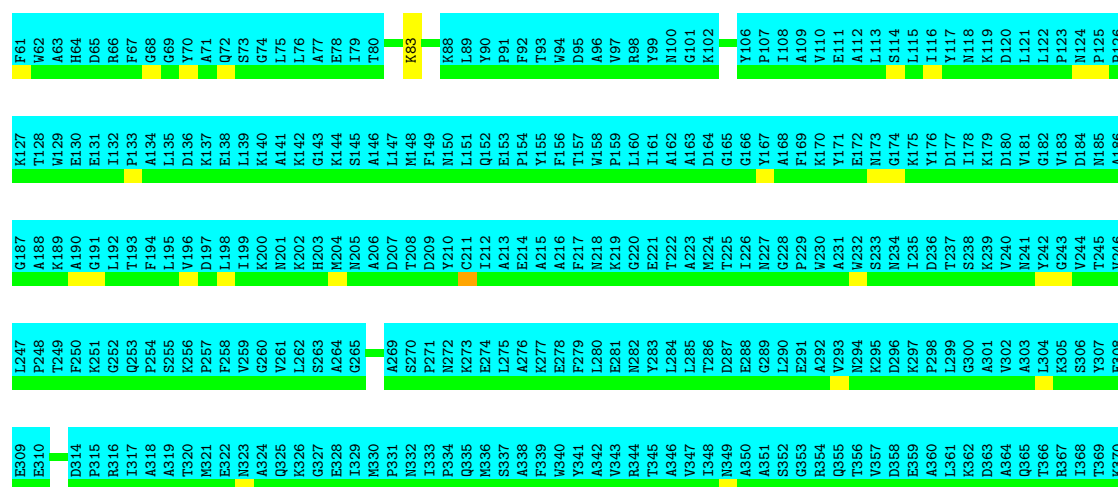


4.2.7 Score per residue for model 7

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

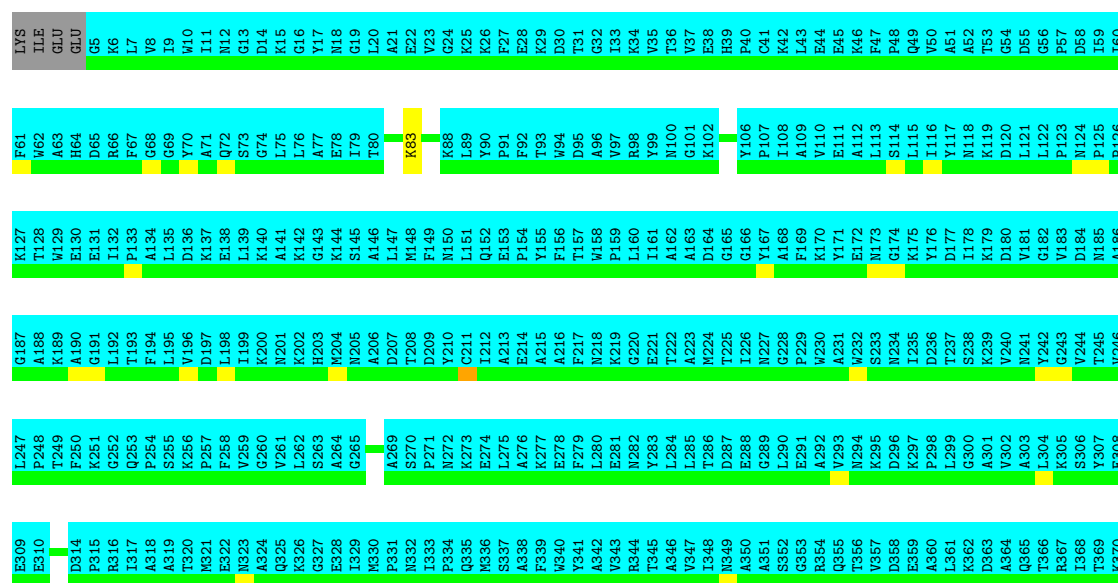




4.2.8 Score per residue for model 8

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

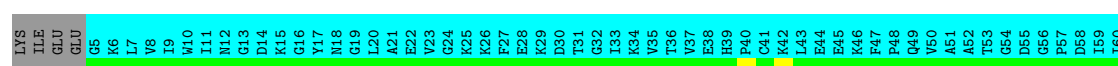
Chain A: . 95%

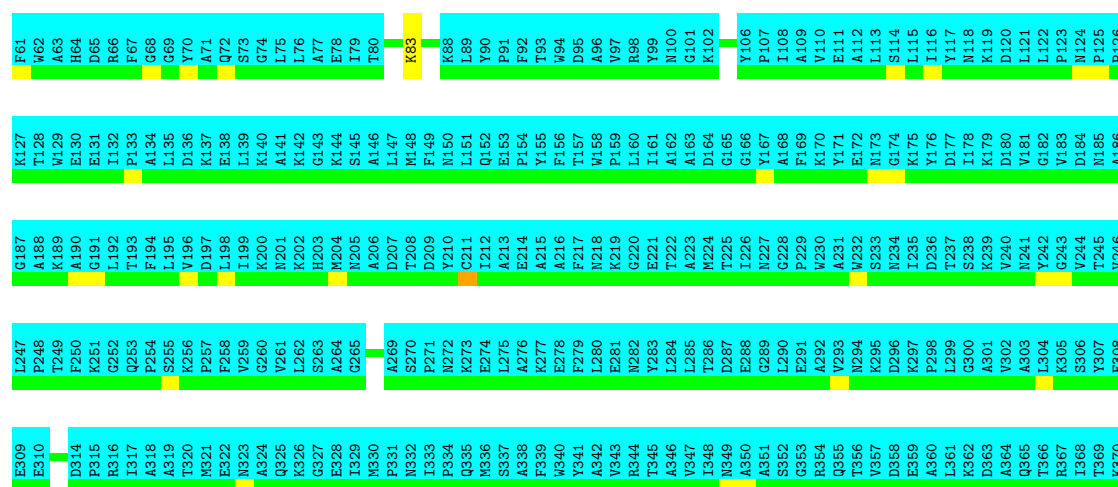


4.2.9 Score per residue for model 9

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

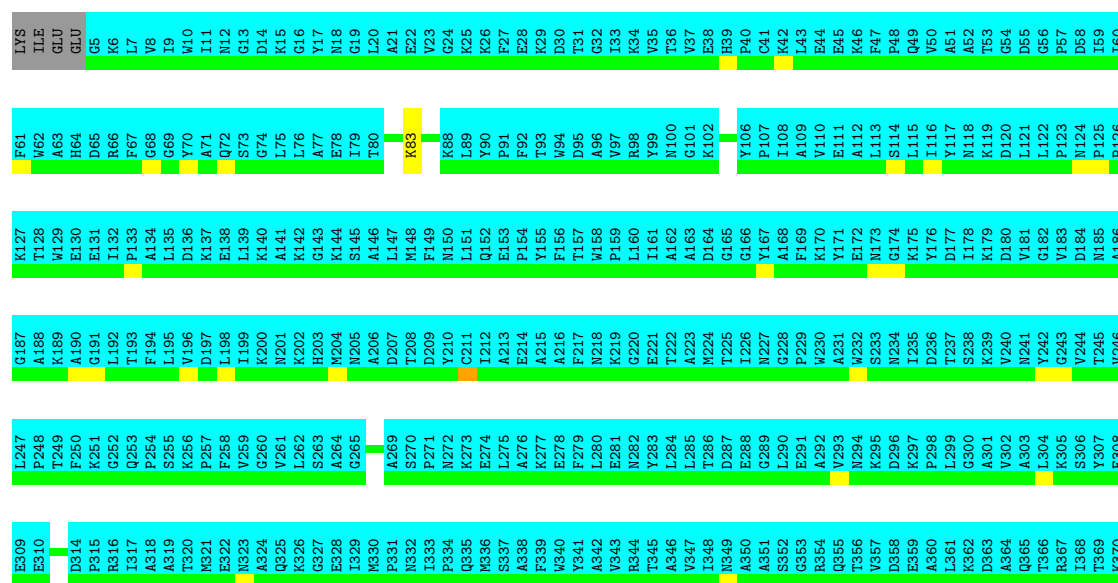




4.2.10 Score per residue for model 10

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

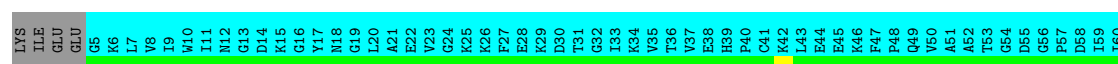
Chain A: . 95%

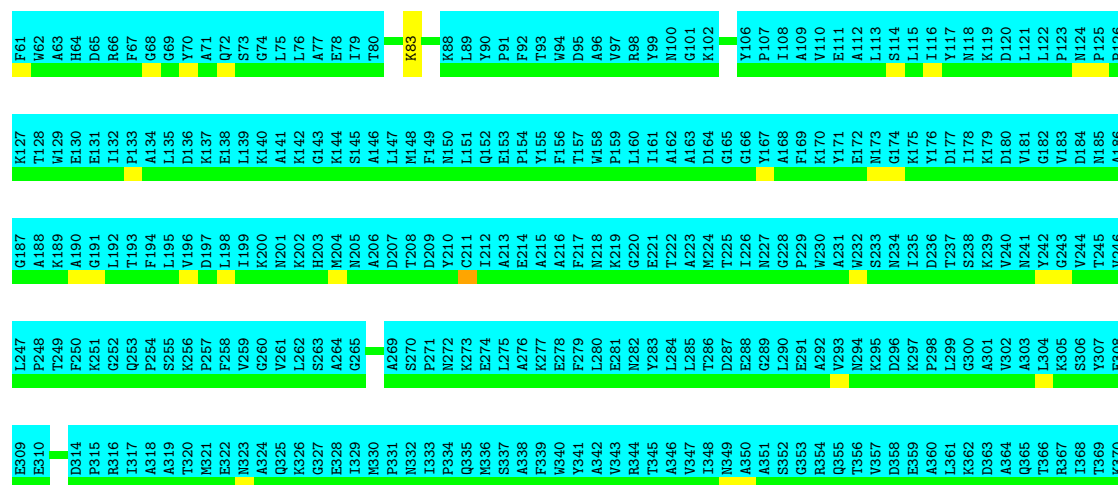


4.2.11 Score per residue for model 11

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

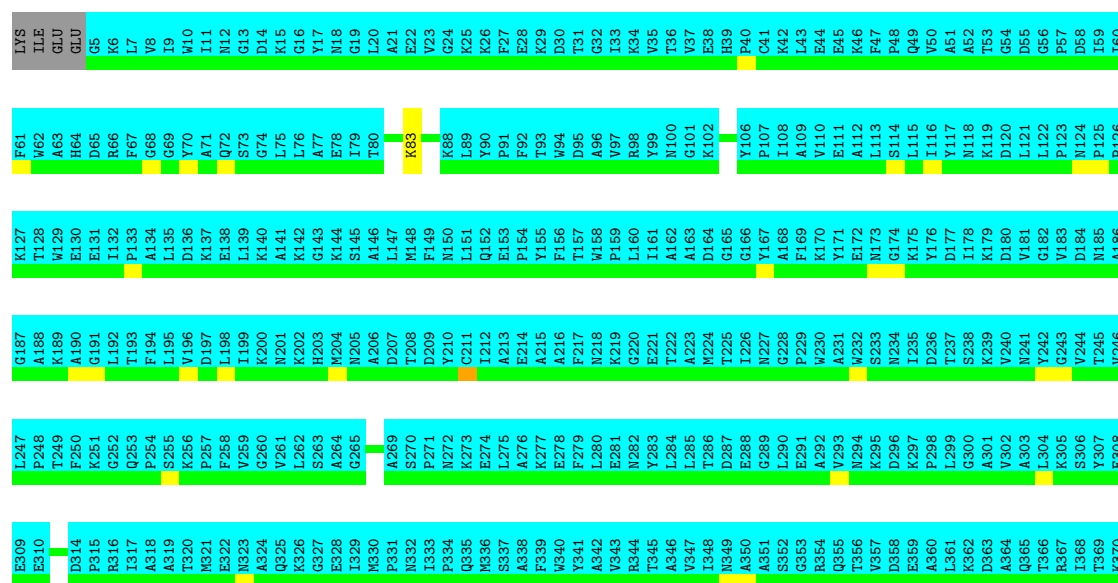




4.2.12 Score per residue for model 12

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

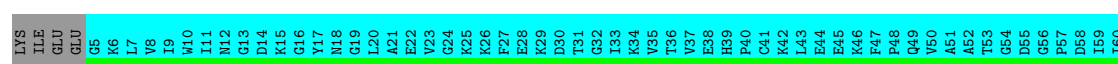
Chain A: . 95%

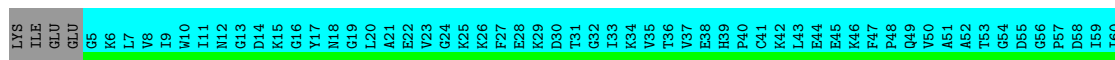


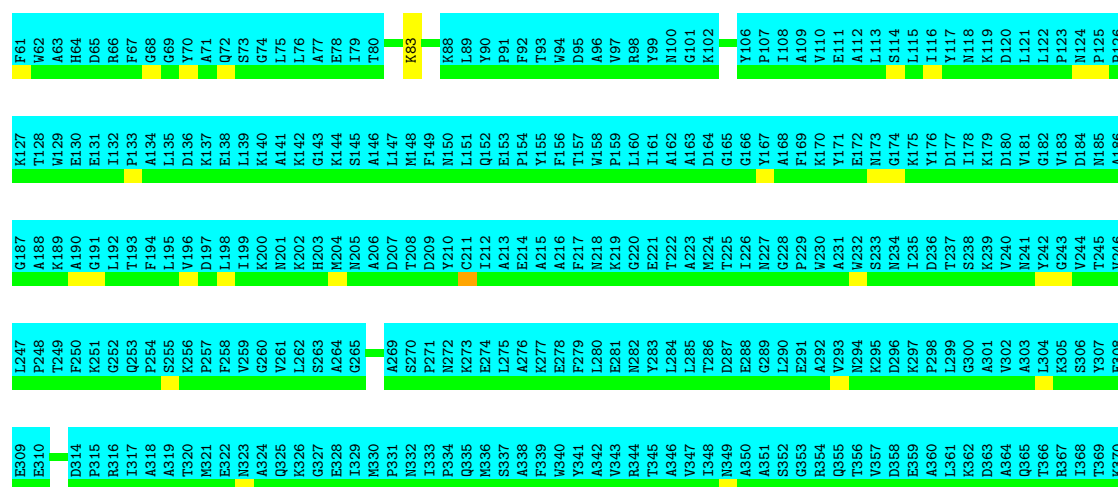
4.2.13 Score per residue for model 13

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%



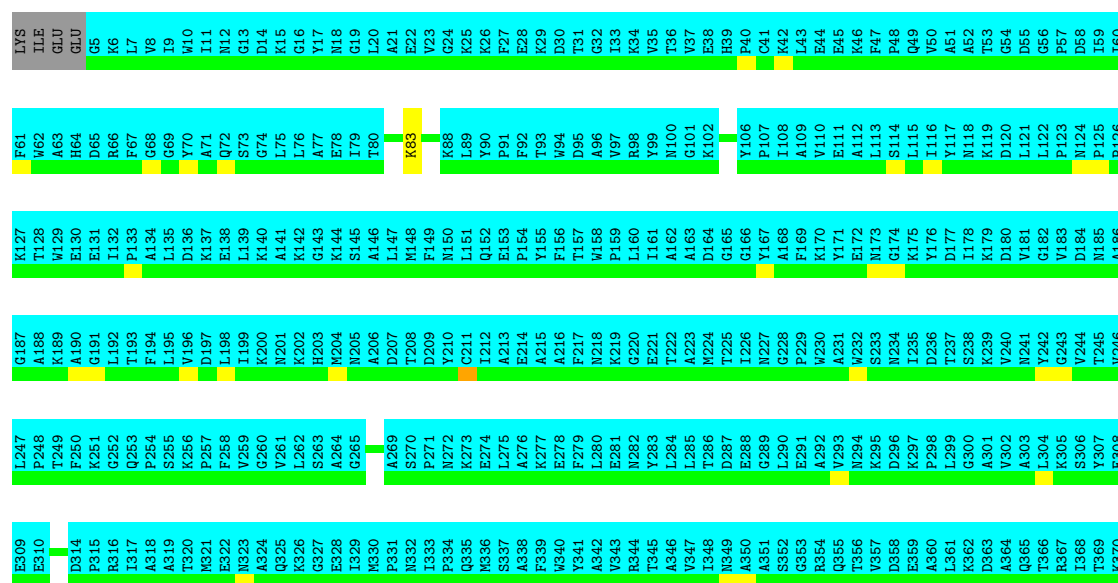




4.2.16 Score per residue for model 16

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

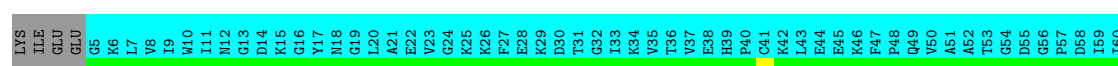
Chain A: . 95%

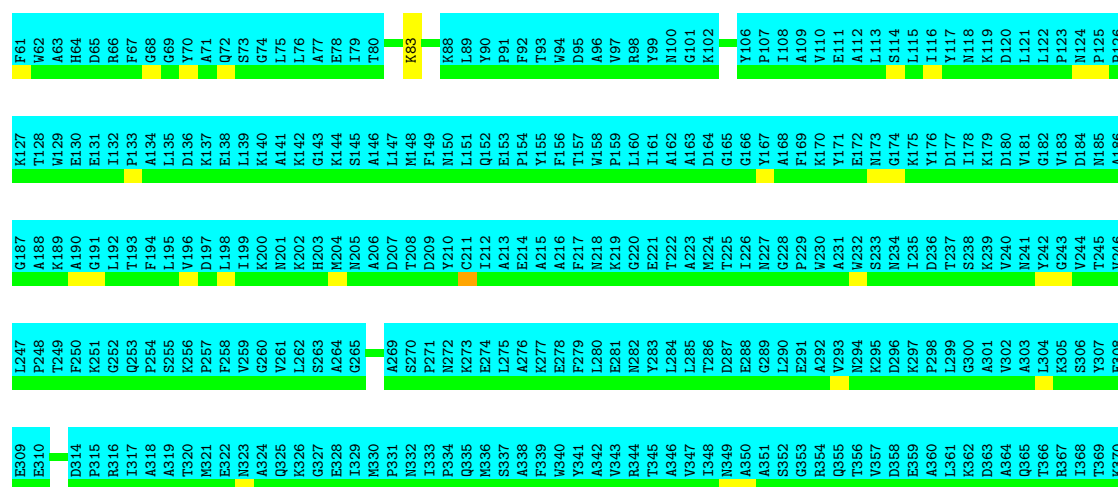


4.2.17 Score per residue for model 17

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

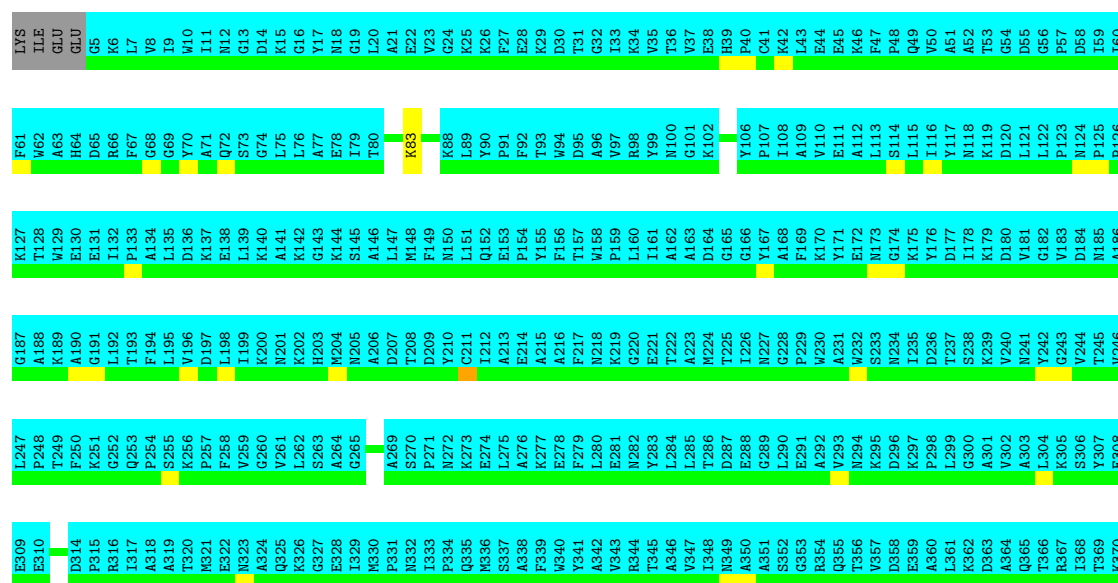




4.2.18 Score per residue for model 18

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

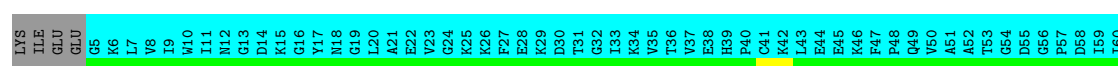
Chain A: . 95%

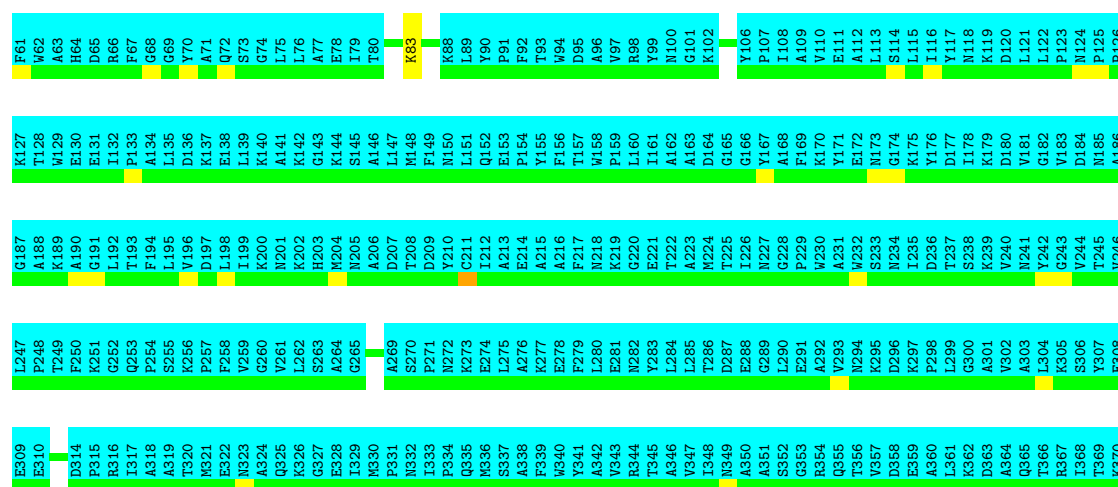


4.2.19 Score per residue for model 19

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

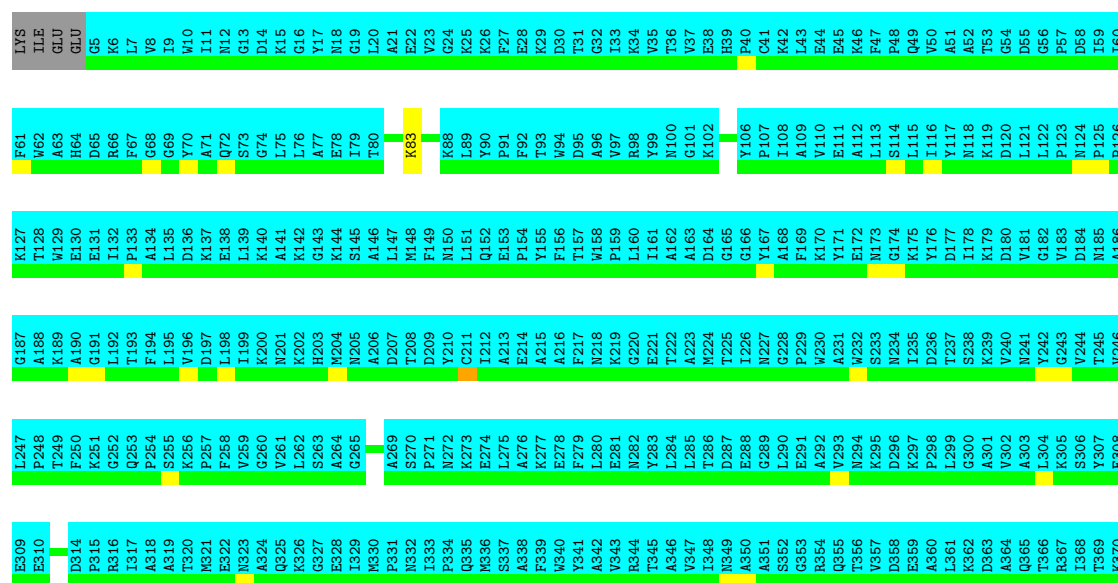




4.2.20 Score per residue for model 20

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

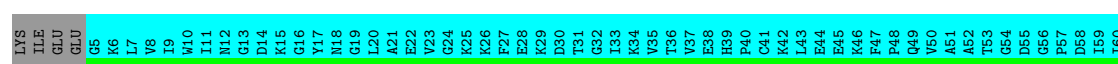
Chain A: . 95%

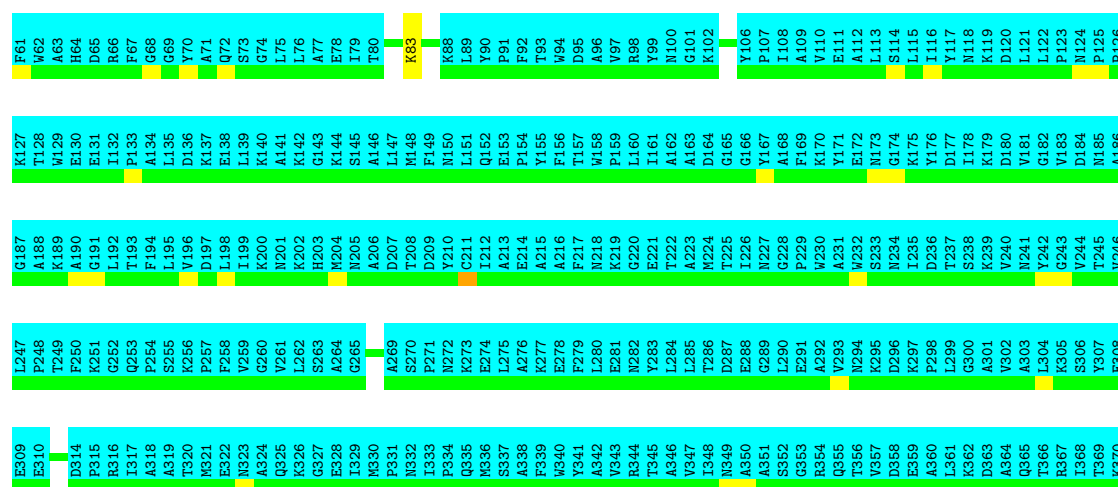


4.2.21 Score per residue for model 21

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

