



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 24, 2023 – 08:13 PM EDT

PDB ID : 5UOB
Title : Structure of human endothelial nitric oxide synthase heme domain in complex with (R)-3-[(2-amino-4-methylquinolin-7-yl)methoxy]-5-(2-(methylamino)propyl)benzotrile
Authors : Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on : 2017-01-31
Resolution : 2.29 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

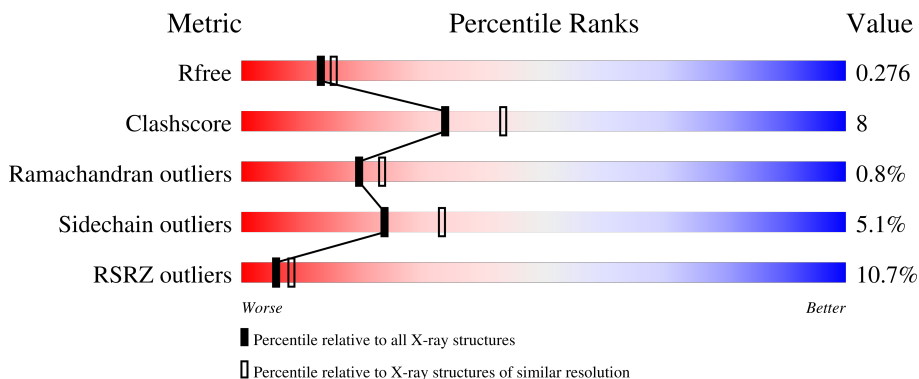
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	A	440	 16% 70% 20% • 8%
1	