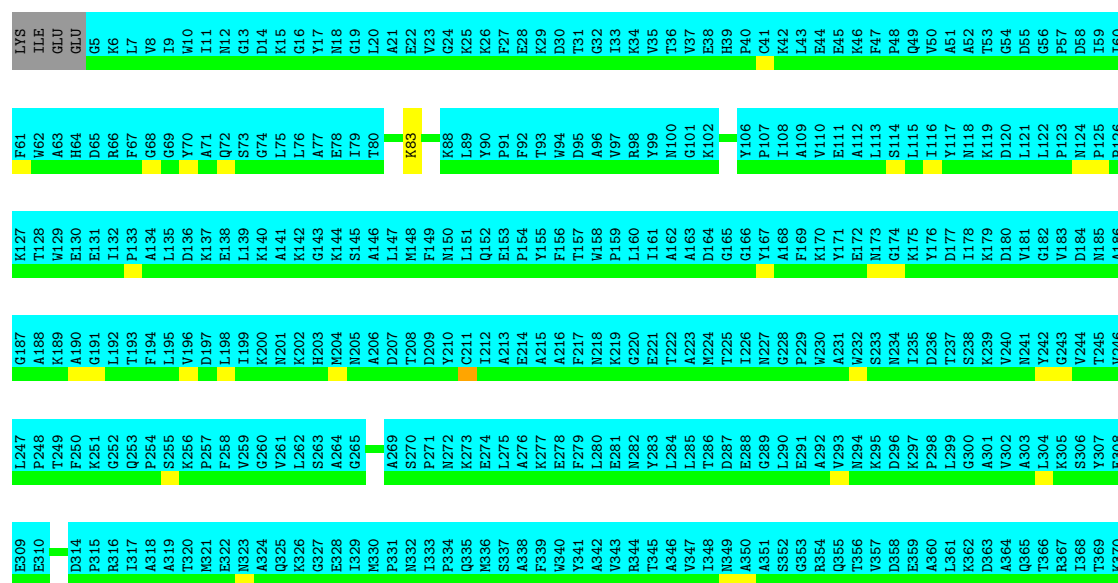




4.2.22 Score per residue for model 22

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

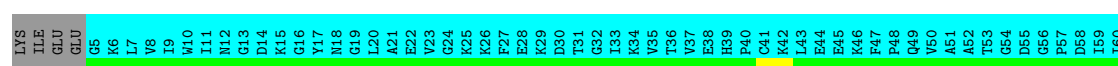
Chain A: . 95%

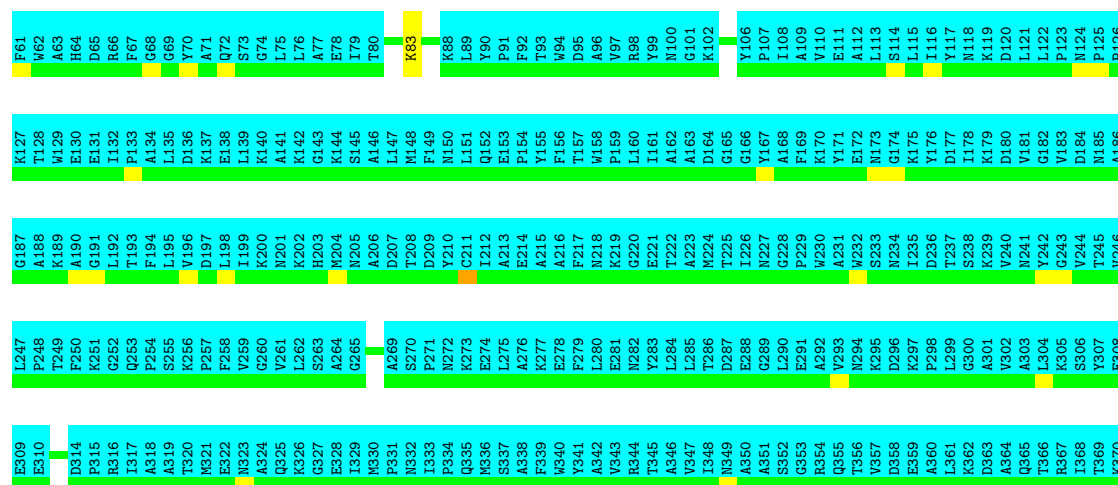


4.2.23 Score per residue for model 23

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

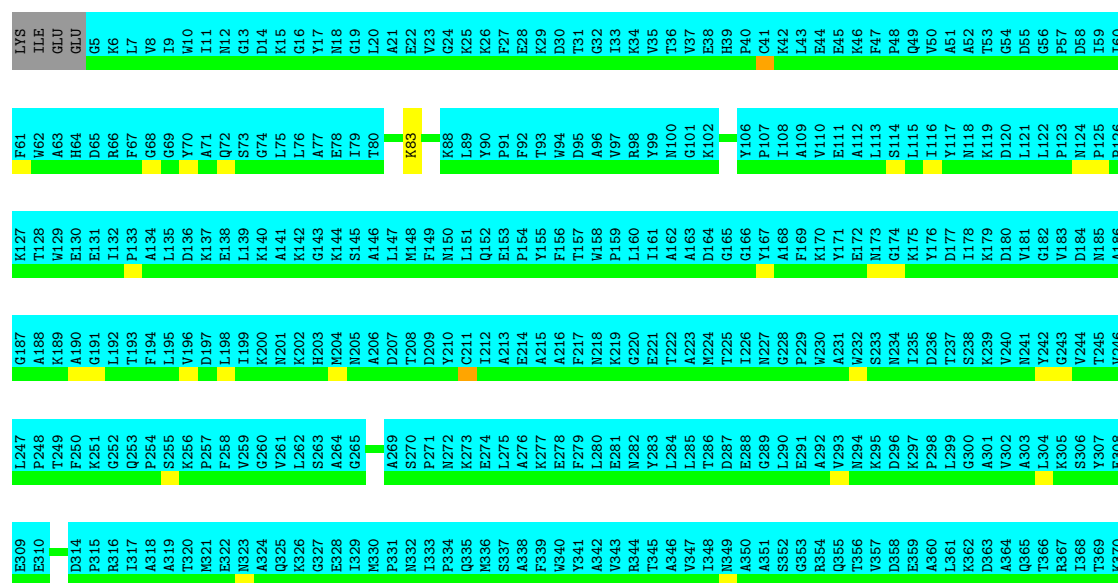




4.2.24 Score per residue for model 24

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

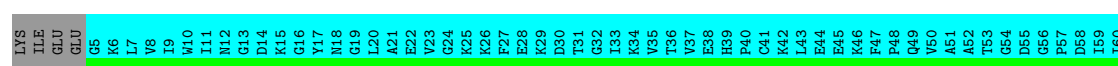
Chain A: . 95%

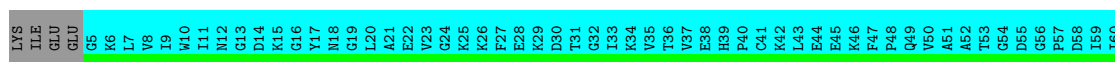


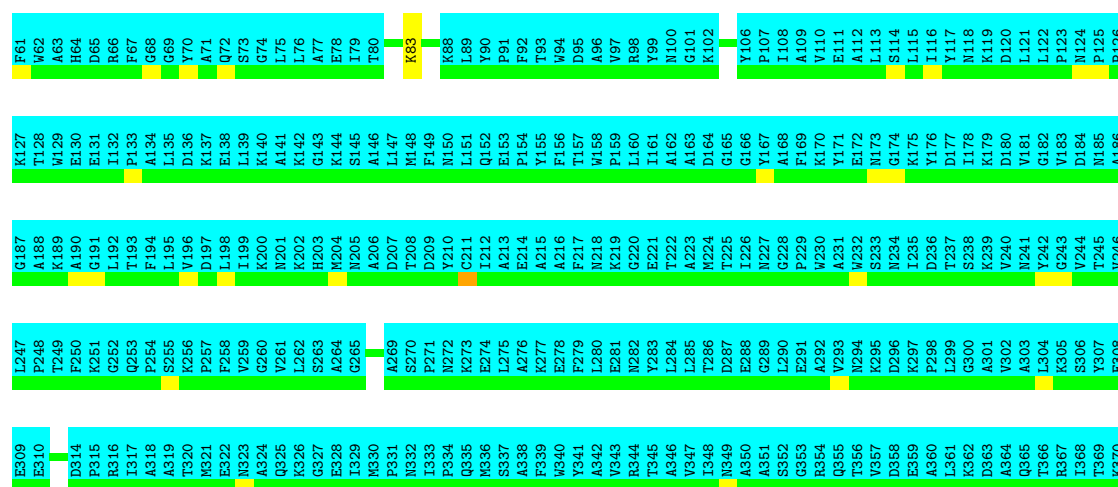
4.2.25 Score per residue for model 25

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%



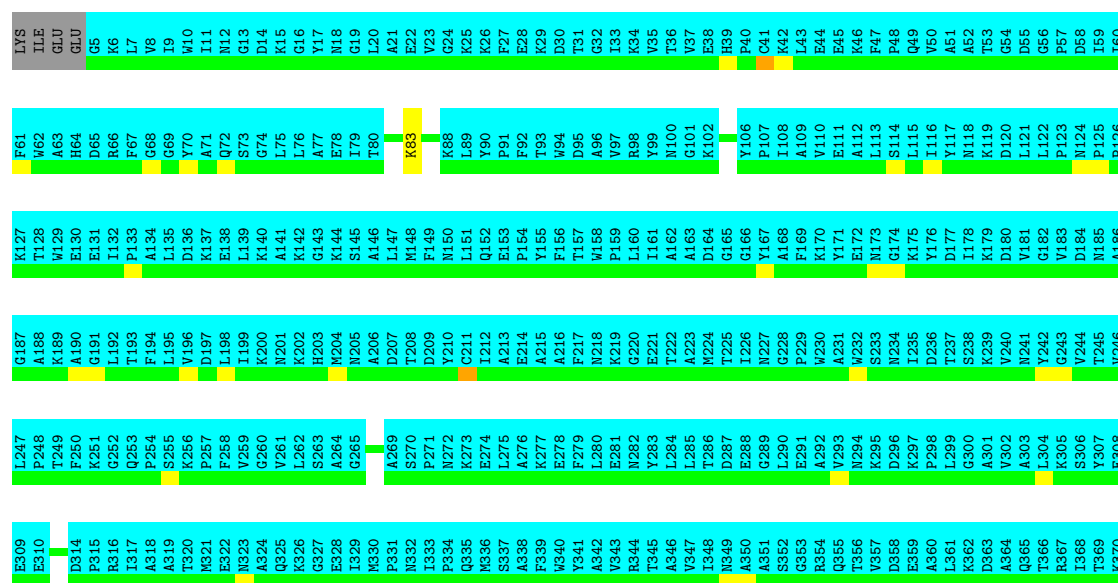




4.2.28 Score per residue for model 28

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

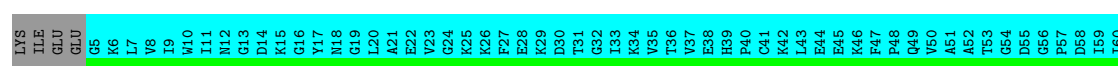
Chain A: . 95%

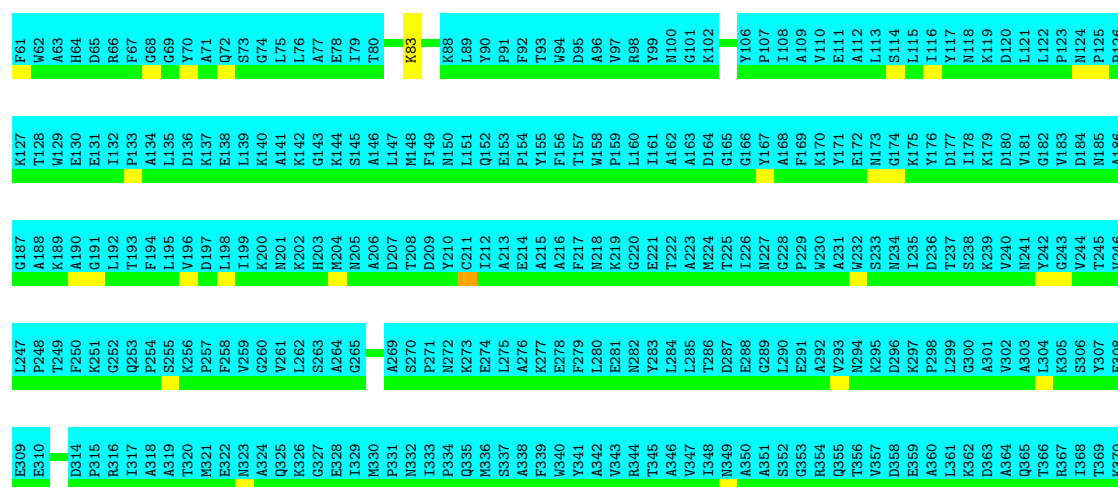


4.2.29 Score per residue for model 29

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

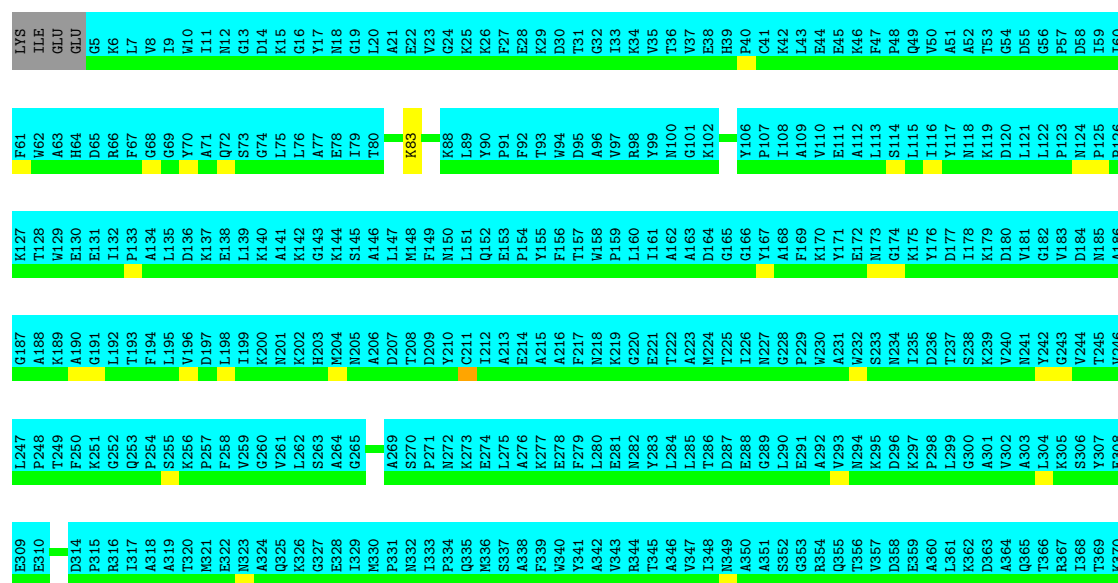




4.2.30 Score per residue for model 30

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

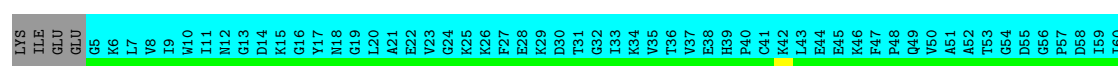
Chain A: . 95%

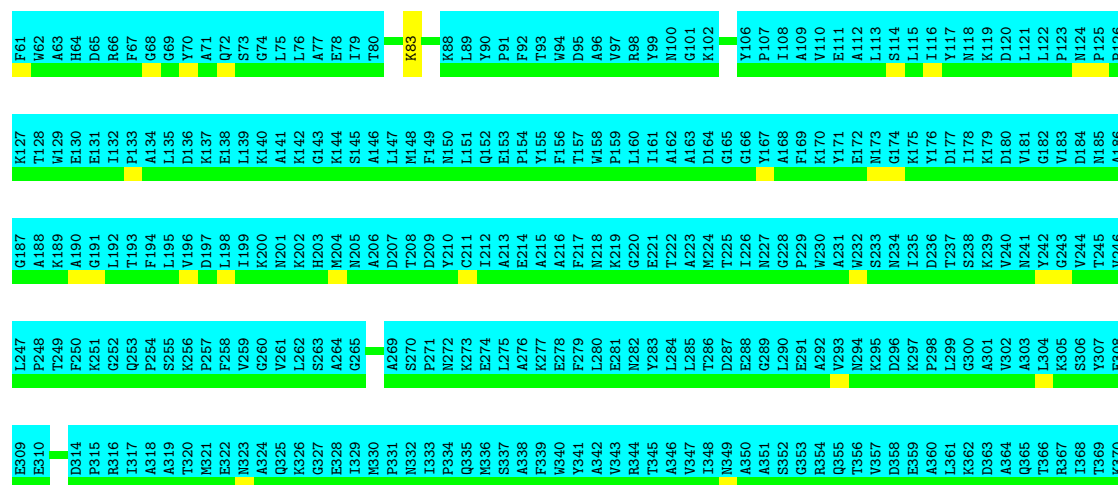


4.2.31 Score per residue for model 31

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

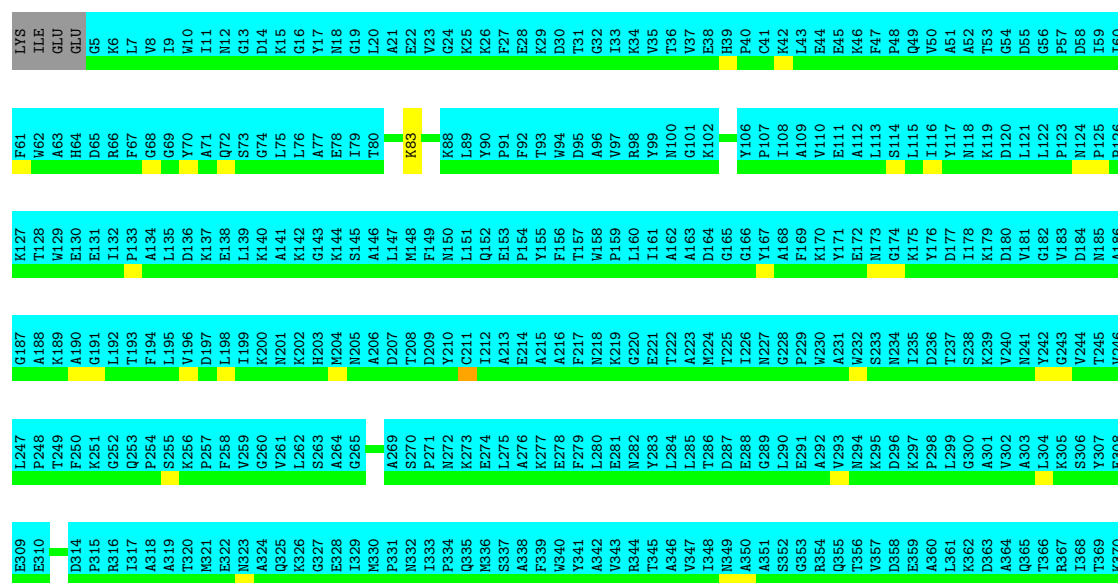




4.2.32 Score per residue for model 32

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

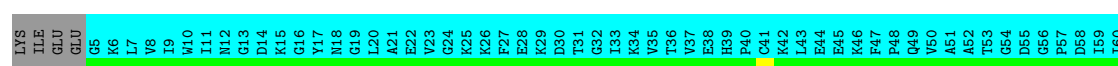
Chain A: . 95%



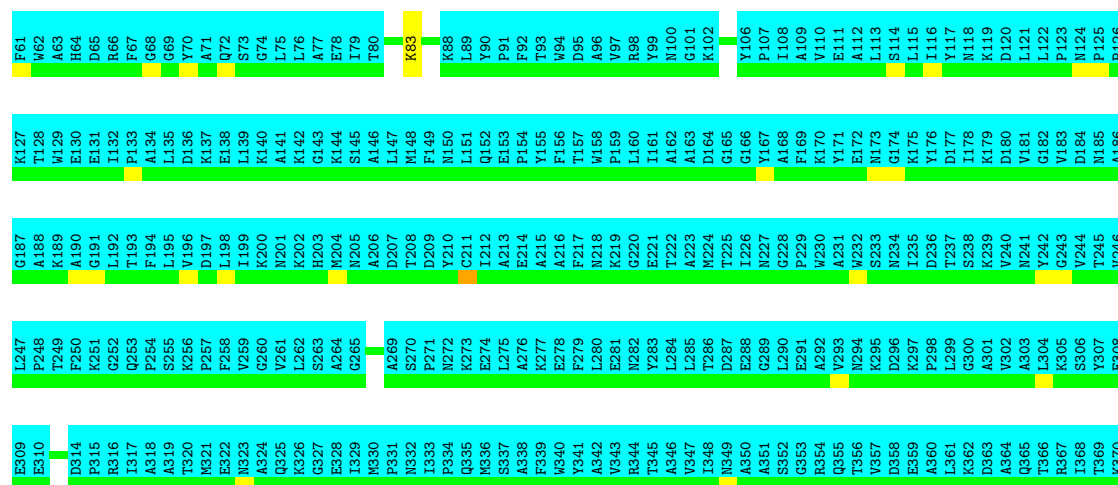
4.2.33 Score per residue for model 33

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%



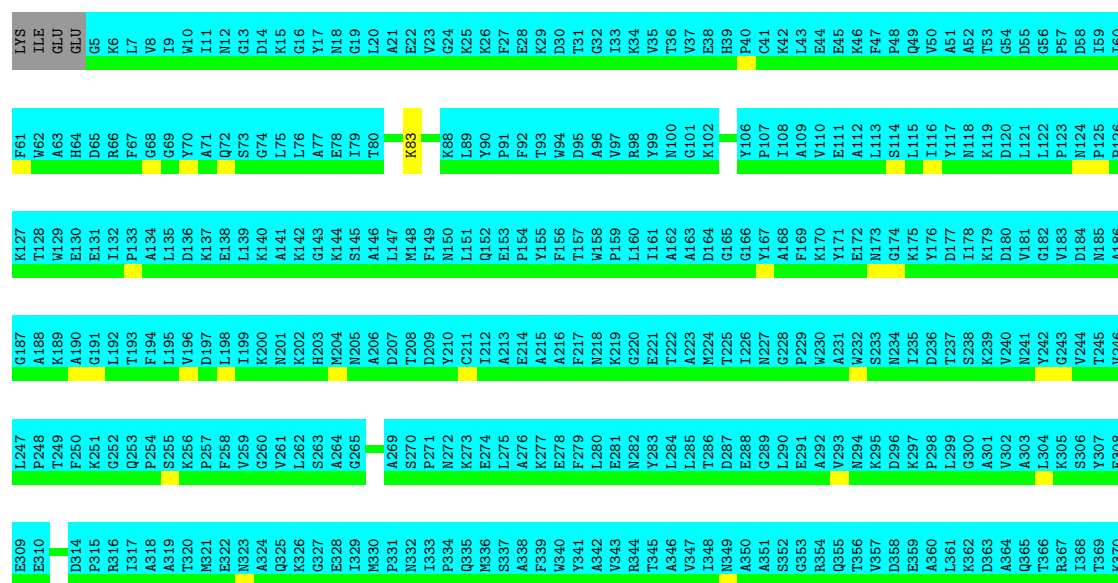




4.2.36 Score per residue for model 36

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

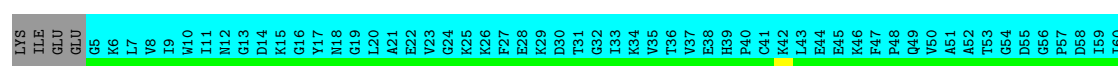
Chain A: . 95%

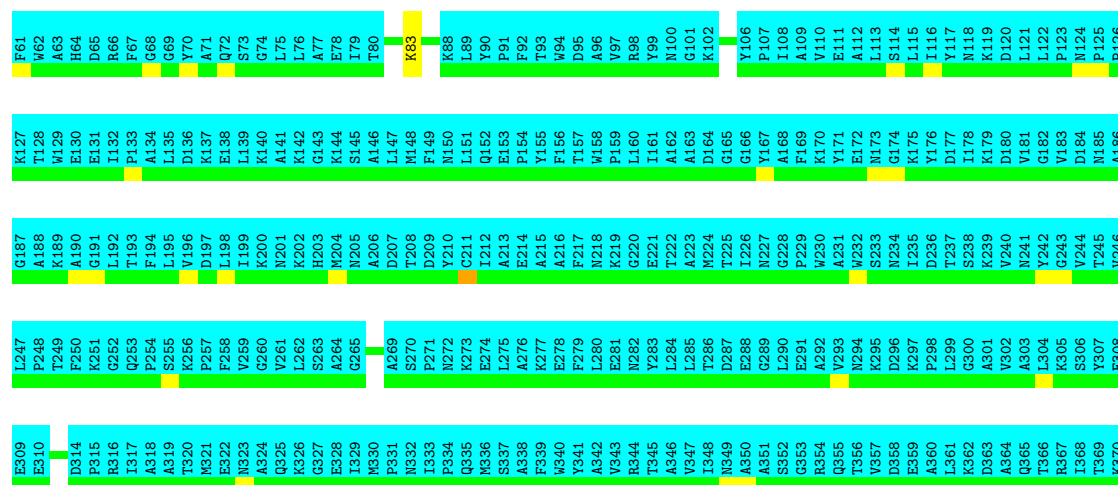


4.2.37 Score per residue for model 37

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

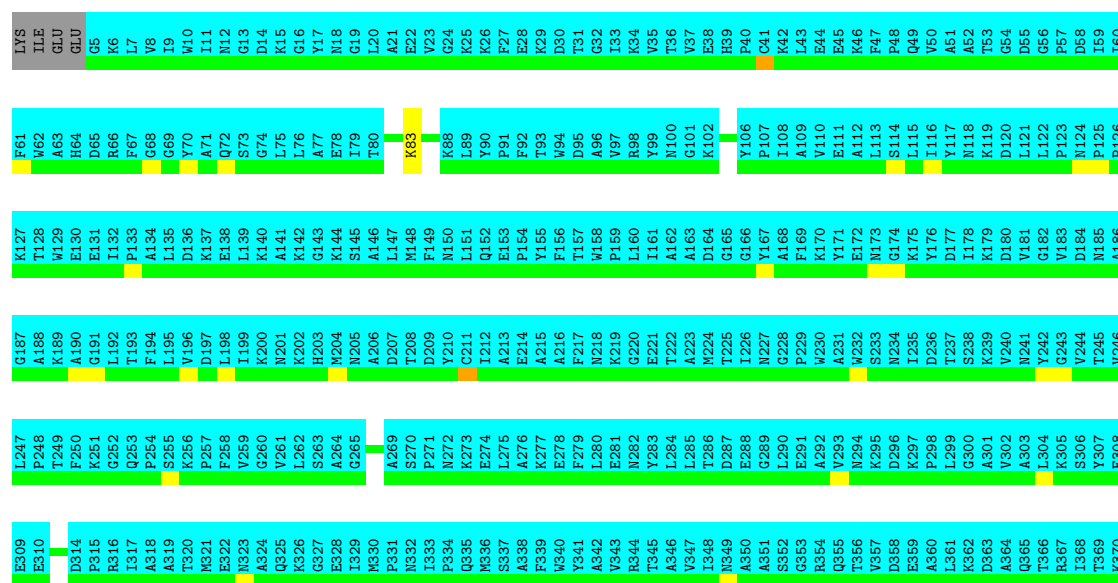




4.2.38 Score per residue for model 38

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

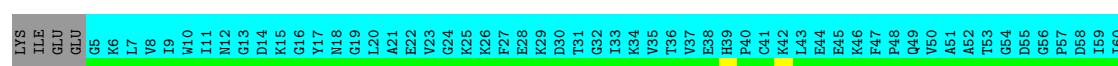
Chain A: . 95%

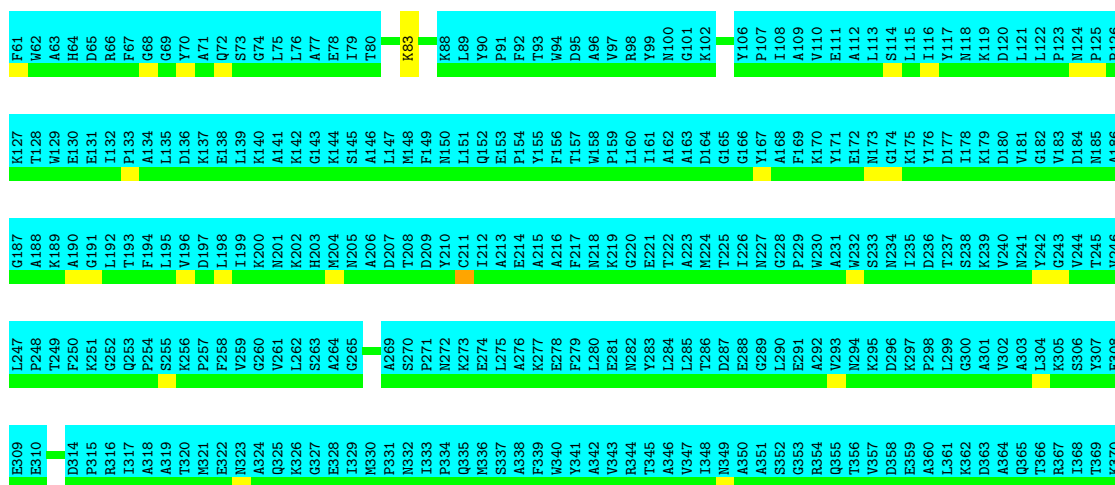


4.2.39 Score per residue for model 39

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

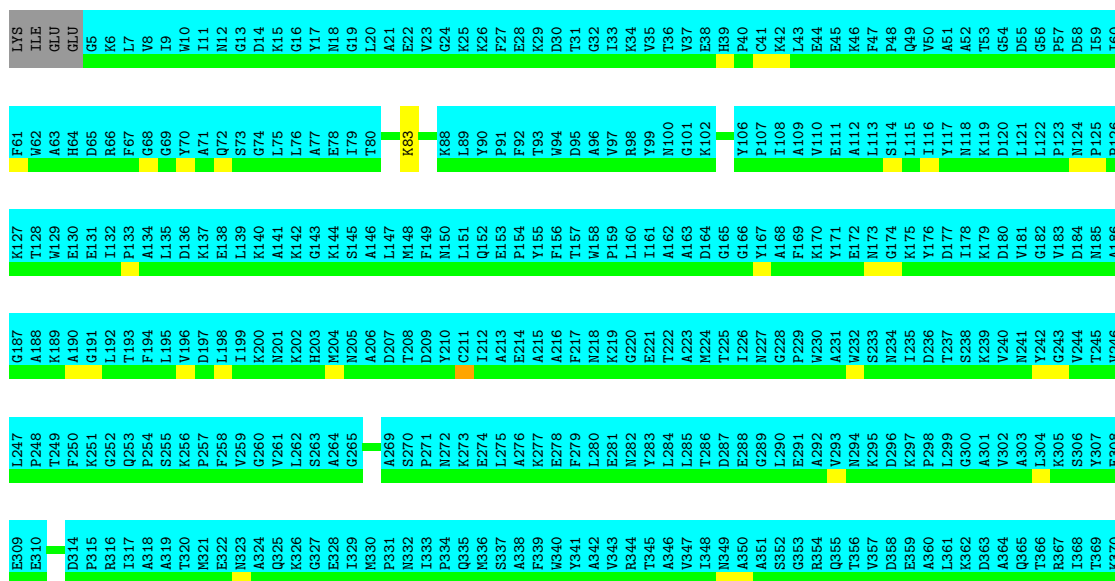




4.2.40 Score per residue for model 40

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

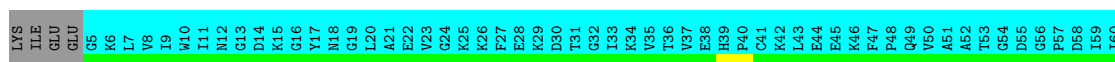
Chain A: . 95%

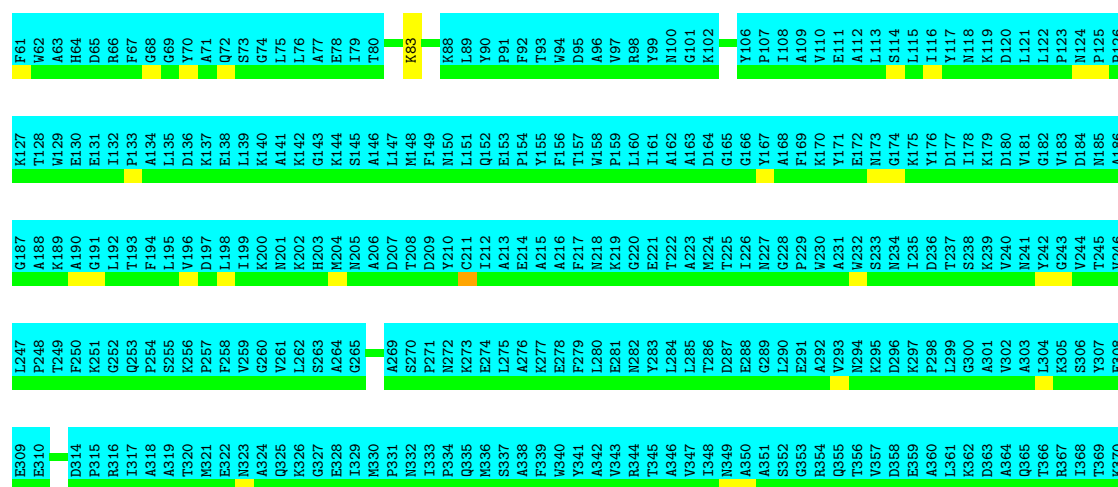


4.2.41 Score per residue for model 41

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

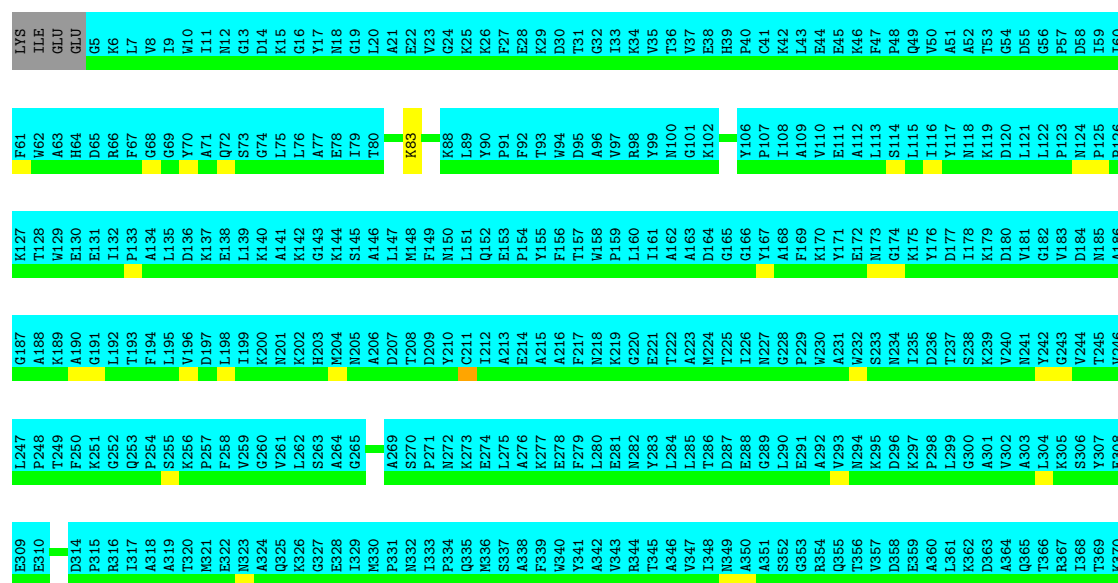




4.2.42 Score per residue for model 42

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

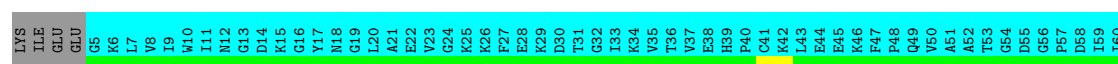
Chain A: . 95%

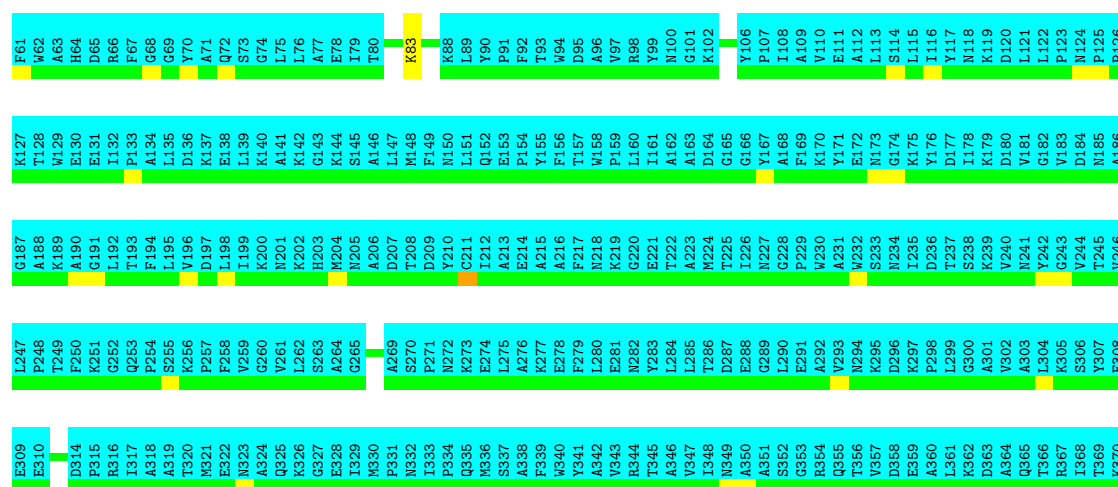


4.2.43 Score per residue for model 43

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

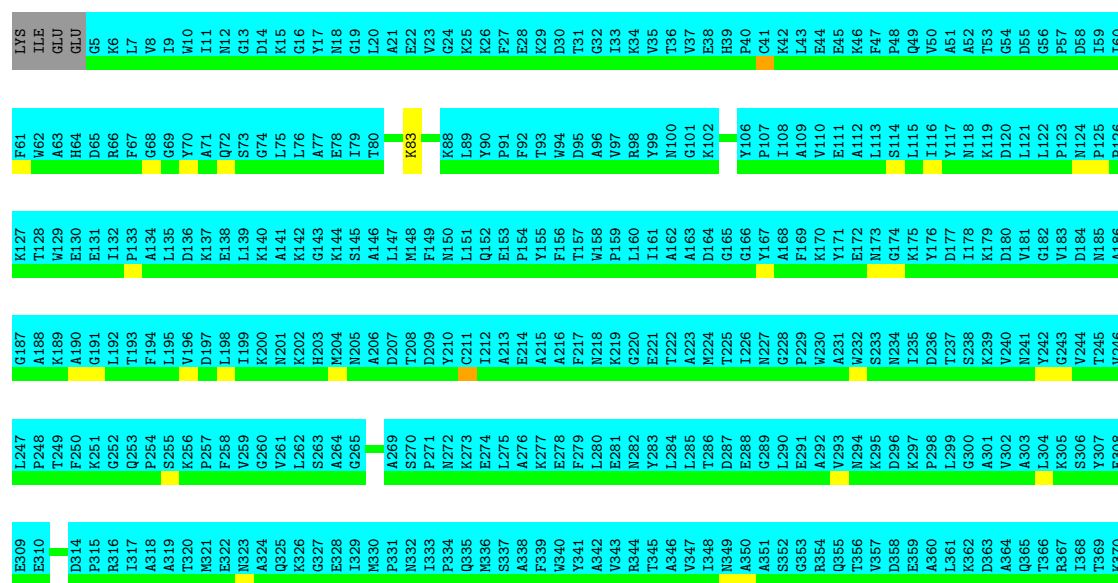




4.2.44 Score per residue for model 44

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

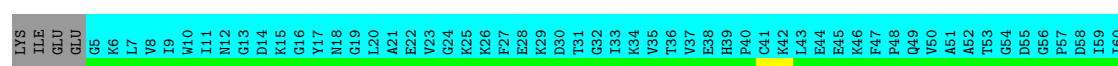
Chain A: . 95%

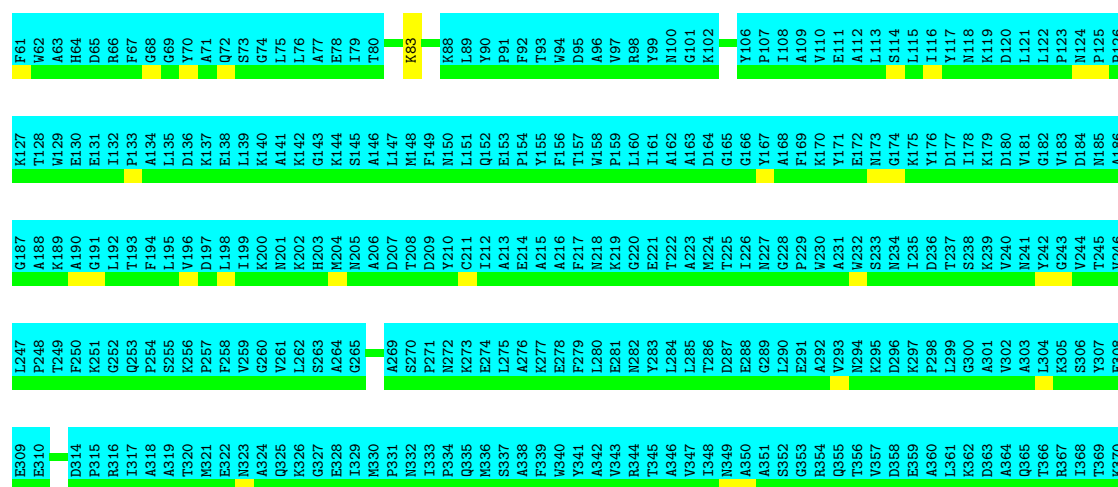


4.2.45 Score per residue for model 45

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

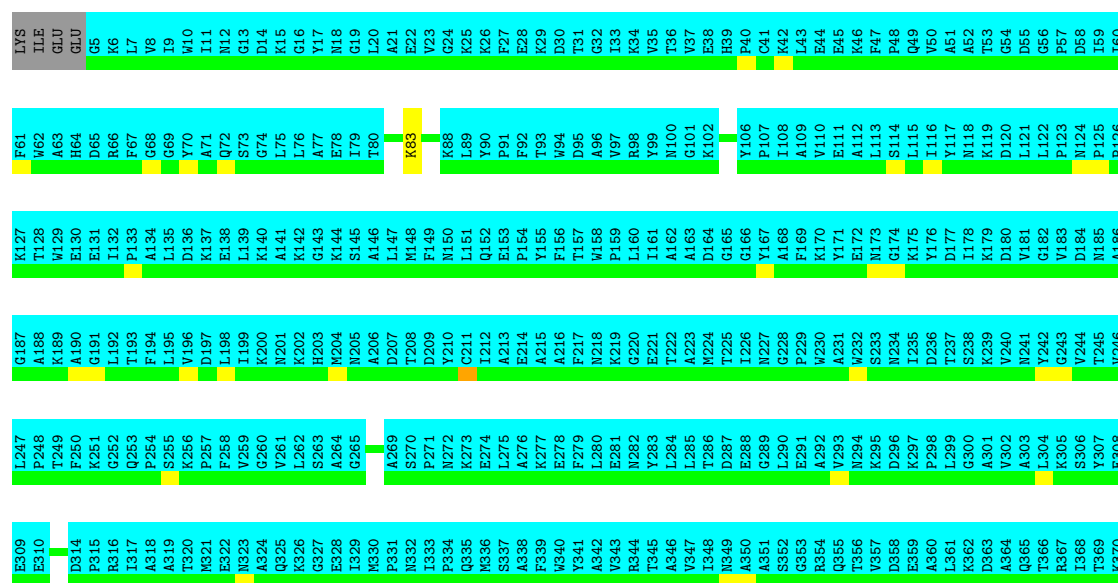




4.2.46 Score per residue for model 46

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

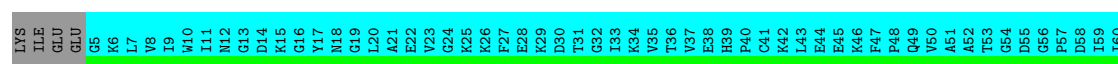
Chain A: . 95%

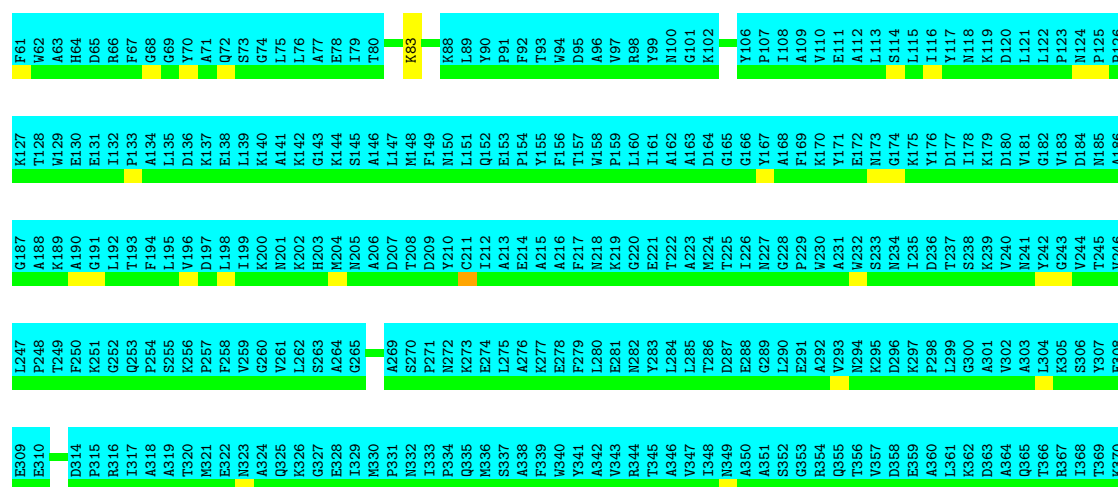


4.2.47 Score per residue for model 47

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

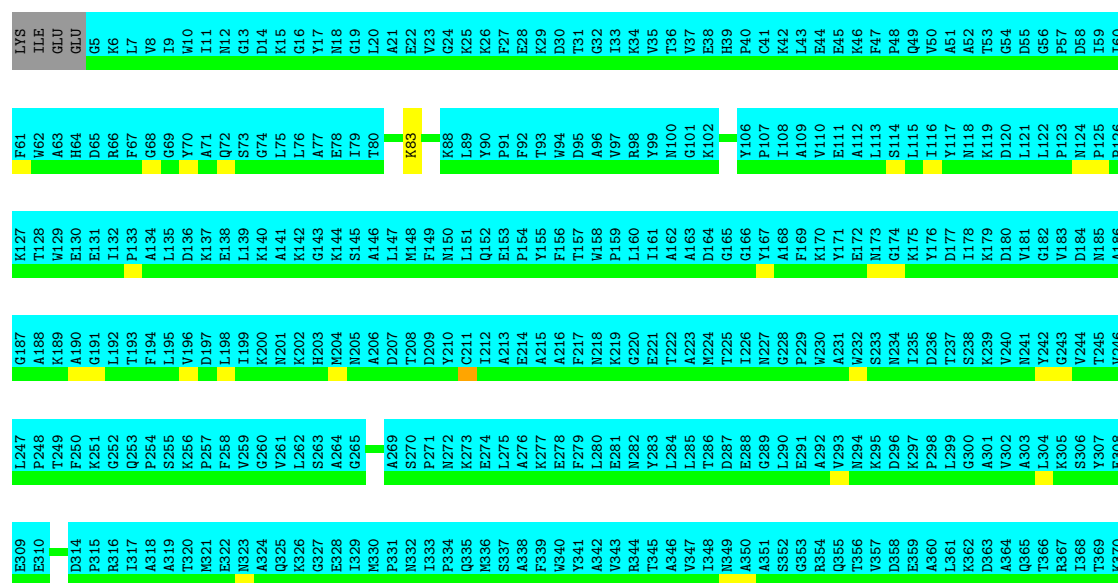




4.2.48 Score per residue for model 48

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

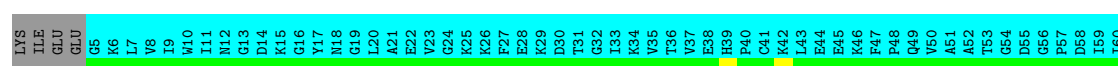
Chain A: . 95%

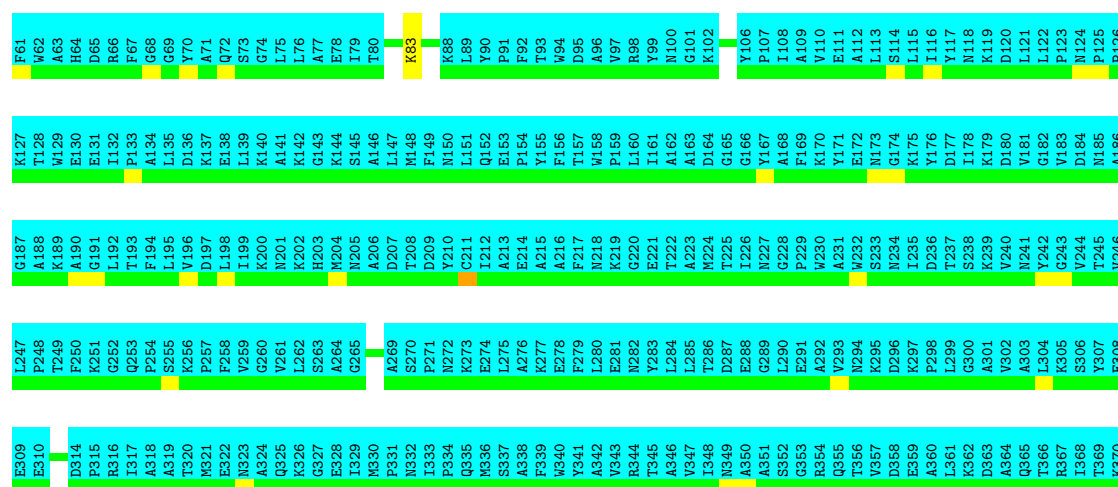


4.2.49 Score per residue for model 49

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%

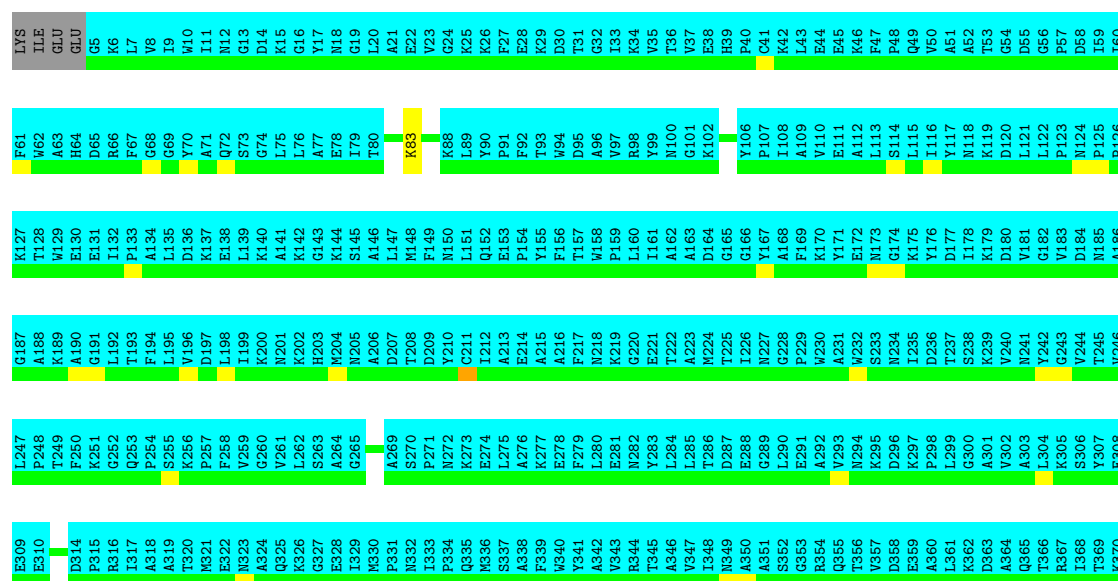




4.2.50 Score per residue for model 50

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A: . 95%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *CONJOINED RIGID BODY/TORSION ANGLE SIMULATED ANNEALING DYNAMICS*.

Of the 100 calculated structures, 50 were deposited, based on the following criterion: *PRE AND VDW ENERGIES*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
NIH	refinement	
Xplor-NIH	structure solution	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MXT

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 (average) 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	A	1.55±0.00	0±0/64 (0.0± 0.0%)	2.12±0.01	2±0/80 (2.5± 0.0%)
All	All	1.55	0/3200 (0.0%)	2.12	100/4000 (2.5%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	83	LYS	CA-C-N	5.08	127.08	120.28	1	50
1	A	83	LYS	C-N-CA	5.08	127.08	120.28	1	50

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	-2113	-424	14	0±0
2	A	432	456	500	14±4
All	All	-84050	1600	25663	696

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 0.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:402[A]:MXT:O11	2:A:402[A]:MXT:H231	0.83	1.73	29	11
2:A:402[B]:MXT:O11	2:A:402[B]:MXT:H231	0.83	1.73	46	12
2:A:401[F]:MXT:H231	2:A:401[F]:MXT:O11	0.83	1.73	24	12
2:A:401[D]:MXT:O11	2:A:401[D]:MXT:H231	0.83	1.73	10	14
2:A:401[A]:MXT:O11	2:A:401[A]:MXT:H231	0.82	1.75	24	6
2:A:401[C]:MXT:H231	2:A:401[C]:MXT:O11	0.81	1.75	2	14
2:A:401[B]:MXT:H231	2:A:401[B]:MXT:O11	0.81	1.73	13	5
2:A:402[D]:MXT:O11	2:A:402[D]:MXT:H231	0.81	1.74	5	9
2:A:402[D]:MXT:H231	2:A:402[D]:MXT:O11	0.81	1.75	43	1
2:A:401[E]:MXT:O11	2:A:401[E]:MXT:H231	0.80	1.73	50	24
2:A:401[F]:MXT:O11	2:A:401[F]:MXT:H231	0.80	1.74	32	4
2:A:401[B]:MXT:O11	2:A:401[B]:MXT:H231	0.78	1.77	34	2
2:A:402[F]:MXT:O11	2:A:402[F]:MXT:H231	0.69	1.86	17	4
2:A:402[D]:MXT:O12	2:A:402[D]:MXT:H231	0.68	1.89	14	12
2:A:401[B]:MXT:H231	2:A:401[B]:MXT:O12	0.68	1.88	45	8
2:A:402[A]:MXT:O12	2:A:402[A]:MXT:H231	0.68	1.89	3	7
2:A:402[E]:MXT:O12	2:A:402[E]:MXT:H231	0.67	1.89	45	20
2:A:402[E]:MXT:H231	2:A:402[E]:MXT:O12	0.67	1.88	49	4
2:A:402[F]:MXT:O12	2:A:402[F]:MXT:H231	0.67	1.88	32	5
2:A:402[F]:MXT:H231	2:A:402[F]:MXT:O12	0.66	1.90	29	13
2:A:401[A]:MXT:O12	2:A:401[A]:MXT:H231	0.66	1.89	40	10
2:A:401[B]:MXT:O12	2:A:401[B]:MXT:H231	0.66	1.88	9	2
2:A:402[C]:MXT:O11	2:A:402[C]:MXT:H231	0.66	1.90	37	2
2:A:402[C]:MXT:O12	2:A:402[C]:MXT:H231	0.66	1.89	3	9
2:A:401[A]:MXT:H231	2:A:401[A]:MXT:O12	0.65	1.91	32	1
2:A:402[E]:MXT:O11	2:A:402[E]:MXT:H231	0.64	1.91	31	1
2:A:402[B]:MXT:H231	2:A:402[B]:MXT:O12	0.63	1.92	44	4
2:A:401[D]:MXT:O12	2:A:401[D]:MXT:H231	0.61	1.94	16	6
2:A:402[B]:MXT:O12	2:A:402[B]:MXT:H231	0.61	1.94	34	2
2:A:401[C]:MXT:O11	2:A:401[C]:MXT:C23	0.58	2.52	49	5
2:A:401[E]:MXT:O11	2:A:401[E]:MXT:C23	0.57	2.52	19	7
2:A:402[D]:MXT:O11	2:A:402[D]:MXT:C23	0.57	2.53	33	3
2:A:401[B]:MXT:C22	2:A:401[B]:MXT:O11	0.57	2.52	37	4
2:A:401[A]:MXT:O11	2:A:401[A]:MXT:C22	0.57	2.53	16	15
2:A:402[A]:MXT:O11	2:A:402[A]:MXT:C23	0.57	2.52	33	5
2:A:401[C]:MXT:C22	2:A:401[C]:MXT:O11	0.57	2.53	32	5
2:A:401[B]:MXT:O11	2:A:401[B]:MXT:C23	0.57	2.52	34	7
2:A:401[D]:MXT:O11	2:A:401[D]:MXT:C22	0.57	2.52	13	6
2:A:401[D]:MXT:O11	2:A:401[D]:MXT:C23	0.57	2.52	4	10
2:A:402[C]:MXT:C22	2:A:402[C]:MXT:O11	0.57	2.53	24	4
2:A:401[A]:MXT:O11	2:A:401[A]:MXT:H221	0.56	2.00	26	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:401[E]:MXT:O12	2:A:401[E]:MXT:H231	0.56	2.00	27	2
2:A:402[B]:MXT:O11	2:A:402[B]:MXT:H221	0.56	2.00	36	3
2:A:402[D]:MXT:O11	2:A:402[D]:MXT:H221	0.56	2.00	49	4
2:A:402[C]:MXT:H231	2:A:402[C]:MXT:O12	0.56	1.89	38	1
2:A:401[F]:MXT:H221	2:A:401[F]:MXT:O11	0.56	2.00	41	1
2:A:401[F]:MXT:H231	2:A:401[F]:MXT:O12	0.56	1.98	22	1
2:A:401[E]:MXT:O11	2:A:401[E]:MXT:H221	0.56	2.00	42	2
2:A:401[F]:MXT:O11	2:A:401[F]:MXT:C23	0.55	2.53	7	10
2:A:402[E]:MXT:O11	2:A:402[E]:MXT:H221	0.55	2.01	18	6
2:A:402[B]:MXT:O11	2:A:402[B]:MXT:C23	0.55	2.52	17	5
2:A:402[D]:MXT:C22	2:A:402[D]:MXT:O11	0.54	2.55	1	1
2:A:401[D]:MXT:O11	2:A:401[D]:MXT:H221	0.54	2.03	47	5
2:A:401[A]:MXT:O11	2:A:401[A]:MXT:C23	0.54	2.55	9	5
2:A:402[C]:MXT:O11	2:A:402[C]:MXT:C22	0.53	2.56	18	2
2:A:401[C]:MXT:O12	2:A:401[C]:MXT:H231	0.52	2.02	31	1
2:A:402[F]:MXT:C22	2:A:402[F]:MXT:O11	0.52	2.57	47	2
2:A:401[F]:MXT:O11	2:A:401[F]:MXT:C22	0.52	2.57	41	2
2:A:402[E]:MXT:O11	2:A:402[E]:MXT:C22	0.52	2.58	48	6
2:A:402[D]:MXT:O11	2:A:402[D]:MXT:C22	0.51	2.58	22	4
2:A:402[B]:MXT:C22	2:A:402[B]:MXT:O11	0.51	2.59	4	1
2:A:402[C]:MXT:O11	2:A:402[C]:MXT:H221	0.51	2.05	28	2
2:A:402[F]:MXT:O11	2:A:402[F]:MXT:C22	0.51	2.58	33	5
2:A:402[E]:MXT:C22	2:A:402[E]:MXT:O11	0.51	2.59	32	1
2:A:401[F]:MXT:C22	2:A:401[F]:MXT:O11	0.51	2.59	1	1
2:A:401[D]:MXT:C23	2:A:401[D]:MXT:O11	0.50	2.59	41	1
2:A:401[C]:MXT:O11	2:A:401[C]:MXT:H221	0.49	2.05	32	1
2:A:401[F]:MXT:O11	2:A:401[F]:MXT:H221	0.49	2.06	29	1
2:A:402[B]:MXT:C23	2:A:402[B]:MXT:O11	0.49	2.61	38	2
2:A:402[A]:MXT:O11	2:A:402[A]:MXT:C22	0.49	2.60	49	2
2:A:401[B]:MXT:O11	2:A:401[B]:MXT:H221	0.49	2.07	11	3
2:A:402[A]:MXT:O11	2:A:402[A]:MXT:H221	0.48	2.07	4	1
2:A:401[E]:MXT:O11	2:A:401[E]:MXT:C22	0.48	2.61	42	2
2:A:401[B]:MXT:O11	2:A:401[B]:MXT:C22	0.48	2.61	29	3
2:A:402[F]:MXT:C23	2:A:402[F]:MXT:O11	0.47	2.62	45	1
2:A:401[B]:MXT:O11	2:A:401[B]:MXT:H222	0.47	2.10	29	3
2:A:402[E]:MXT:O11	2:A:402[E]:MXT:H222	0.46	2.10	43	5
2:A:401[D]:MXT:O11	2:A:401[D]:MXT:H222	0.46	2.10	42	3
2:A:402[F]:MXT:H222	2:A:402[F]:MXT:O11	0.46	2.10	19	3
2:A:402[B]:MXT:H222	2:A:402[B]:MXT:O11	0.46	2.11	30	1
2:A:402[F]:MXT:O11	2:A:402[F]:MXT:H221	0.46	2.09	30	1
2:A:402[F]:MXT:O11	2:A:402[F]:MXT:H222	0.46	2.10	49	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:402[D]:MXT:H222	2:A:402[D]:MXT:O11	0.46	2.10	10	1
2:A:401[A]:MXT:H222	2:A:401[A]:MXT:O11	0.46	2.11	34	1
2:A:402[B]:MXT:O11	2:A:402[B]:MXT:H222	0.46	2.11	4	1
2:A:401[C]:MXT:O11	2:A:401[C]:MXT:H222	0.46	2.11	1	8
2:A:401[B]:MXT:H222	2:A:401[B]:MXT:O11	0.46	2.11	44	3
2:A:402[E]:MXT:O11	2:A:402[E]:MXT:C23	0.46	2.63	42	1
2:A:402[A]:MXT:H222	2:A:402[A]:MXT:O11	0.46	2.11	27	1
2:A:401[A]:MXT:O11	2:A:401[A]:MXT:H222	0.45	2.11	8	1
2:A:402[B]:MXT:O11	2:A:402[B]:MXT:C22	0.45	2.63	36	3
2:A:402[C]:MXT:H222	2:A:402[C]:MXT:O11	0.45	2.11	49	1
2:A:401[F]:MXT:O11	2:A:401[F]:MXT:H222	0.45	2.11	1	2
2:A:402[D]:MXT:O11	2:A:402[D]:MXT:H222	0.45	2.11	22	2
2:A:401[E]:MXT:H222	2:A:401[E]:MXT:O11	0.45	2.12	11	2
2:A:402[E]:MXT:H222	2:A:402[E]:MXT:O11	0.44	2.11	17	4
2:A:402[C]:MXT:O11	2:A:402[C]:MXT:H222	0.44	2.12	15	2
2:A:402[A]:MXT:O11	2:A:402[A]:MXT:H222	0.44	2.11	49	1
2:A:402[A]:MXT:O12	2:A:402[A]:MXT:C22	0.44	2.66	38	8
2:A:402[C]:MXT:C22	2:A:402[C]:MXT:O12	0.44	2.66	31	1
2:A:401[B]:MXT:C23	2:A:401[B]:MXT:O11	0.43	2.65	15	1
2:A:401[E]:MXT:C22	2:A:401[E]:MXT:O12	0.43	2.66	38	1
2:A:401[E]:MXT:O12	2:A:401[E]:MXT:C22	0.43	2.66	6	3
2:A:402[F]:MXT:O12	2:A:402[F]:MXT:C23	0.43	2.67	6	3
2:A:401[B]:MXT:O12	2:A:401[B]:MXT:C23	0.43	2.67	17	4
2:A:402[A]:MXT:O12	2:A:402[A]:MXT:C23	0.43	2.67	43	1
2:A:401[D]:MXT:O12	2:A:401[D]:MXT:C23	0.43	2.66	16	3
2:A:402[B]:MXT:O12	2:A:402[B]:MXT:C22	0.43	2.66	20	2
2:A:401[A]:MXT:O12	2:A:401[A]:MXT:C22	0.43	2.67	23	2
2:A:401[B]:MXT:O12	2:A:401[B]:MXT:C22	0.43	2.66	32	4
2:A:401[F]:MXT:O12	2:A:401[F]:MXT:C22	0.43	2.66	40	7
2:A:401[B]:MXT:C22	2:A:401[B]:MXT:O12	0.43	2.66	36	2
2:A:402[A]:MXT:C22	2:A:402[A]:MXT:O12	0.43	2.66	16	1
2:A:402[B]:MXT:O12	2:A:402[B]:MXT:C23	0.43	2.66	43	2
2:A:402[C]:MXT:O12	2:A:402[C]:MXT:C23	0.43	2.67	6	3
2:A:401[C]:MXT:O11	2:A:401[C]:MXT:C22	0.43	2.66	9	3
2:A:402[B]:MXT:C22	2:A:402[B]:MXT:O12	0.43	2.66	15	1
2:A:402[F]:MXT:O12	2:A:402[F]:MXT:C22	0.43	2.66	5	3
2:A:402[E]:MXT:O12	2:A:402[E]:MXT:C23	0.43	2.66	41	8
2:A:402[E]:MXT:O12	2:A:402[E]:MXT:C22	0.43	2.67	21	2
2:A:402[C]:MXT:O12	2:A:402[C]:MXT:C22	0.42	2.66	36	5
2:A:402[D]:MXT:O12	2:A:402[D]:MXT:C23	0.42	2.67	28	4
2:A:401[A]:MXT:C22	2:A:401[A]:MXT:O12	0.42	2.67	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:401[C]:MXT:O11	2:A:401[C]:MXT:H231	0.42	2.13	27	2
2:A:401[F]:MXT:O12	2:A:401[F]:MXT:H231	0.42	2.13	29	1
2:A:401[D]:MXT:O12	2:A:401[D]:MXT:C22	0.42	2.68	27	1
2:A:401[F]:MXT:H221	2:A:401[F]:MXT:O12	0.42	2.15	3	1
2:A:401[C]:MXT:O12	2:A:401[C]:MXT:C22	0.41	2.66	28	1
2:A:402[A]:MXT:O12	2:A:402[A]:MXT:H221	0.41	2.16	23	3
2:A:401[D]:MXT:O12	2:A:401[D]:MXT:H221	0.41	2.16	46	1
2:A:402[D]:MXT:O12	2:A:402[D]:MXT:C22	0.41	2.68	15	1
2:A:402[D]:MXT:H231	2:A:402[D]:MXT:O12	0.41	2.15	41	1
2:A:401[A]:MXT:O12	2:A:401[A]:MXT:C23	0.41	2.70	10	2
2:A:401[F]:MXT:O12	2:A:401[F]:MXT:H221	0.41	2.15	45	2
2:A:402[A]:MXT:H221	2:A:402[A]:MXT:O12	0.41	2.16	44	1
2:A:401[A]:MXT:O12	2:A:401[A]:MXT:H221	0.40	2.16	7	1
2:A:402[B]:MXT:O12	2:A:402[B]:MXT:H221	0.40	2.16	13	1
2:A:401[E]:MXT:O12	2:A:401[E]:MXT:H221	0.40	2.15	17	1
2:A:402[B]:MXT:H221	2:A:402[B]:MXT:O12	0.40	2.16	39	1

6.3 Torsion angles [i](#)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	A	16/370 (4%)	15±0 (94±0%)	1±0 (6±0%)	0±0 (0±0%)	100	100
All	All	800/18500 (4%)	750 (94%)	50 (6%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. 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	A	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	MXT	A	401[D]	1	19,19,19	1.81±0.00	5±0 (26±0%)
2	MXT	A	401[C]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	402[E]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	401[V]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	402[Y]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	402[C]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	401[Y]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	402[W]	1	19,19,19	1.83±0.00	5±0 (26±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	MXT	A	402[X]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	401[A]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	402[Z]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	401[Z]	1	19,19,19	1.84±0.00	5±0 (26±0%)
2	MXT	A	402[V]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	402[U]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	401[F]	1	19,19,19	1.84±0.00	5±0 (26±0%)
2	MXT	A	401[U]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	401[B]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	402[B]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	402[A]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	401[X]	1	19,19,19	1.81±0.00	5±0 (26±0%)
2	MXT	A	401[E]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	402[F]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	401[W]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	402[D]	1	19,19,19	1.82±0.00	5±0 (26±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	MXT	A	401[D]	1	27,31,31	1.22±0.01	4±0 (13±1%)
2	MXT	A	401[C]	1	27,31,31	1.23±0.01	3±0 (11±0%)
2	MXT	A	402[E]	1	27,31,31	1.25±0.01	4±0 (14±1%)
2	MXT	A	401[V]	1	27,31,31	1.23±0.01	3±0 (12±1%)
2	MXT	A	402[Y]	1	27,31,31	1.25±0.01	4±0 (14±1%)
2	MXT	A	402[C]	1	27,31,31	1.24±0.01	4±0 (14±0%)
2	MXT	A	401[Y]	1	27,31,31	1.22±0.01	3±1 (10±2%)
2	MXT	A	402[W]	1	27,31,31	1.24±0.01	4±0 (14±1%)
2	MXT	A	402[X]	1	27,31,31	1.25±0.01	4±0 (13±1%)
2	MXT	A	401[A]	1	27,31,31	1.23±0.01	3±0 (11±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
2	MXT	A	402[Z]	1	27,31,31	1.21±0.01	3±1 (11±2%)
2	MXT	A	401[Z]	1	27,31,31	1.24±0.01	4±0 (14±1%)
2	MXT	A	402[V]	1	27,31,31	1.21±0.01	3±1 (11±2%)
2	MXT	A	402[U]	1	27,31,31	1.23±0.01	3±0 (11±0%)
2	MXT	A	401[F]	1	27,31,31	1.24±0.01	4±0 (13±1%)
2	MXT	A	401[U]	1	27,31,31	1.23±0.01	3±0 (11±1%)
2	MXT	A	401[B]	1	27,31,31	1.23±0.01	3±0 (12±1%)
2	MXT	A	402[B]	1	27,31,31	1.21±0.01	3±0 (11±1%)
2	MXT	A	402[A]	1	27,31,31	1.23±0.01	3±0 (11±0%)
2	MXT	A	401[X]	1	27,31,31	1.22±0.01	4±0 (13±1%)
2	MXT	A	401[E]	1	27,31,31	1.22±0.01	3±1 (11±1%)
2	MXT	A	402[F]	1	27,31,31	1.21±0.01	3±1 (10±2%)
2	MXT	A	401[W]	1	27,31,31	1.23±0.01	3±0 (11±0%)
2	MXT	A	402[D]	1	27,31,31	1.25±0.01	4±0 (13±1%)

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	MXT	A	401[D]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[A]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[X]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[W]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[C]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[D]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[V]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[F]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[V]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[B]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[B]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[W]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[Z]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[Z]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[F]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[A]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[Y]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[U]	1	-	0±0,4,39,39	0±0,2,2,2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MXT	A	402[Y]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[X]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[U]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[E]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[E]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[C]	1	-	0±0,4,39,39	0±0,2,2,2

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	401[A]	MXT	O2-N2	3.84	1.22	1.43	24	50
2	A	402[D]	MXT	O2-N2	3.84	1.22	1.43	49	50
2	A	401[U]	MXT	O2-N2	3.84	1.22	1.43	17	50
2	A	402[C]	MXT	O2-N2	3.84	1.22	1.43	21	50
2	A	402[U]	MXT	O2-N2	3.84	1.22	1.43	9	50
2	A	401[E]	MXT	O2-N2	3.84	1.22	1.43	36	50
2	A	401[Z]	MXT	O2-N2	3.84	1.22	1.43	29	50
2	A	402[A]	MXT	O2-N2	3.84	1.22	1.43	6	50
2	A	402[X]	MXT	O2-N2	3.84	1.22	1.43	5	50
2	A	402[Y]	MXT	O2-N2	3.84	1.22	1.43	35	50
2	A	402[Z]	MXT	O2-N2	3.84	1.22	1.43	45	50
2	A	401[Y]	MXT	O2-N2	3.84	1.22	1.43	6	50
2	A	402[F]	MXT	O2-N2	3.84	1.22	1.43	46	50
2	A	401[F]	MXT	O2-N2	3.83	1.22	1.43	43	50
2	A	402[E]	MXT	O2-N2	3.83	1.22	1.43	19	50
2	A	402[W]	MXT	O2-N2	3.83	1.22	1.43	48	50
2	A	402[B]	MXT	O2-N2	3.83	1.22	1.43	20	50
2	A	402[V]	MXT	O2-N2	3.83	1.22	1.43	46	50
2	A	401[V]	MXT	O2-N2	3.82	1.22	1.43	40	50
2	A	401[D]	MXT	O2-N2	3.82	1.22	1.43	42	50
2	A	401[B]	MXT	O2-N2	3.82	1.22	1.43	23	50
2	A	401[C]	MXT	O2-N2	3.82	1.22	1.43	9	50
2	A	401[W]	MXT	O2-N2	3.82	1.23	1.43	11	50
2	A	401[X]	MXT	O2-N2	3.82	1.23	1.43	48	50
2	A	401[F]	MXT	C24-N2	3.26	1.53	1.48	8	50
2	A	401[Z]	MXT	C24-N2	3.25	1.53	1.48	48	50
2	A	402[B]	MXT	C24-N2	3.24	1.53	1.48	10	50
2	A	402[E]	MXT	C24-N2	3.24	1.53	1.48	16	50
2	A	402[Y]	MXT	C24-N2	3.24	1.53	1.48	21	50
2	A	402[V]	MXT	C24-N2	3.23	1.53	1.48	29	50
2	A	401[V]	MXT	C24-N2	3.22	1.53	1.48	49	50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	402[X]	MXT	C24-N2	3.22	1.53	1.48	30	50
2	A	401[F]	MXT	C27-N2	3.22	1.53	1.48	32	50
2	A	401[U]	MXT	C27-N2	3.22	1.53	1.48	31	50
2	A	401[B]	MXT	C24-N2	3.21	1.53	1.48	44	50
2	A	402[F]	MXT	C24-N2	3.21	1.53	1.48	25	50
2	A	401[Y]	MXT	C24-N2	3.21	1.53	1.48	7	50
2	A	402[D]	MXT	C24-N2	3.20	1.53	1.48	39	50
2	A	402[C]	MXT	C24-N2	3.20	1.53	1.48	47	50
2	A	401[C]	MXT	C24-N2	3.19	1.53	1.48	2	50
2	A	401[Z]	MXT	C27-N2	3.20	1.53	1.48	31	50
2	A	402[Z]	MXT	C24-N2	3.19	1.53	1.48	10	50
2	A	402[W]	MXT	C24-N2	3.18	1.53	1.48	21	50
2	A	401[E]	MXT	C24-N2	3.18	1.53	1.48	1	50
2	A	402[U]	MXT	C27-N2	3.18	1.53	1.48	7	50
2	A	402[A]	MXT	C24-N2	3.17	1.53	1.48	9	50
2	A	401[A]	MXT	C27-N2	3.17	1.53	1.48	2	50
2	A	402[A]	MXT	C27-N2	3.17	1.53	1.48	1	50
2	A	401[U]	MXT	C24-N2	3.17	1.53	1.48	10	50
2	A	401[W]	MXT	C24-N2	3.16	1.53	1.48	18	50
2	A	402[W]	MXT	C27-N2	3.16	1.53	1.48	6	50
2	A	401[A]	MXT	C24-N2	3.16	1.53	1.48	21	50
2	A	402[C]	MXT	C27-N2	3.16	1.53	1.48	6	50
2	A	402[Z]	MXT	C27-N2	3.16	1.53	1.48	36	50
2	A	401[D]	MXT	C27-N2	3.15	1.52	1.48	22	50
2	A	401[E]	MXT	C27-N2	3.14	1.52	1.48	5	50
2	A	401[X]	MXT	C27-N2	3.14	1.52	1.48	33	50
2	A	402[U]	MXT	C24-N2	3.14	1.52	1.48	18	50
2	A	401[Y]	MXT	C27-N2	3.13	1.52	1.48	6	50
2	A	401[W]	MXT	C27-N2	3.12	1.52	1.48	30	50
2	A	402[F]	MXT	C27-N2	3.13	1.52	1.48	12	50
2	A	401[V]	MXT	C27-N2	3.12	1.52	1.48	15	50
2	A	401[B]	MXT	C27-N2	3.11	1.52	1.48	9	50
2	A	402[X]	MXT	C27-N2	3.11	1.52	1.48	41	50
2	A	402[B]	MXT	C27-N2	3.11	1.52	1.48	48	50
2	A	402[D]	MXT	C27-N2	3.10	1.52	1.48	28	50
2	A	402[V]	MXT	C27-N2	3.10	1.52	1.48	31	50
2	A	401[C]	MXT	C27-N2	3.09	1.52	1.48	38	50
2	A	402[E]	MXT	C27-N2	3.09	1.52	1.48	50	50
2	A	401[X]	MXT	C24-N2	3.08	1.52	1.48	27	50
2	A	401[D]	MXT	C24-N2	3.08	1.52	1.48	45	50
2	A	402[Y]	MXT	C27-N2	3.07	1.52	1.48	12	50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	401[A]	MXT	C14-N1	2.47	1.44	1.39	23	50
2	A	402[E]	MXT	C14-N1	2.45	1.44	1.39	22	50
2	A	401[C]	MXT	C14-N1	2.45	1.44	1.39	21	50
2	A	402[Y]	MXT	C14-N1	2.44	1.44	1.39	18	50
2	A	401[U]	MXT	C14-N1	2.44	1.44	1.39	27	50
2	A	401[W]	MXT	C14-N1	2.43	1.44	1.39	38	50
2	A	402[D]	MXT	C14-N1	2.42	1.43	1.39	35	50
2	A	402[X]	MXT	C14-N1	2.41	1.43	1.39	32	50
2	A	401[B]	MXT	C14-N1	2.41	1.43	1.39	24	50
2	A	401[X]	MXT	C14-N1	2.41	1.43	1.39	14	50
2	A	402[C]	MXT	C14-N1	2.41	1.43	1.39	46	50
2	A	402[V]	MXT	C14-N1	2.40	1.43	1.39	50	50
2	A	401[D]	MXT	C14-N1	2.40	1.43	1.39	45	50
2	A	401[V]	MXT	C14-N1	2.40	1.43	1.39	33	50
2	A	402[A]	MXT	C14-N1	2.39	1.43	1.39	49	50
2	A	402[W]	MXT	C14-N1	2.39	1.43	1.39	5	50
2	A	402[B]	MXT	C14-N1	2.38	1.43	1.39	41	50
2	A	401[Z]	MXT	C14-N1	2.38	1.43	1.39	16	50
2	A	402[U]	MXT	C14-N1	2.37	1.43	1.39	26	50
2	A	401[F]	MXT	C14-N1	2.36	1.43	1.39	39	50
2	A	402[F]	MXT	C14-N1	2.34	1.43	1.39	7	50
2	A	402[Z]	MXT	C14-N1	2.34	1.43	1.39	1	50
2	A	401[Y]	MXT	C14-N1	2.33	1.43	1.39	12	50
2	A	401[E]	MXT	C14-N1	2.31	1.43	1.39	21	50
2	A	402[Y]	MXT	C13-N1	2.22	1.43	1.39	7	50
2	A	401[F]	MXT	C13-N1	2.21	1.43	1.39	9	50
2	A	401[Z]	MXT	C13-N1	2.21	1.43	1.39	6	50
2	A	402[E]	MXT	C13-N1	2.20	1.43	1.39	2	50
2	A	402[D]	MXT	C13-N1	2.19	1.43	1.39	50	50
2	A	401[Y]	MXT	C13-N1	2.19	1.43	1.39	31	50
2	A	402[C]	MXT	C13-N1	2.18	1.43	1.39	46	50
2	A	401[E]	MXT	C13-N1	2.18	1.43	1.39	30	50
2	A	402[W]	MXT	C13-N1	2.18	1.43	1.39	48	50
2	A	402[X]	MXT	C13-N1	2.17	1.43	1.39	21	50
2	A	402[A]	MXT	C13-N1	2.16	1.43	1.39	19	50
2	A	402[U]	MXT	C13-N1	2.16	1.43	1.39	15	50
2	A	401[X]	MXT	C13-N1	2.14	1.43	1.39	17	50
2	A	401[C]	MXT	C13-N1	2.14	1.43	1.39	40	50
2	A	401[V]	MXT	C13-N1	2.14	1.43	1.39	14	50
2	A	401[D]	MXT	C13-N1	2.13	1.43	1.39	30	50
2	A	402[Z]	MXT	C13-N1	2.13	1.43	1.39	26	50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	402[V]	MXT	C13-N1	2.13	1.43	1.39	5	50
2	A	402[B]	MXT	C13-N1	2.13	1.43	1.39	48	50
2	A	402[F]	MXT	C13-N1	2.13	1.43	1.39	45	50
2	A	401[A]	MXT	C13-N1	2.13	1.43	1.39	40	50
2	A	401[W]	MXT	C13-N1	2.12	1.43	1.39	42	50
2	A	401[B]	MXT	C13-N1	2.12	1.43	1.39	50	50
2	A	401[U]	MXT	C13-N1	2.11	1.43	1.39	38	50

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	402[X]	MXT	C13-N1-C14	3.73	110.14	112.48	31	50
2	A	402[D]	MXT	C13-N1-C14	3.68	110.17	112.48	1	50
2	A	402[E]	MXT	C13-N1-C14	3.67	110.17	112.48	45	50
2	A	402[Y]	MXT	C13-N1-C14	3.66	110.18	112.48	38	50
2	A	401[F]	MXT	C13-N1-C14	3.63	110.20	112.48	33	50
2	A	401[Z]	MXT	C13-N1-C14	3.63	110.20	112.48	10	50
2	A	401[C]	MXT	C13-N1-C14	3.61	110.21	112.48	7	50
2	A	402[W]	MXT	C13-N1-C14	3.61	110.22	112.48	16	50
2	A	402[U]	MXT	C13-N1-C14	3.59	110.22	112.48	39	50
2	A	402[A]	MXT	C13-N1-C14	3.59	110.22	112.48	21	50
2	A	401[W]	MXT	C13-N1-C14	3.59	110.23	112.48	38	50
2	A	401[B]	MXT	C13-N1-C14	3.59	110.23	112.48	2	50
2	A	402[C]	MXT	C13-N1-C14	3.58	110.23	112.48	46	50
2	A	401[V]	MXT	C13-N1-C14	3.57	110.23	112.48	10	50
2	A	401[A]	MXT	C13-N1-C14	3.54	110.26	112.48	17	50
2	A	401[Y]	MXT	C13-N1-C14	3.54	110.26	112.48	27	50
2	A	401[U]	MXT	C13-N1-C14	3.53	110.26	112.48	5	50
2	A	401[E]	MXT	C13-N1-C14	3.51	110.27	112.48	30	50
2	A	402[B]	MXT	C13-N1-C14	3.50	110.28	112.48	15	50
2	A	402[V]	MXT	C13-N1-C14	3.49	110.29	112.48	47	50
2	A	401[D]	MXT	C13-N1-C14	3.49	110.29	112.48	3	50
2	A	401[X]	MXT	C13-N1-C14	3.48	110.30	112.48	11	50
2	A	402[F]	MXT	C13-N1-C14	3.45	110.31	112.48	42	50
2	A	402[Z]	MXT	C13-N1-C14	3.42	110.33	112.48	43	50
2	A	401[A]	MXT	C11-C13-N1	2.22	109.88	107.98	17	50
2	A	401[U]	MXT	C11-C13-N1	2.22	109.88	107.98	27	50
2	A	402[W]	MXT	C11-C13-N1	2.20	109.86	107.98	38	50
2	A	402[X]	MXT	C11-C13-N1	2.20	109.86	107.98	31	50
2	A	401[B]	MXT	C11-C13-N1	2.20	109.86	107.98	42	50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	401[V]	MXT	C11-C13-N1	2.19	109.86	107.98	42	50
2	A	402[Y]	MXT	C11-C13-N1	2.18	109.85	107.98	3	50
2	A	401[F]	MXT	C11-C13-N1	2.18	109.84	107.98	12	50
2	A	402[D]	MXT	C11-C13-N1	2.18	109.84	107.98	31	50
2	A	401[Z]	MXT	C11-C13-N1	2.18	109.84	107.98	41	50
2	A	402[E]	MXT	C11-C13-N1	2.18	109.84	107.98	20	50
2	A	402[C]	MXT	C11-C13-N1	2.17	109.84	107.98	35	50
2	A	402[A]	MXT	C11-C13-N1	2.16	109.83	107.98	21	50
2	A	401[W]	MXT	C11-C13-N1	2.14	109.81	107.98	15	50
2	A	402[U]	MXT	C11-C13-N1	2.14	109.81	107.98	4	50
2	A	401[C]	MXT	C11-C13-N1	2.13	109.80	107.98	34	49
2	A	402[B]	MXT	C11-C13-N1	2.12	109.79	107.98	4	45
2	A	401[U]	MXT	C27-C23-C21	2.11	117.82	113.50	3	50
2	A	402[V]	MXT	C11-C13-N1	2.10	109.78	107.98	38	43
2	A	401[A]	MXT	C27-C23-C21	2.10	117.79	113.50	42	50
2	A	402[A]	MXT	C27-C23-C21	2.10	117.79	113.50	28	50
2	A	402[F]	MXT	C27-C23-C21	2.10	117.79	113.50	9	50
2	A	402[U]	MXT	C27-C23-C21	2.10	117.79	113.50	10	50
2	A	402[D]	MXT	C27-C23-C21	2.10	117.78	113.50	17	50
2	A	402[Z]	MXT	C27-C23-C21	2.10	117.78	113.50	11	50
2	A	401[C]	MXT	C27-C23-C21	2.09	117.78	113.50	49	50
2	A	401[W]	MXT	C27-C23-C21	2.09	117.77	113.50	27	50
2	A	401[Y]	MXT	C27-C23-C21	2.09	117.77	113.50	41	50
2	A	401[B]	MXT	C27-C23-C21	2.09	117.77	113.50	49	50
2	A	401[D]	MXT	C23-C27-N2	2.09	111.30	108.66	1	50
2	A	401[V]	MXT	C27-C23-C21	2.09	117.77	113.50	7	50
2	A	401[Y]	MXT	C11-C13-N1	2.09	109.77	107.98	2	38
2	A	401[E]	MXT	C11-C13-N1	2.08	109.76	107.98	6	41
2	A	401[X]	MXT	C23-C27-N2	2.08	111.30	108.66	45	50
2	A	402[B]	MXT	C27-C23-C21	2.08	117.76	113.50	28	50
2	A	402[X]	MXT	C27-C23-C21	2.08	117.76	113.50	29	50
2	A	402[F]	MXT	C11-C13-N1	2.08	109.76	107.98	47	35
2	A	401[Z]	MXT	C27-C23-C21	2.08	117.75	113.50	3	50
2	A	401[E]	MXT	C27-C23-C21	2.08	117.75	113.50	16	50
2	A	402[V]	MXT	C27-C23-C21	2.08	117.75	113.50	13	50
2	A	402[Z]	MXT	C11-C13-N1	2.08	109.76	107.98	13	35
2	A	401[F]	MXT	C27-C23-C21	2.08	117.75	113.50	27	50
2	A	401[X]	MXT	C11-C13-N1	2.08	109.76	107.98	50	33
2	A	401[D]	MXT	C11-C13-N1	2.08	109.76	107.98	25	26
2	A	402[Y]	MXT	C27-C23-C21	2.07	117.73	113.50	5	50
2	A	402[E]	MXT	C27-C23-C21	2.07	117.73	113.50	15	50

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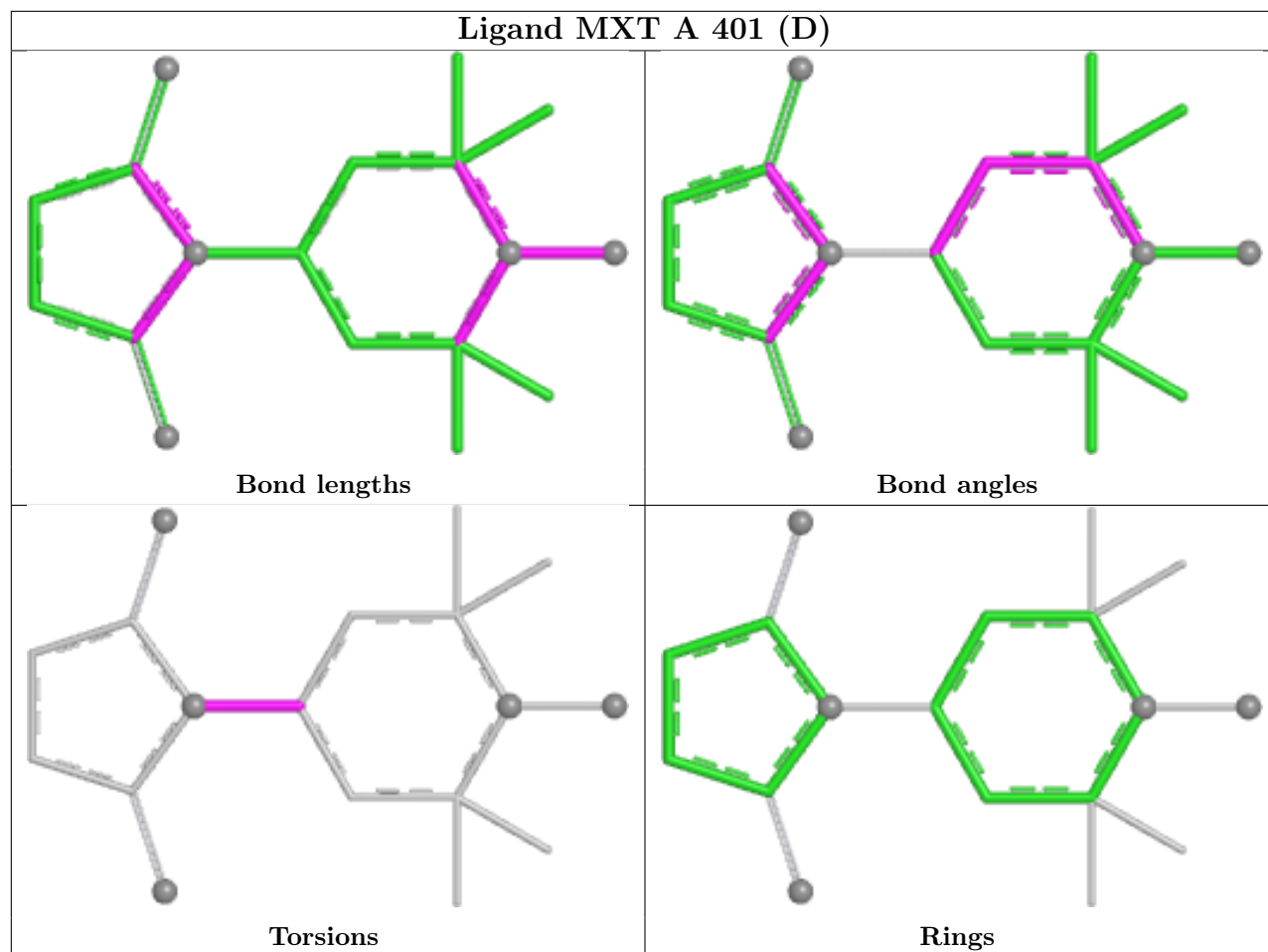
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	402[C]	MXT	C27-C23-C21	2.07	117.73	113.50	25	50
2	A	402[Y]	MXT	C23-C27-N2	2.06	111.27	108.66	49	42
2	A	402[W]	MXT	C27-C23-C21	2.06	117.71	113.50	7	50
2	A	402[W]	MXT	C23-C27-N2	2.06	111.27	108.66	37	44
2	A	401[D]	MXT	C27-C23-C21	2.06	117.71	113.50	39	50
2	A	401[X]	MXT	C27-C23-C21	2.06	117.70	113.50	8	50
2	A	402[E]	MXT	C23-C27-N2	2.06	111.27	108.66	19	42
2	A	402[C]	MXT	C23-C27-N2	2.05	111.26	108.66	27	47
2	A	401[F]	MXT	C23-C27-N2	2.05	111.26	108.66	38	33
2	A	401[Z]	MXT	C23-C27-N2	2.05	111.25	108.66	27	41
2	A	402[D]	MXT	C23-C27-N2	2.05	111.25	108.66	10	31
2	A	401[B]	MXT	C23-C27-N2	2.04	111.24	108.66	44	24
2	A	401[E]	MXT	C23-C27-N2	2.04	111.24	108.66	2	11
2	A	401[Y]	MXT	C23-C27-N2	2.04	111.24	108.66	11	10
2	A	402[X]	MXT	C23-C27-N2	2.04	111.24	108.66	1	34
2	A	401[V]	MXT	C23-C27-N2	2.03	111.23	108.66	25	24
2	A	402[Z]	MXT	C23-C27-N2	2.03	111.23	108.66	13	17
2	A	402[F]	MXT	C23-C27-N2	2.03	111.22	108.66	42	13
2	A	402[V]	MXT	C23-C27-N2	2.02	111.22	108.66	49	9
2	A	402[B]	MXT	C23-C27-N2	2.02	111.22	108.66	12	8
2	A	401[A]	MXT	C23-C27-N2	2.01	111.21	108.66	21	3
2	A	401[U]	MXT	C23-C27-N2	2.01	111.20	108.66	1	4
2	A	402[A]	MXT	C23-C27-N2	2.00	111.20	108.66	47	1
2	A	402[U]	MXT	C23-C27-N2	2.00	111.20	108.66	48	1

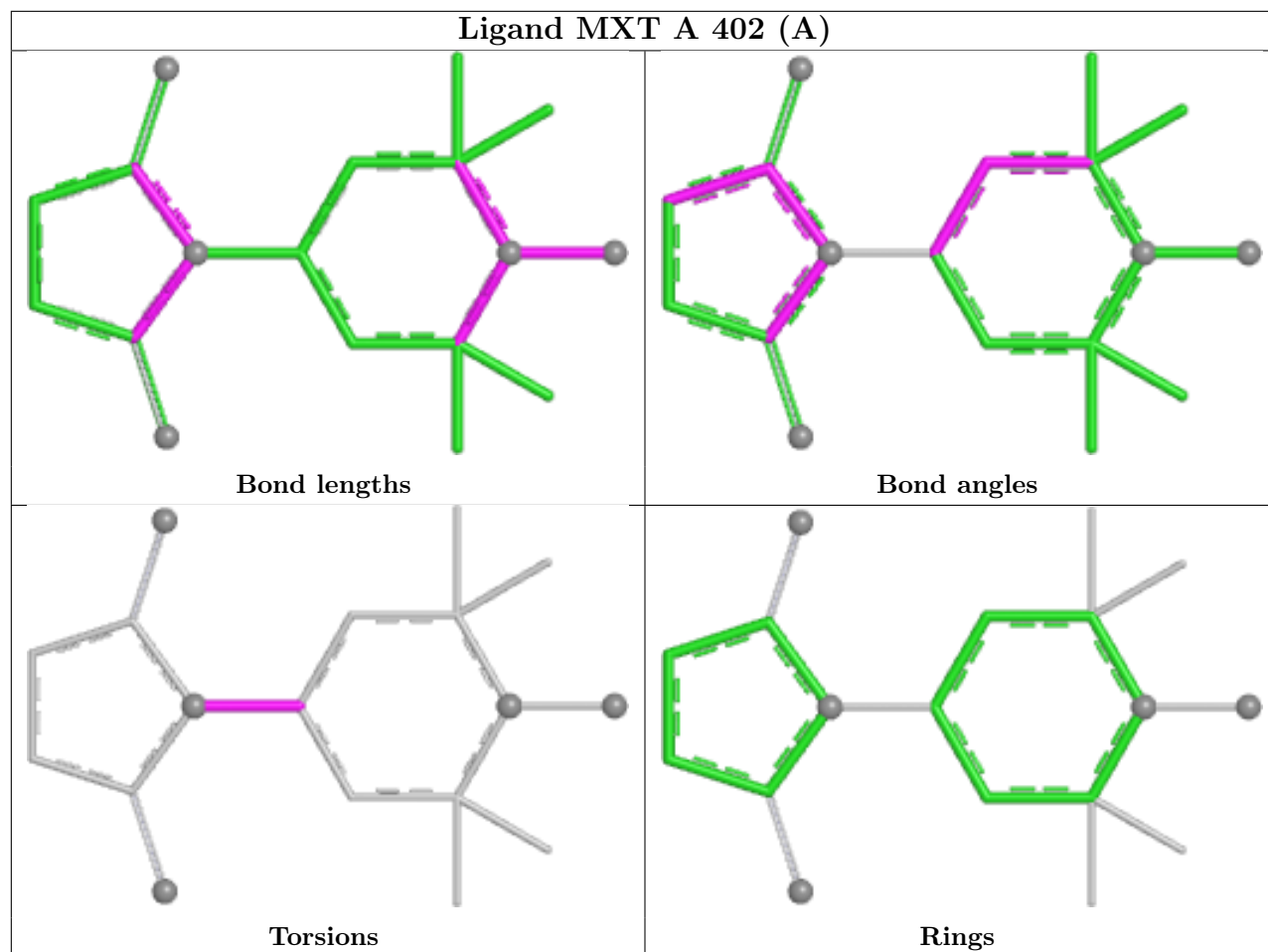
There are no chirality outliers.

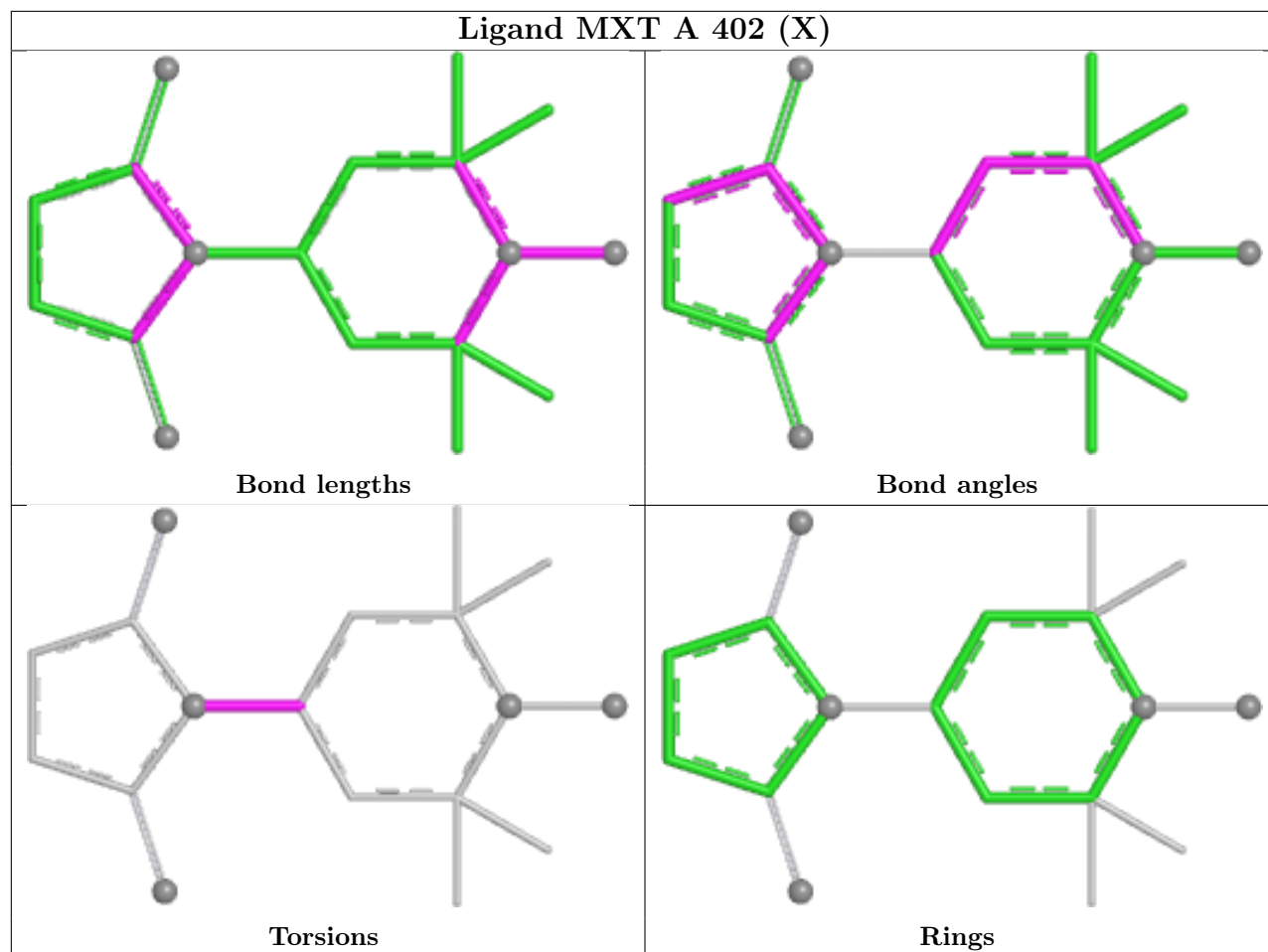
There are no torsion outliers.

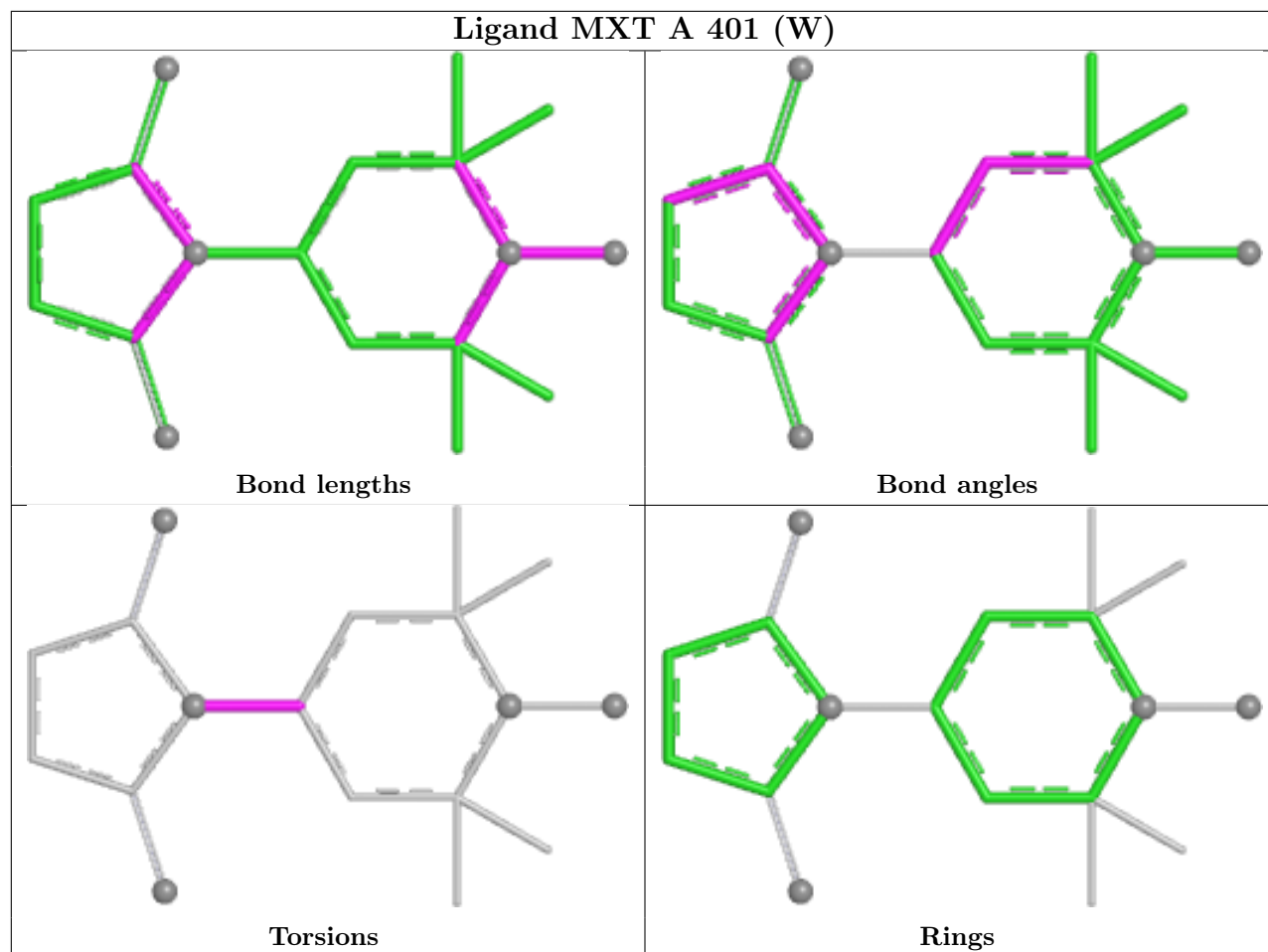
There are no ring outliers.

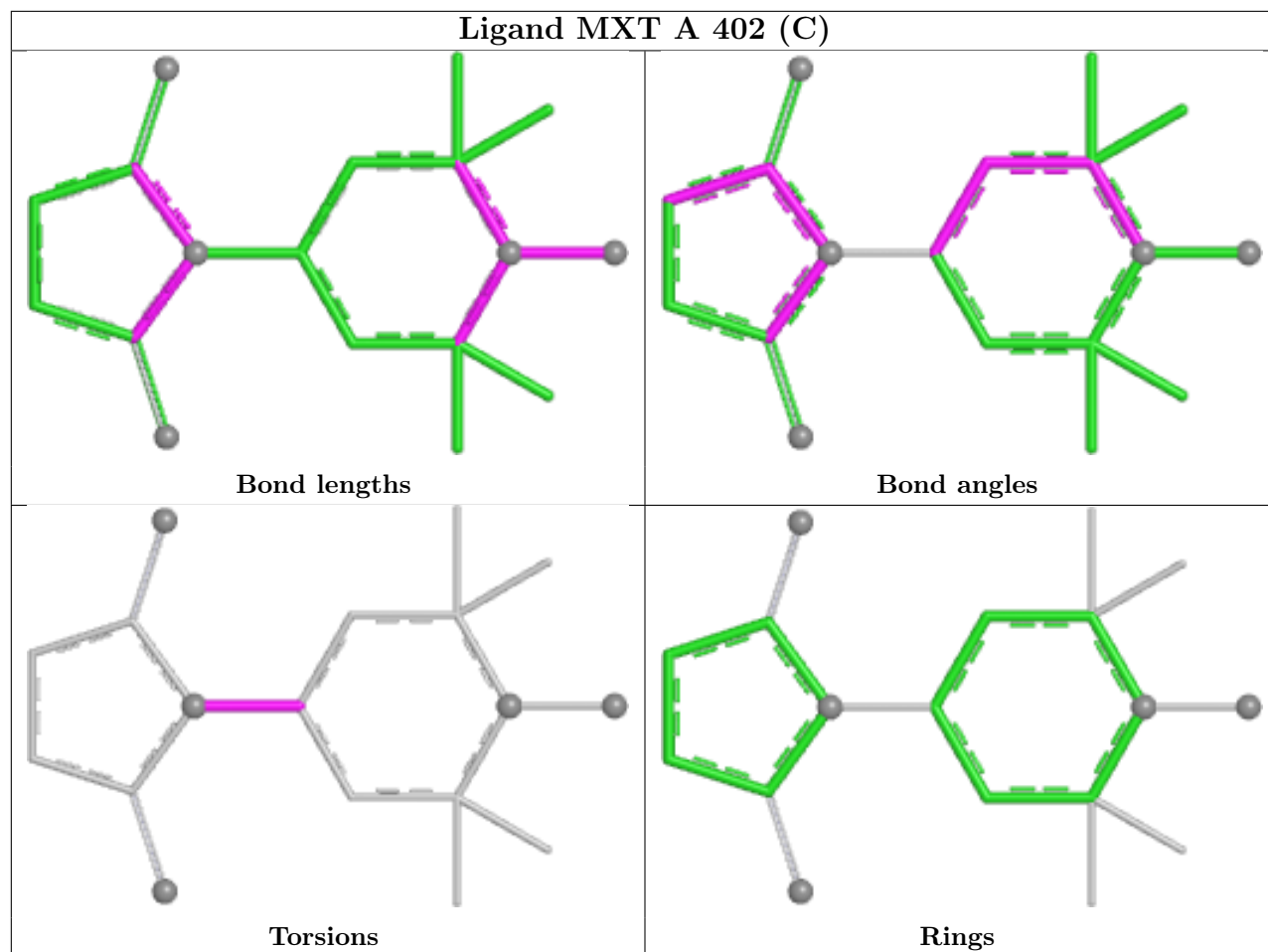
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

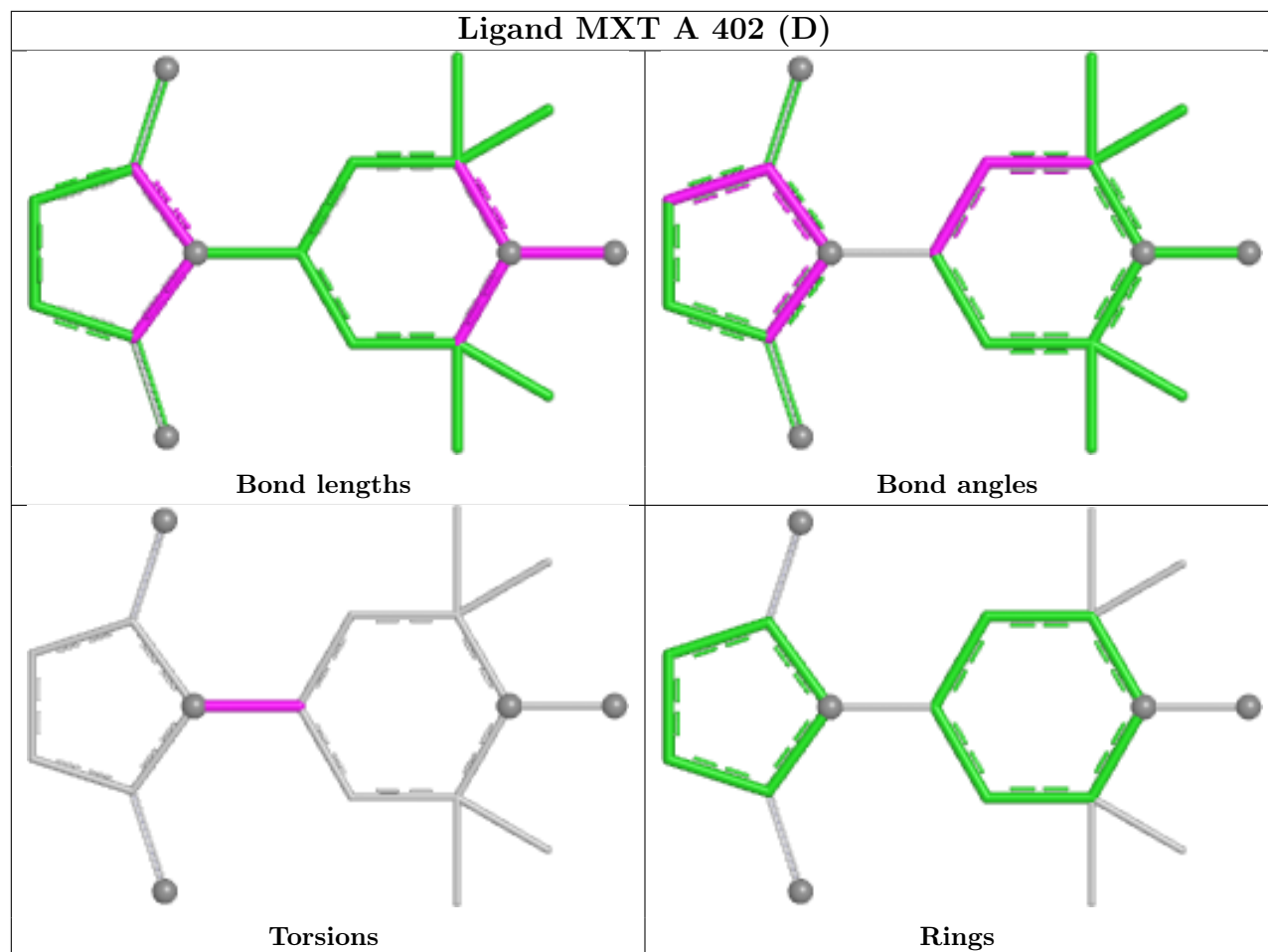


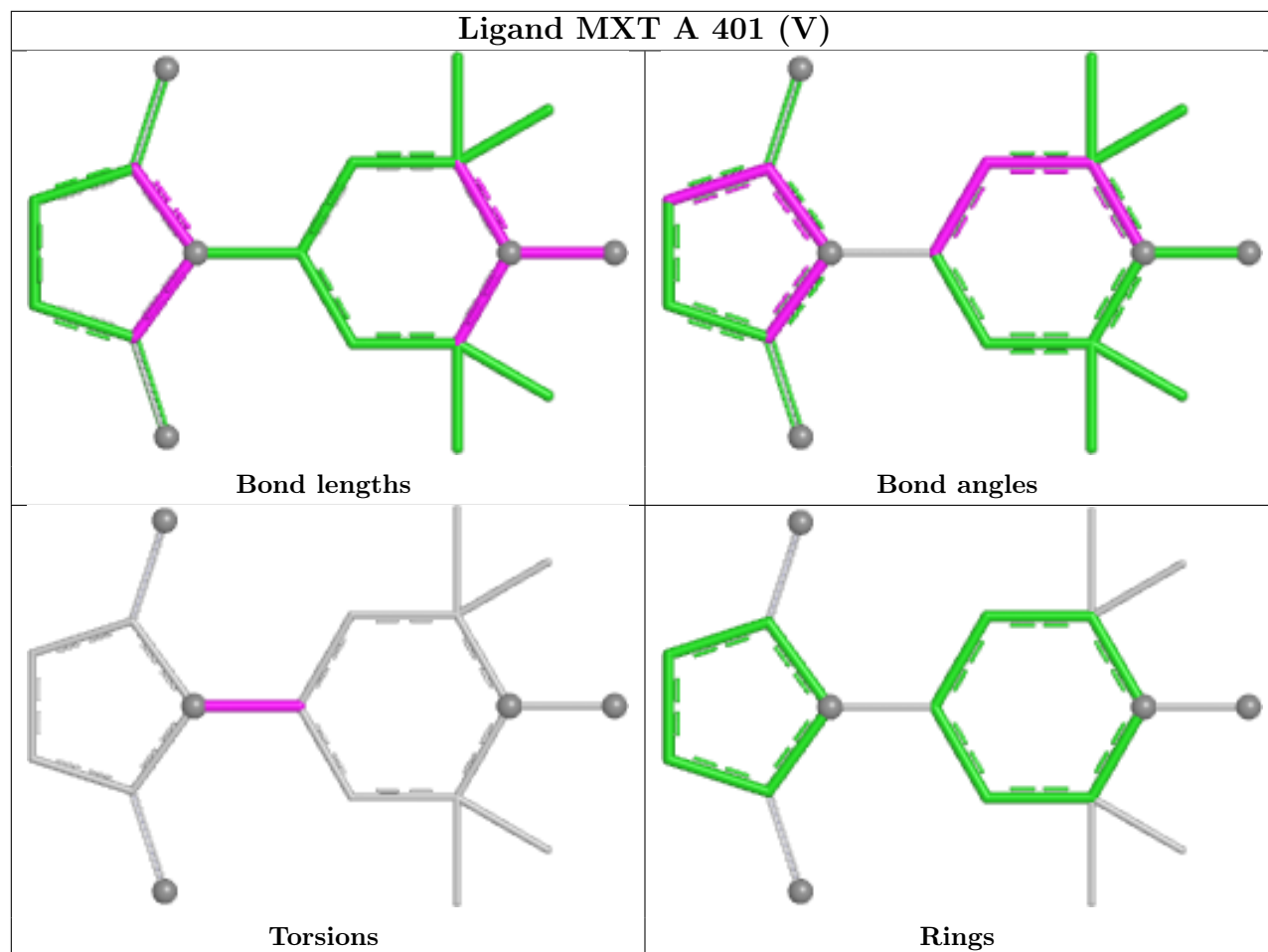


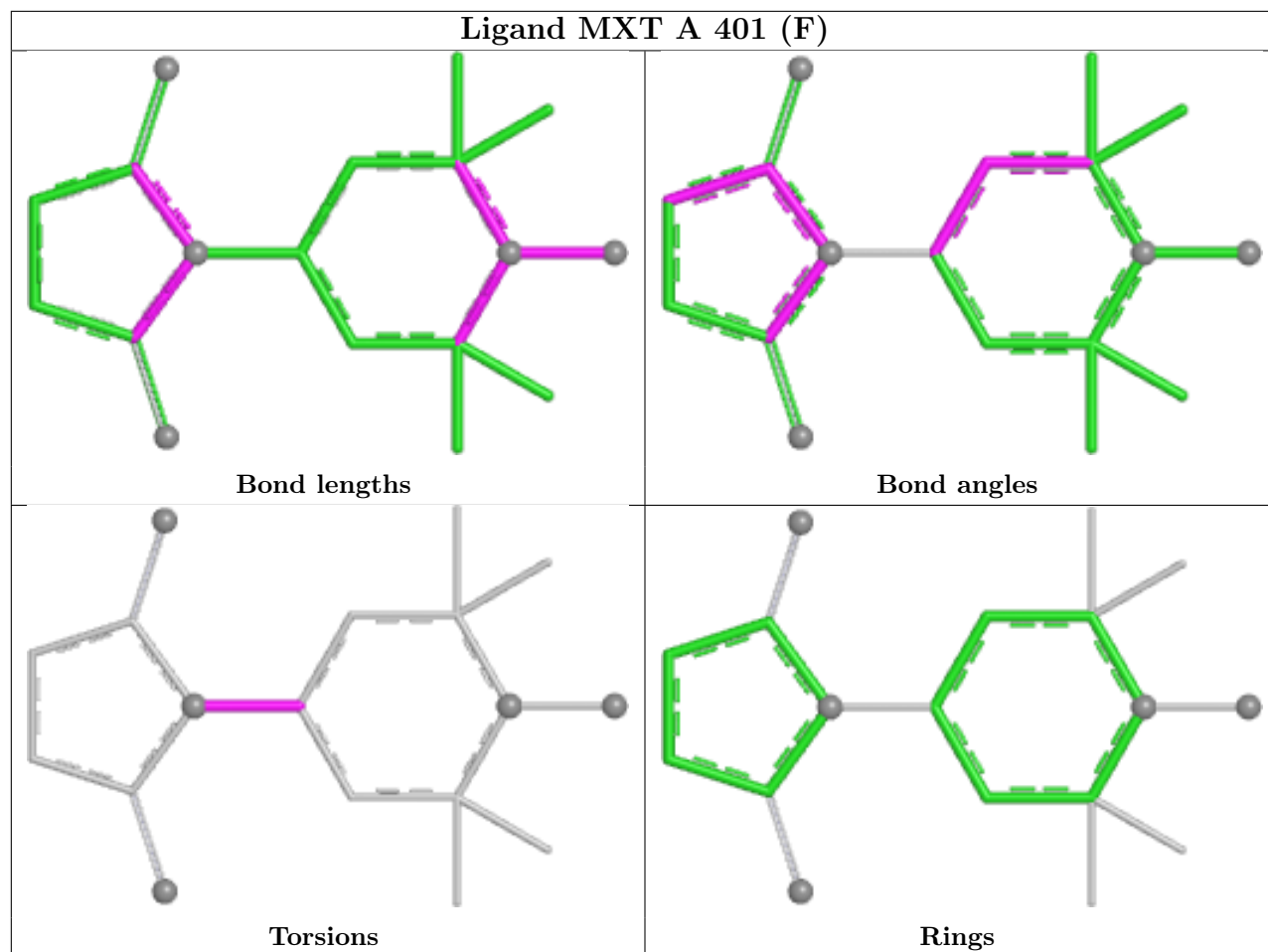


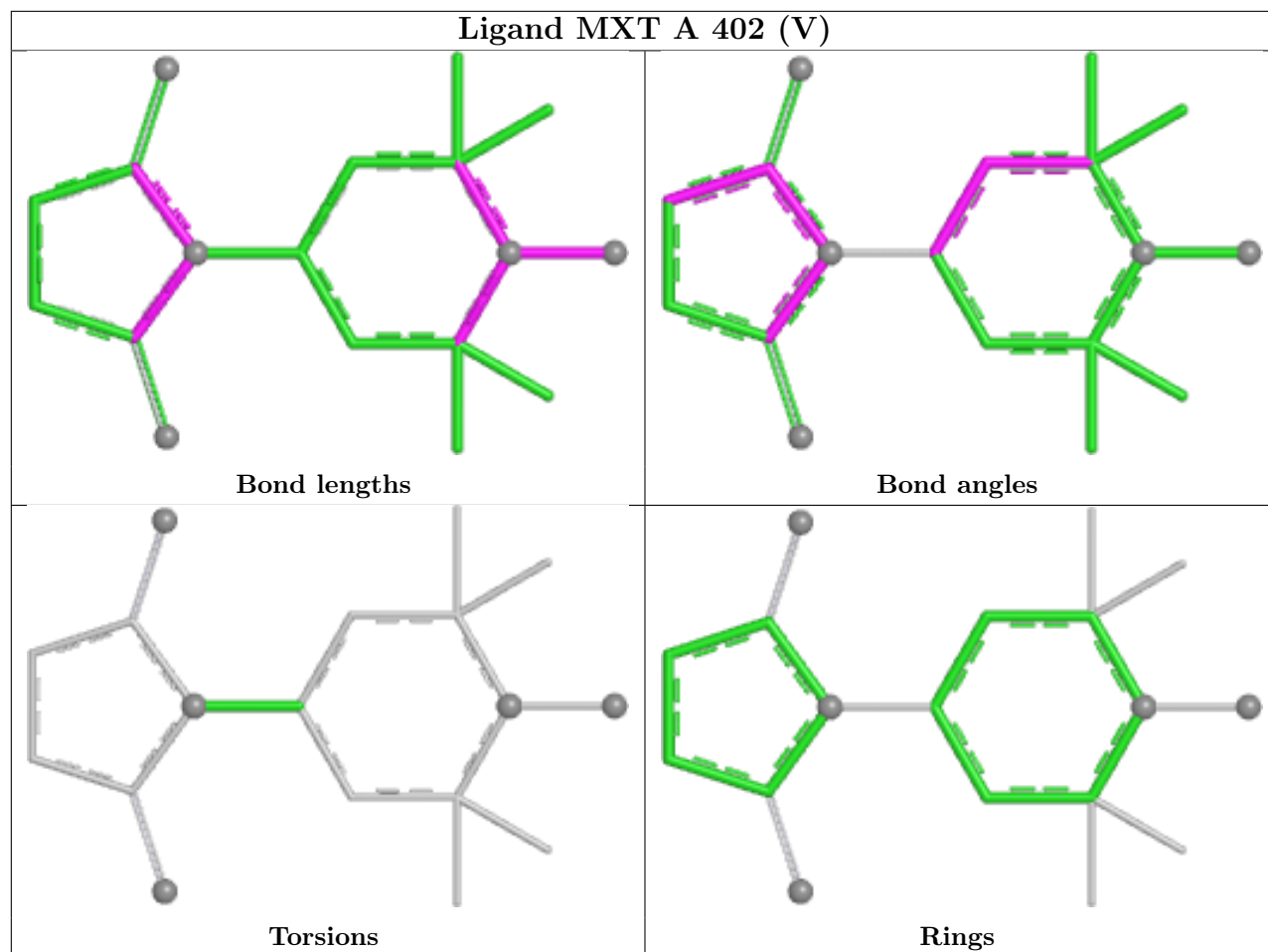


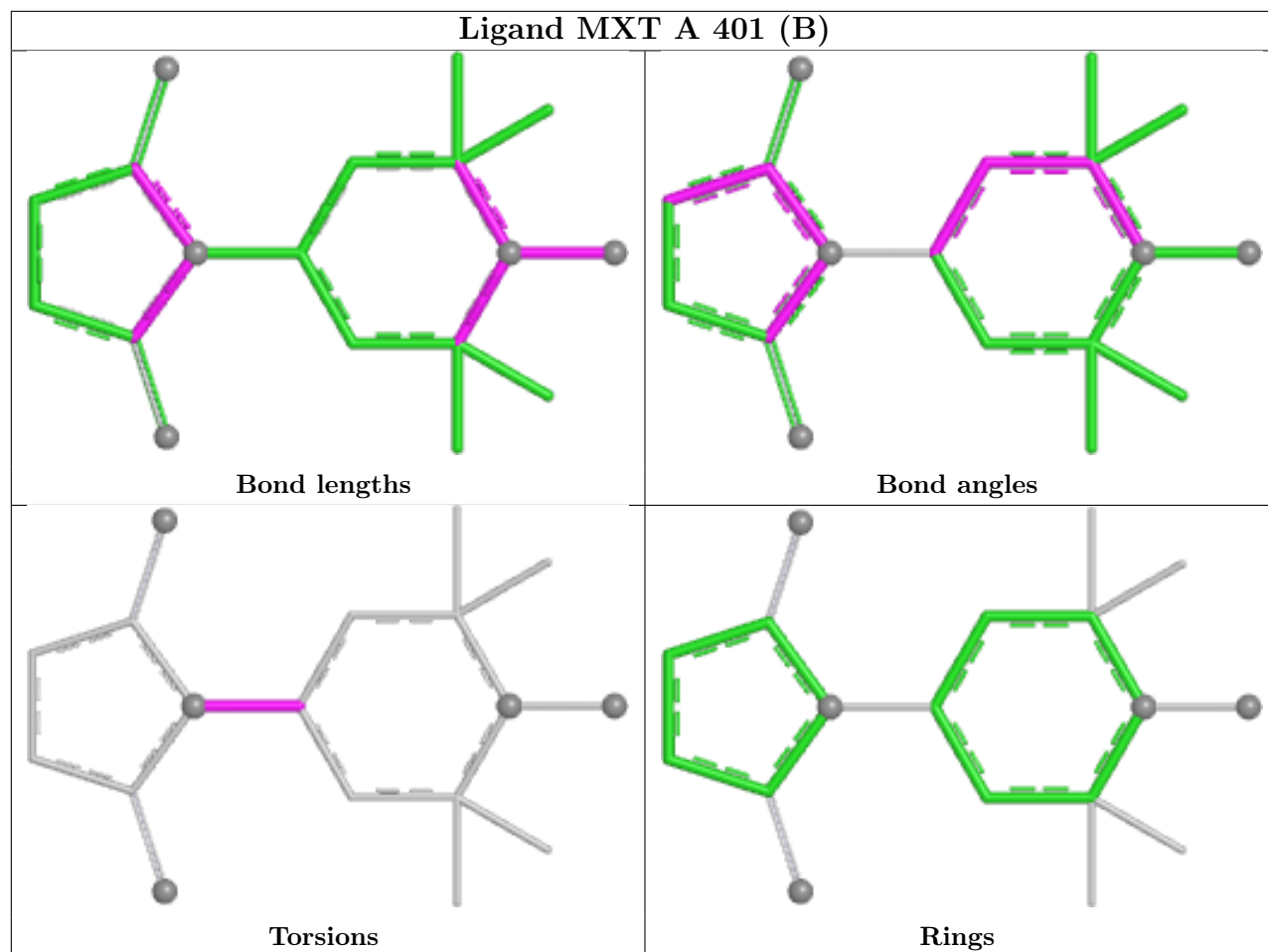


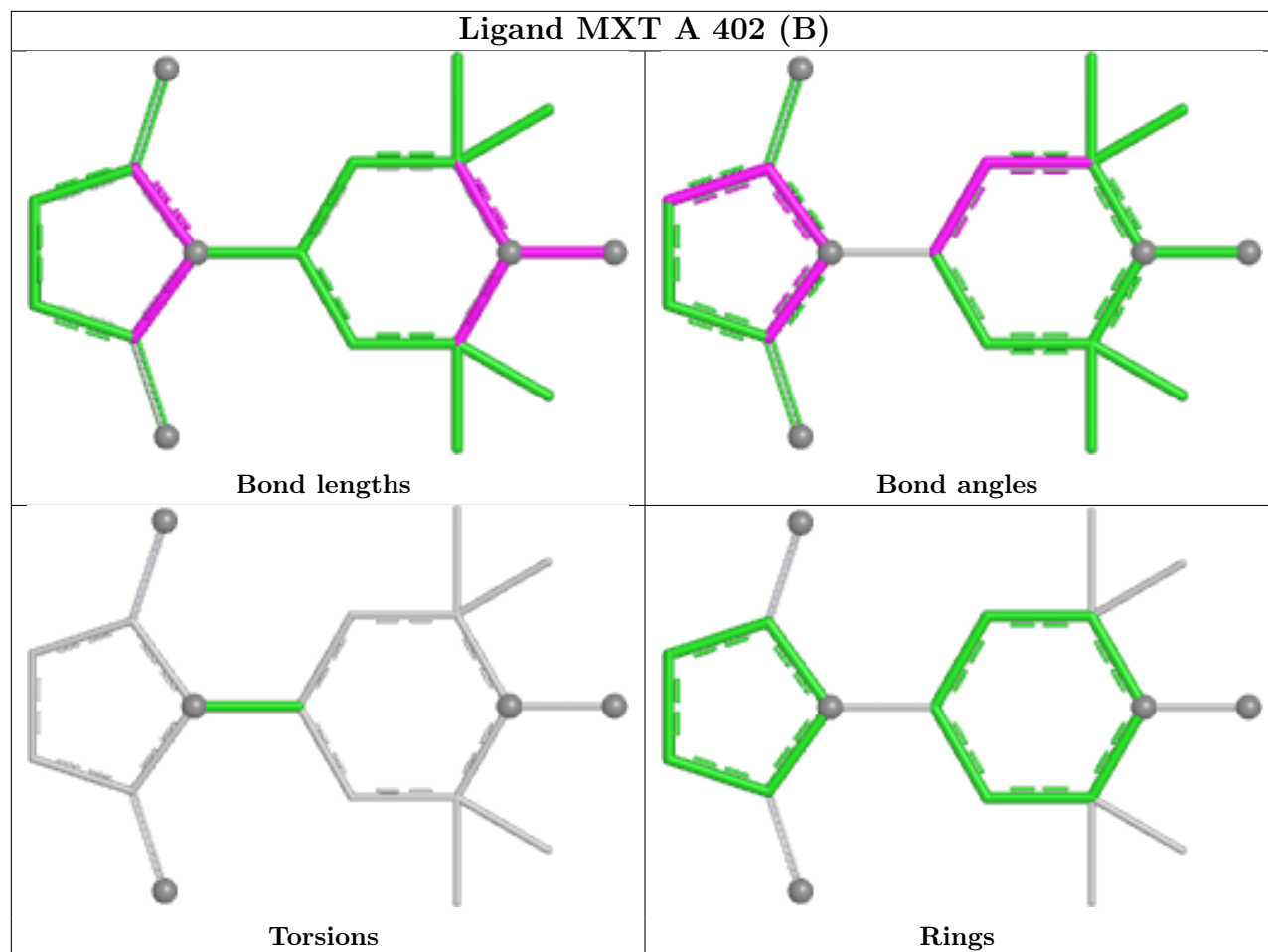


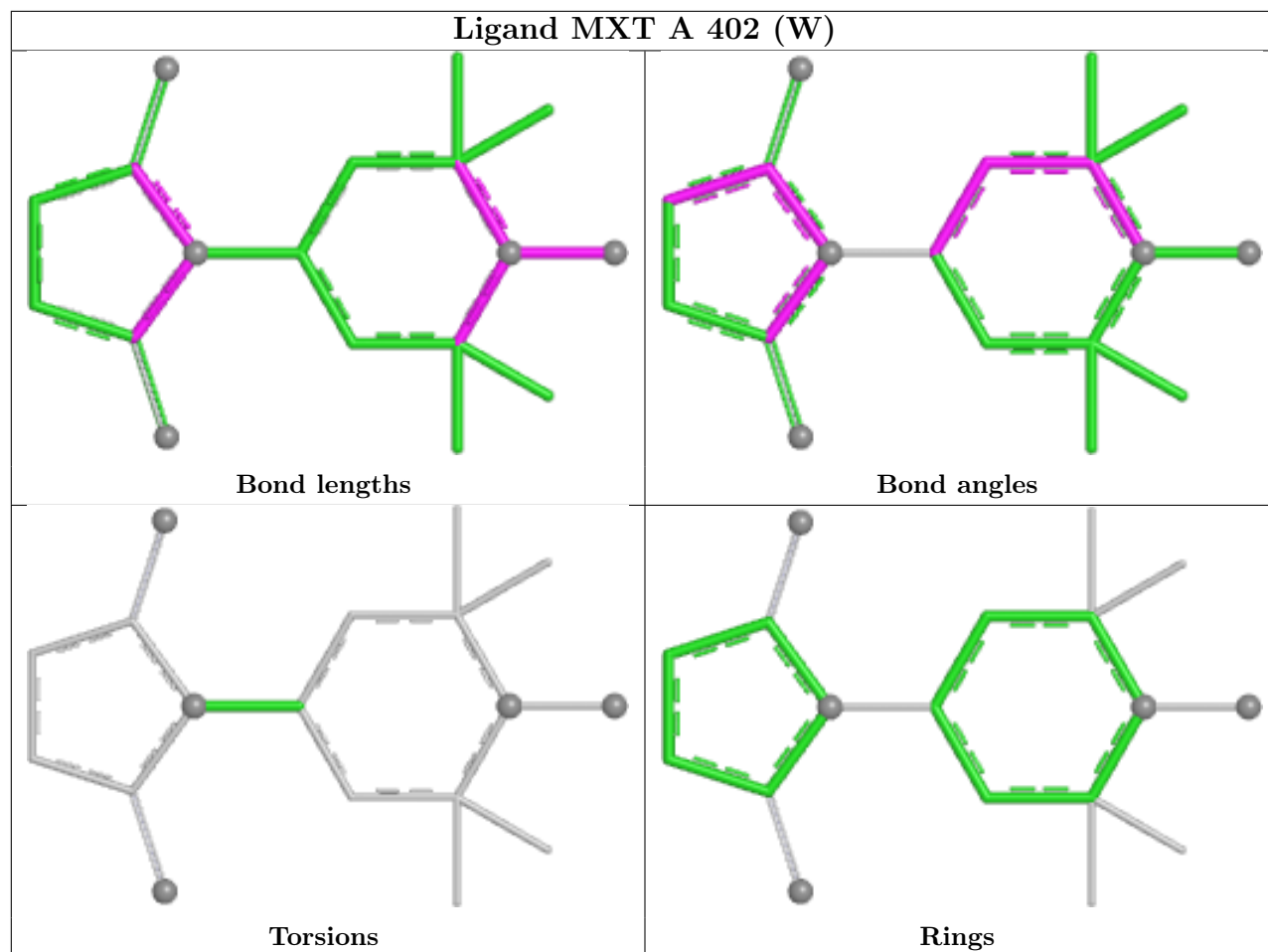


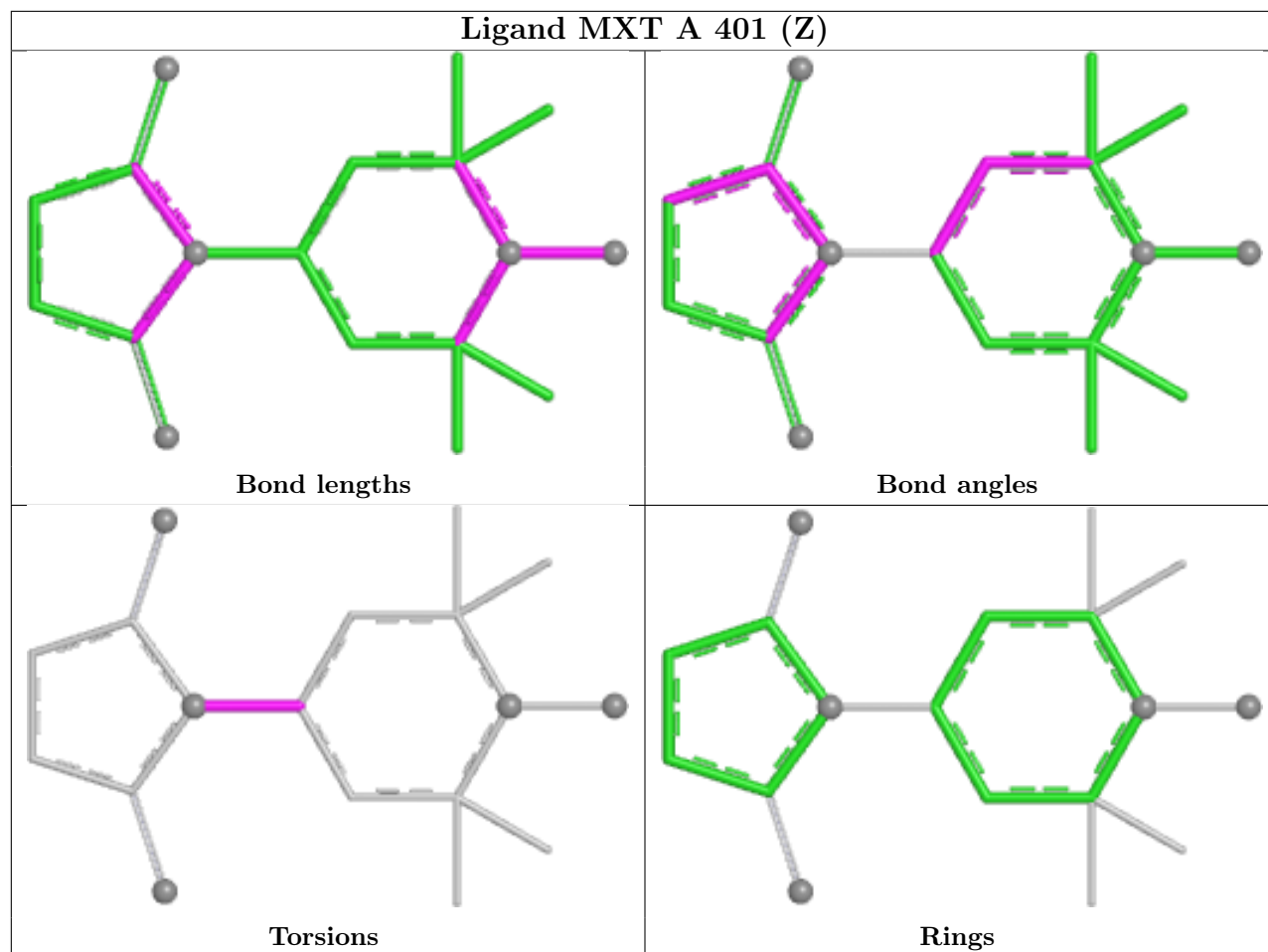


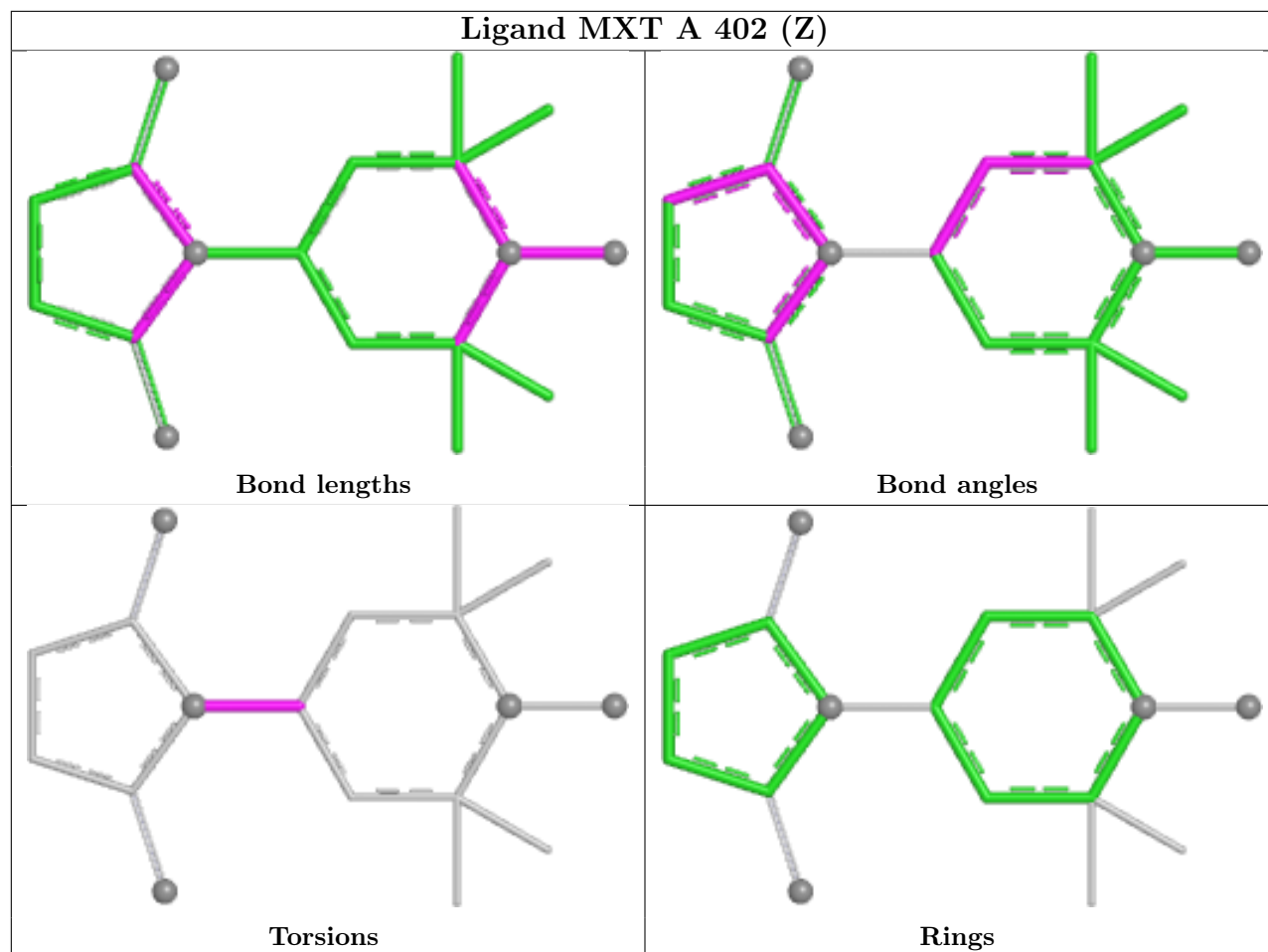


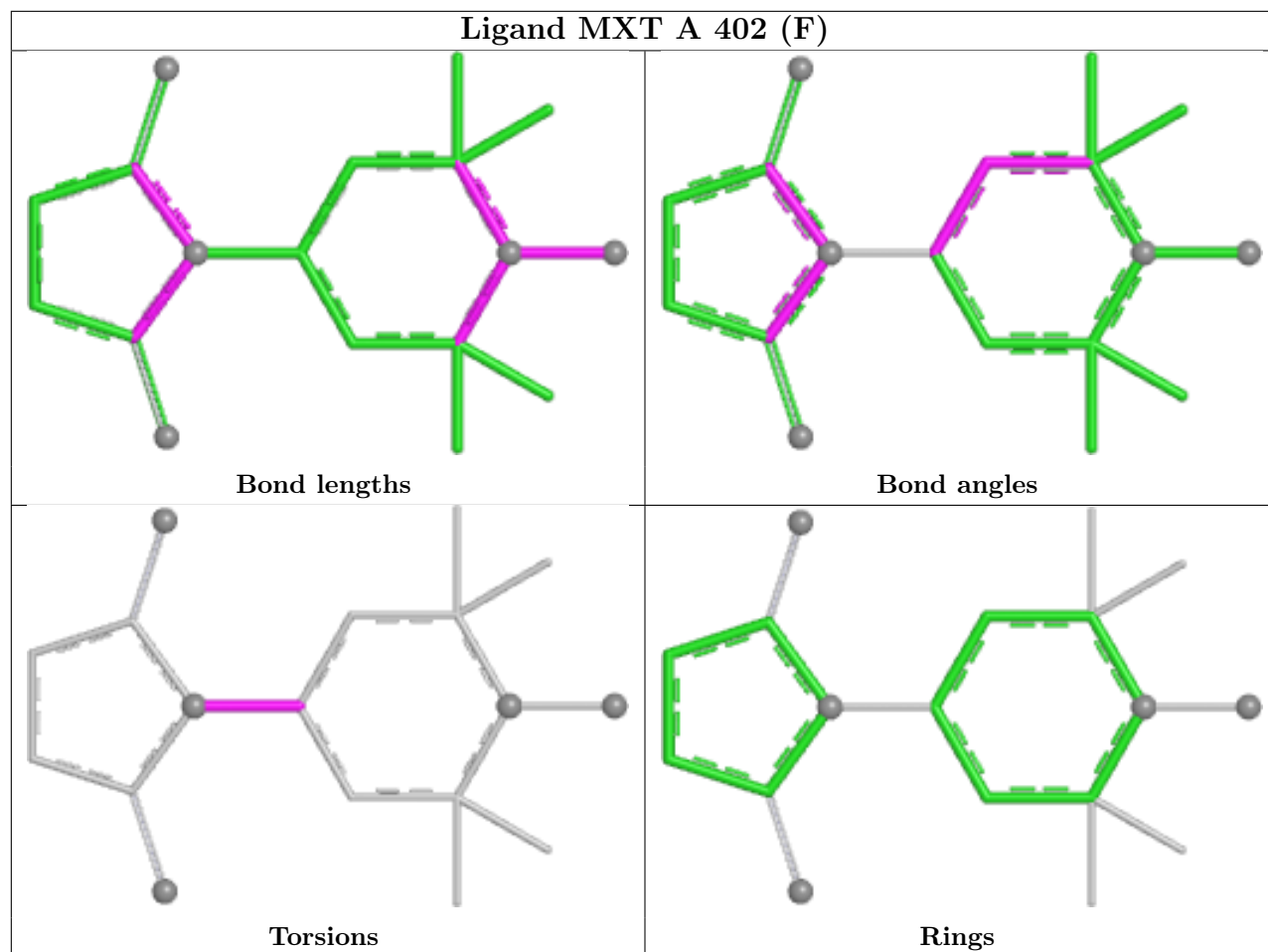


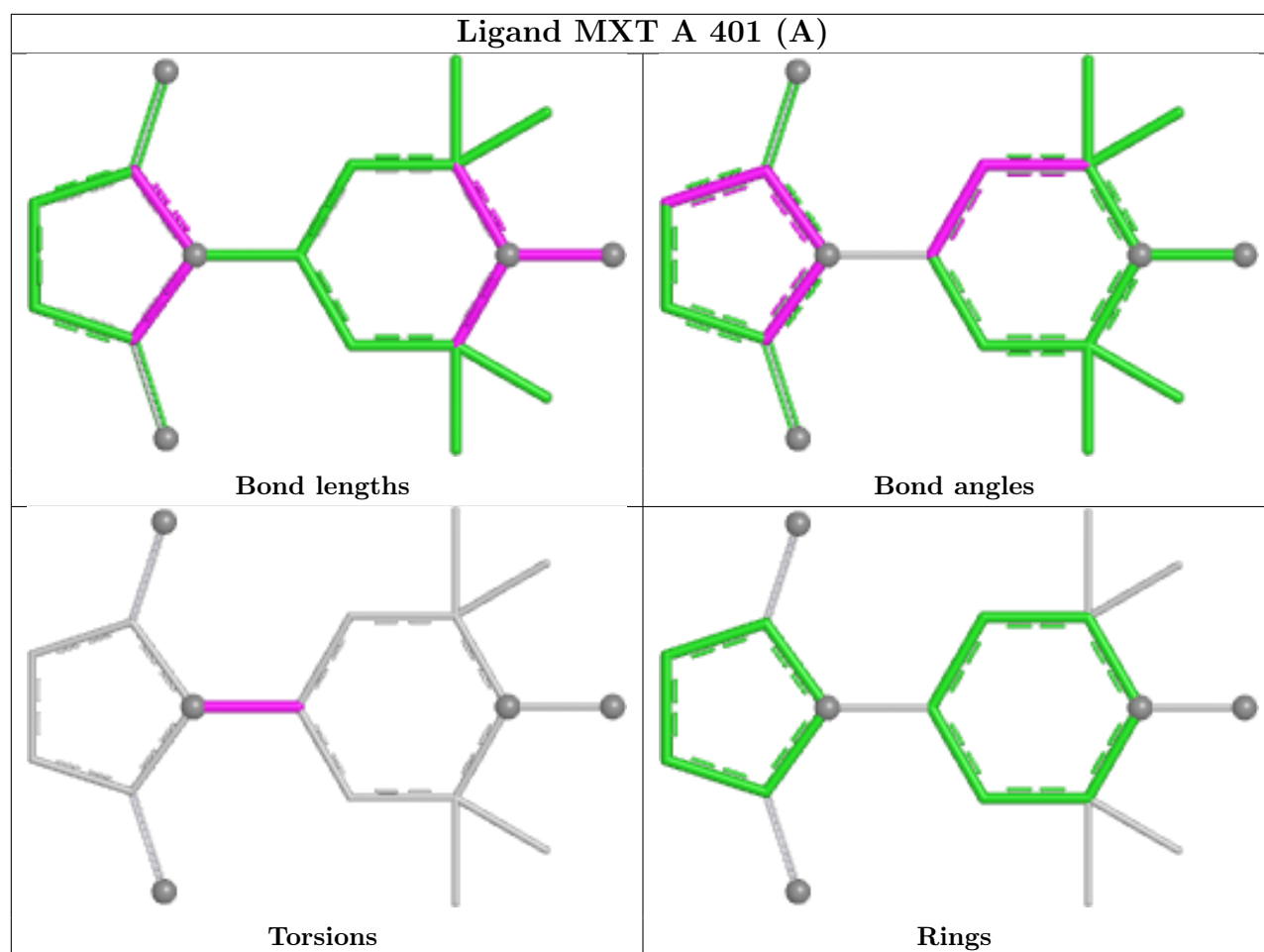


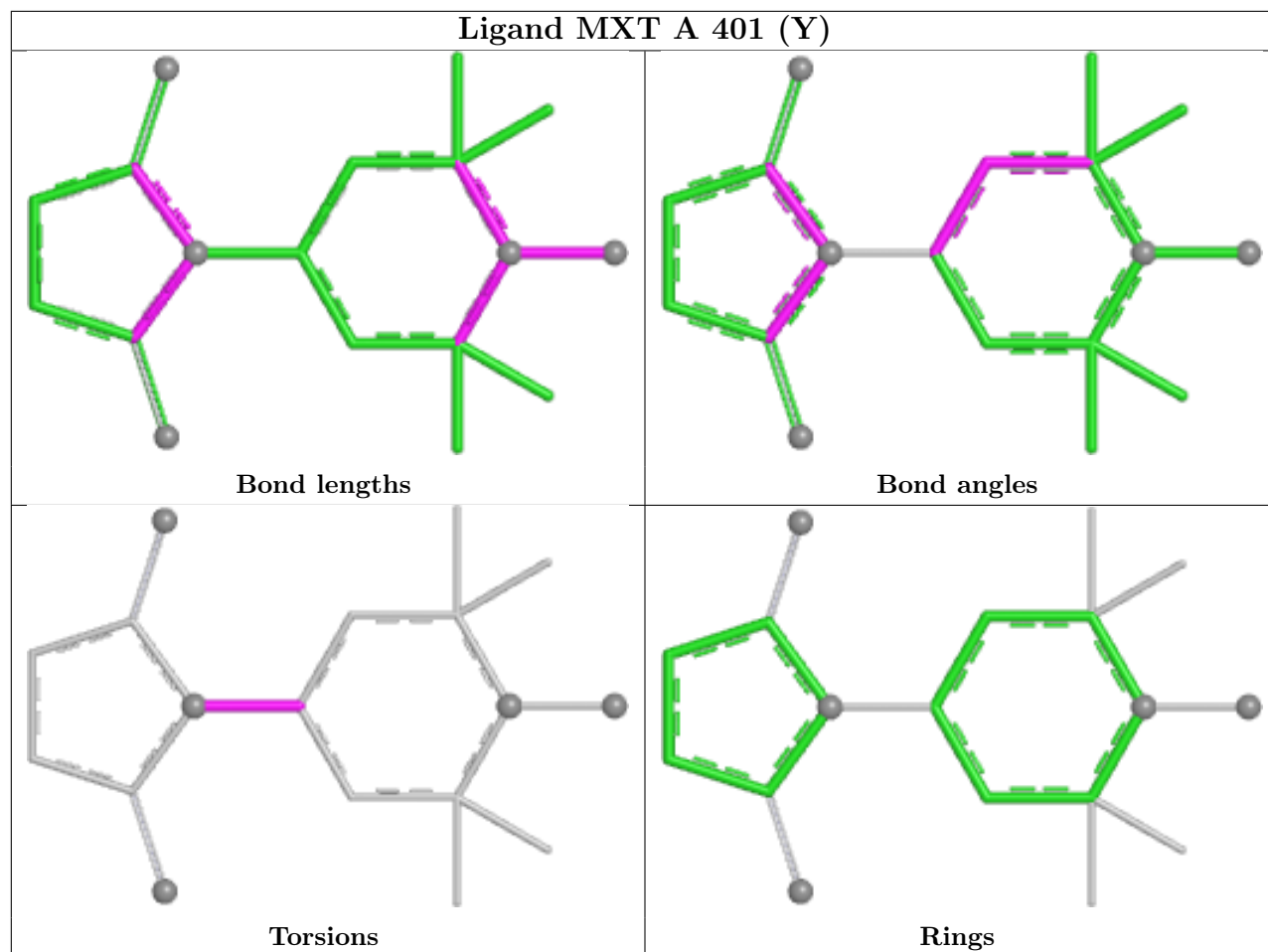


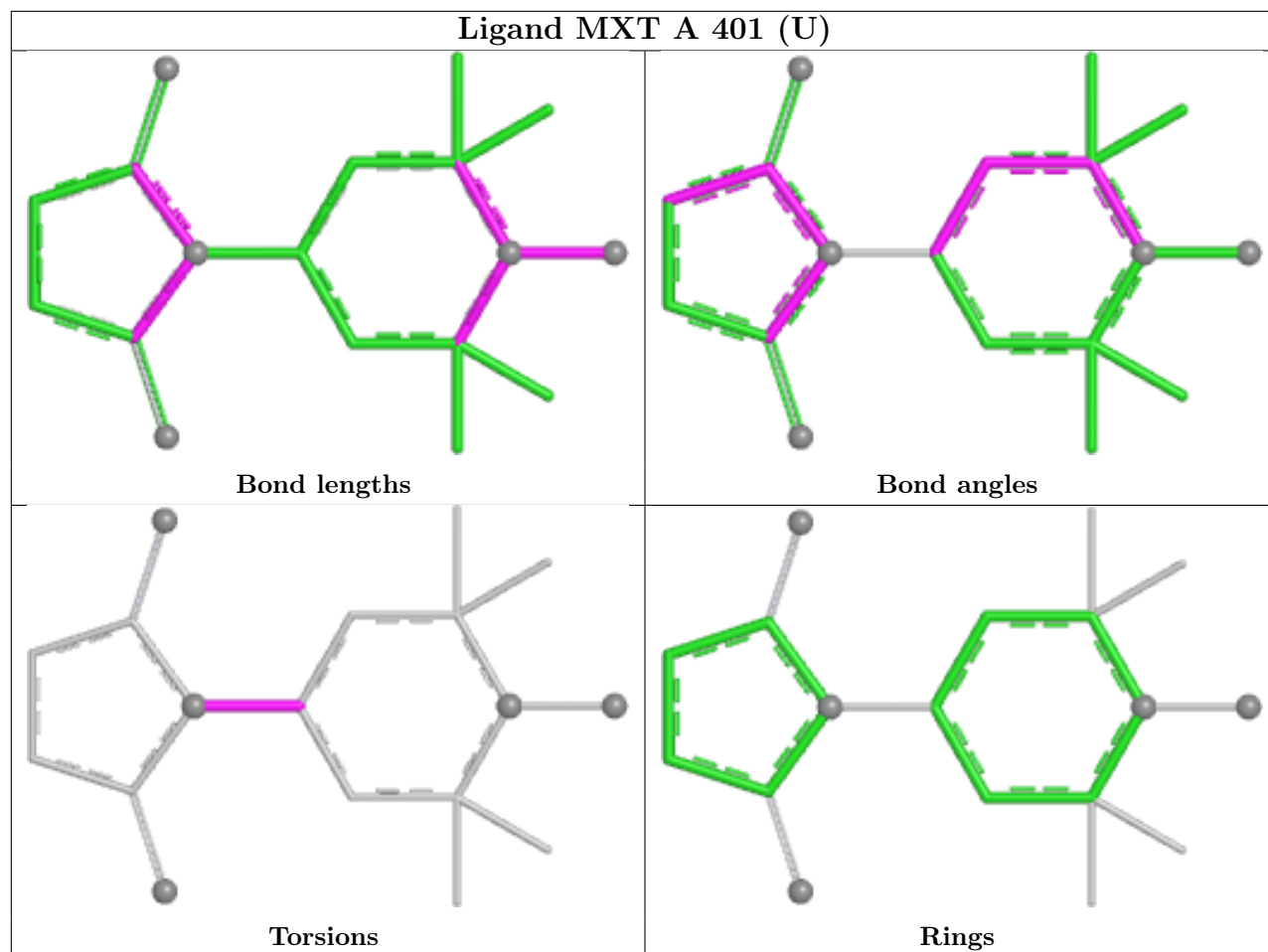


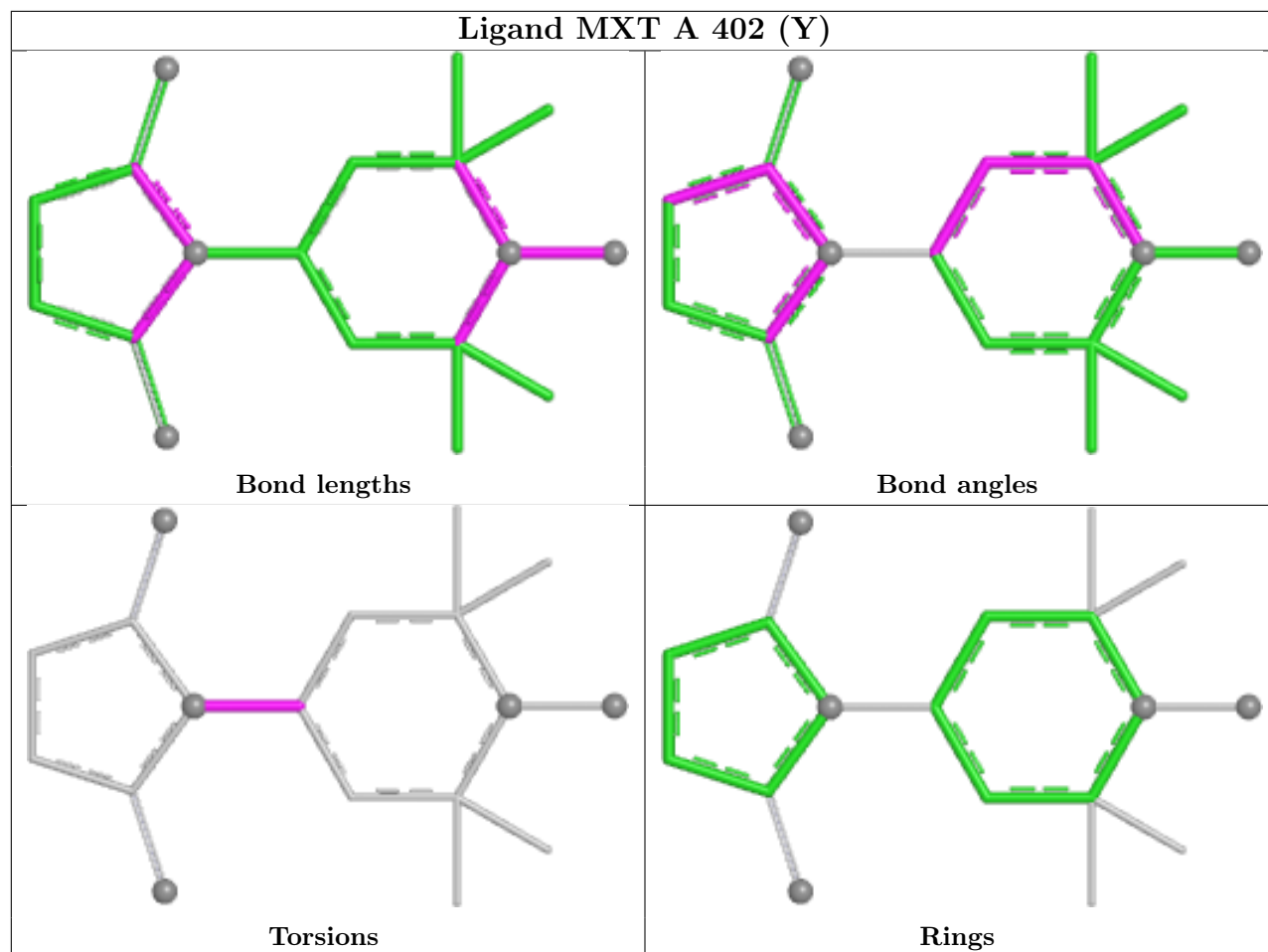


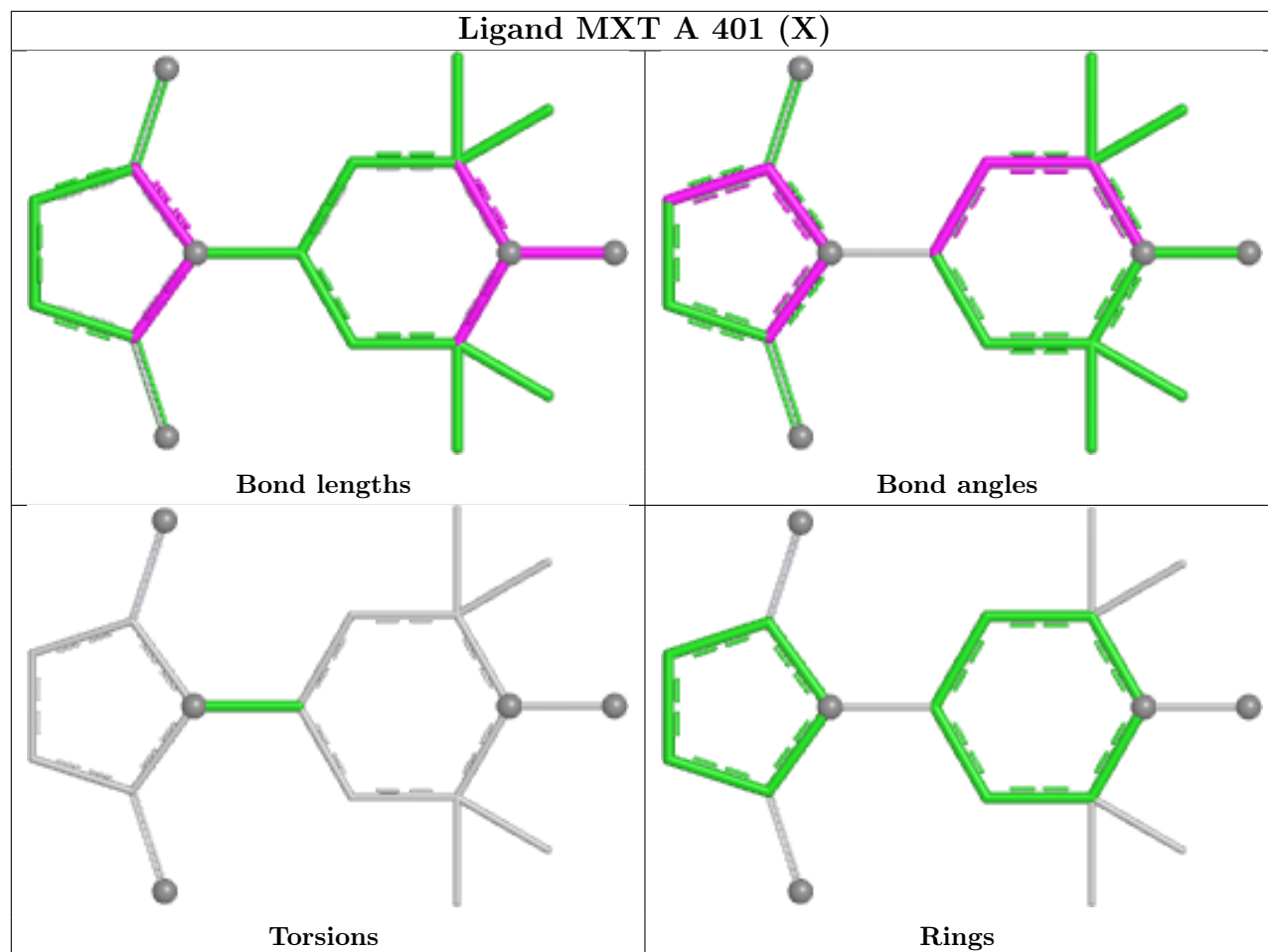


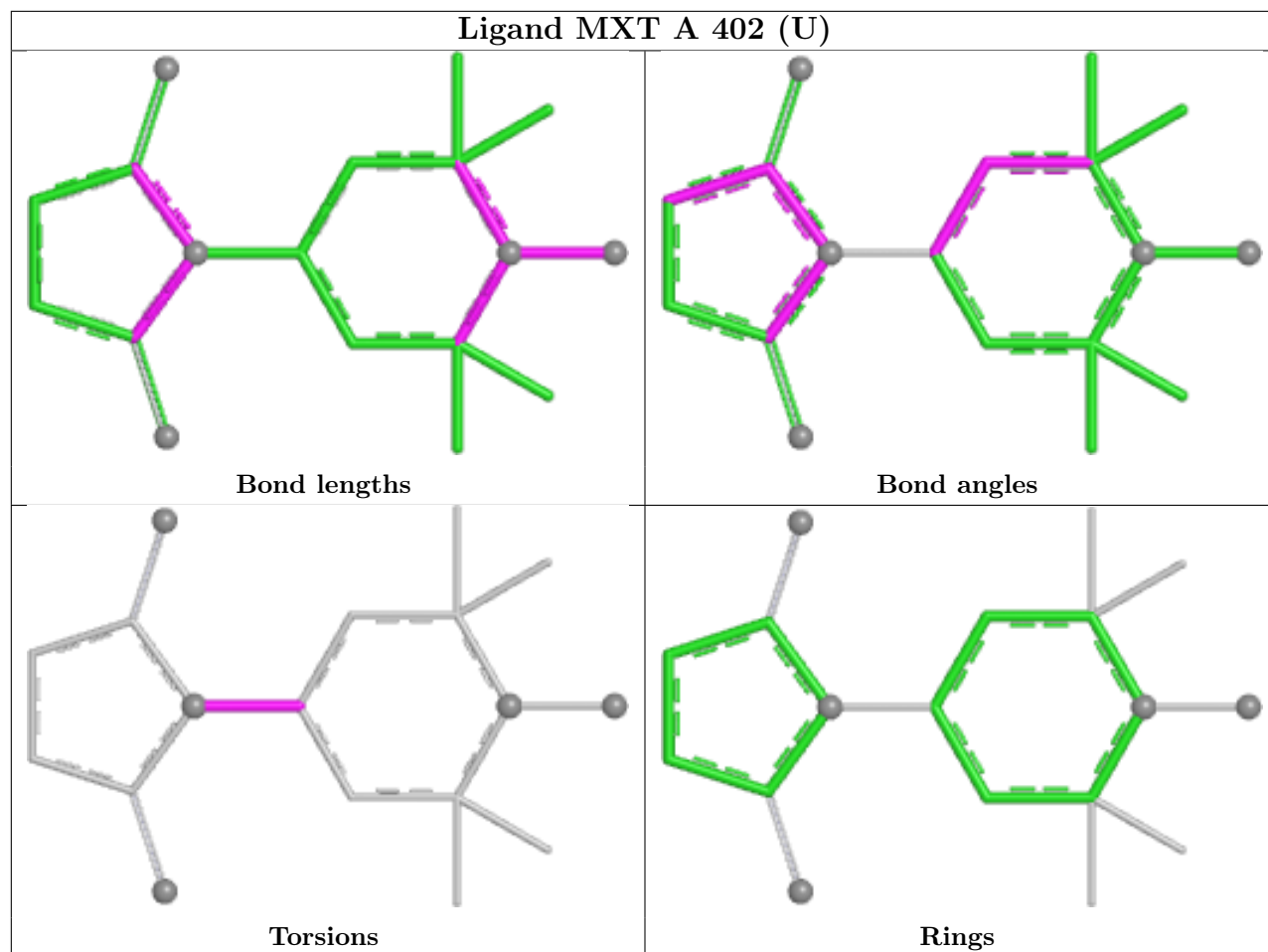


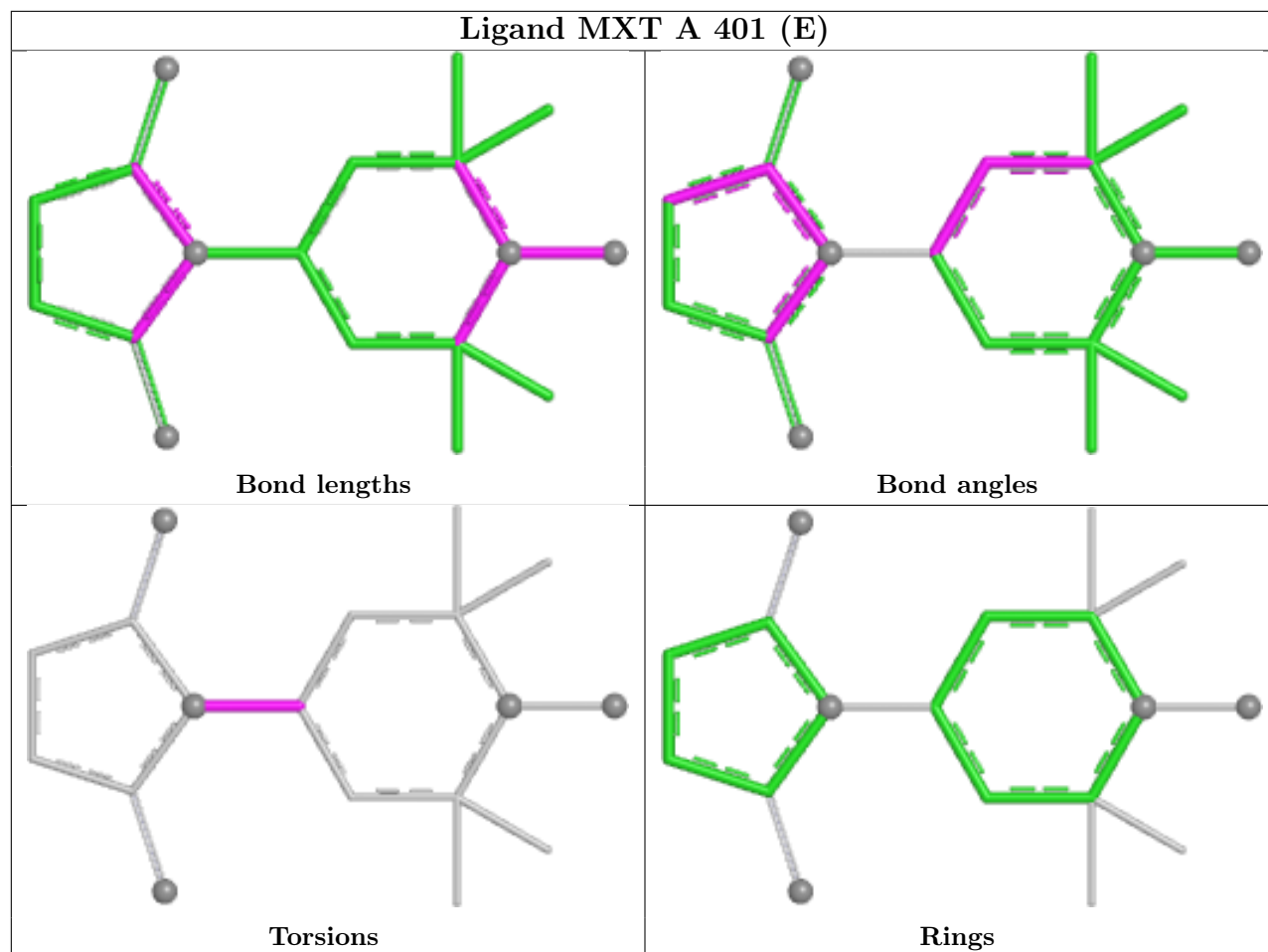


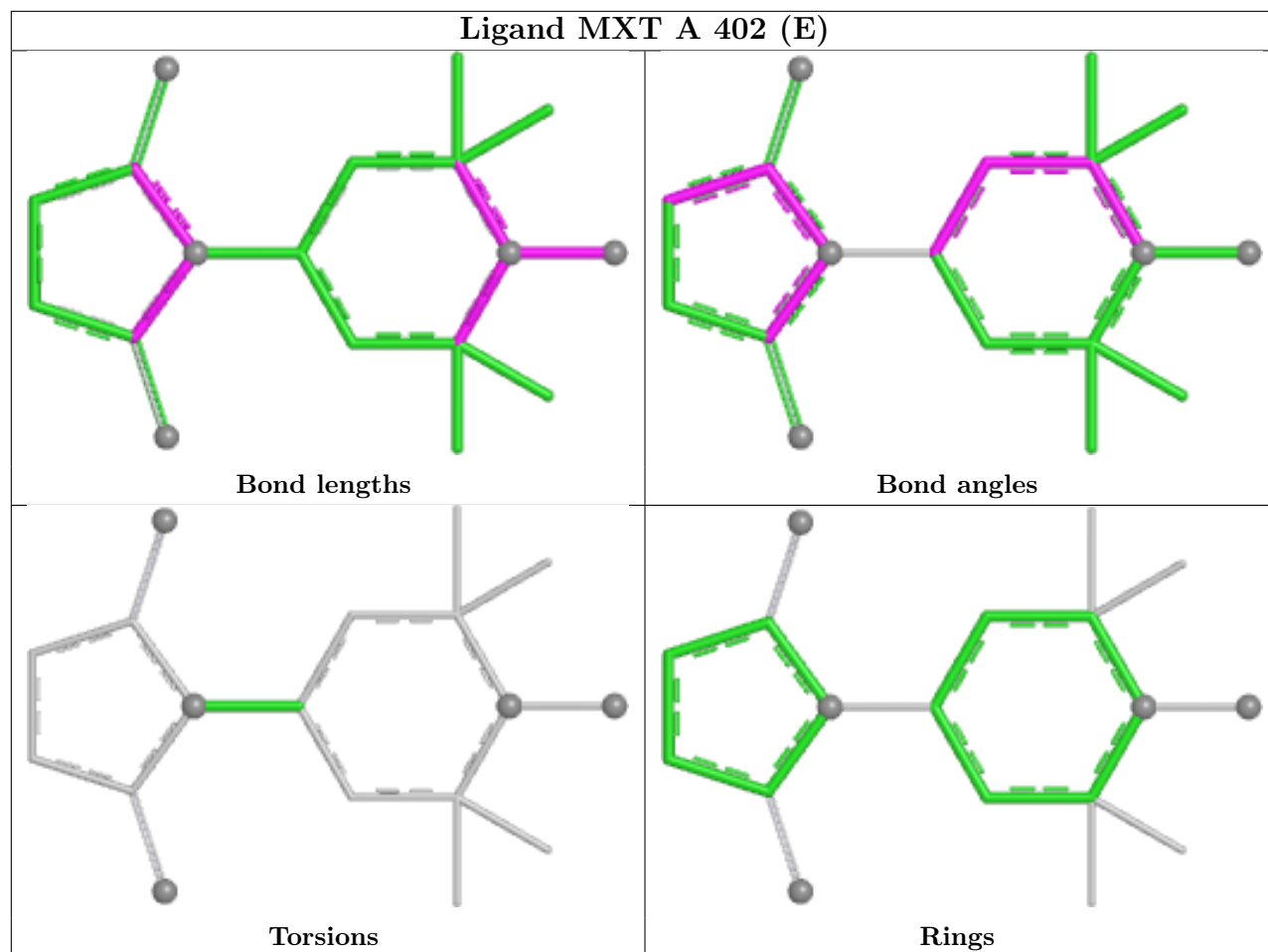


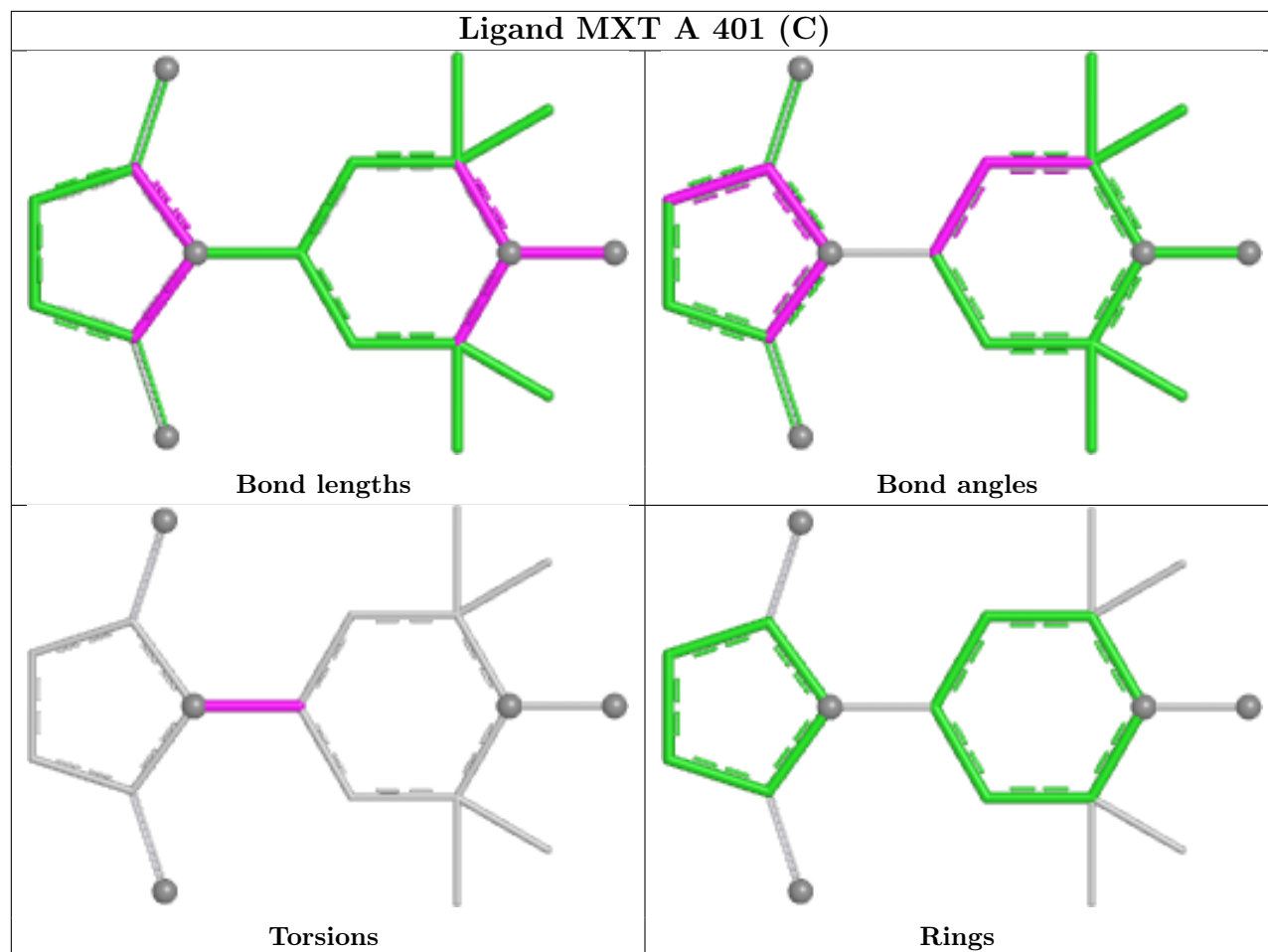












6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided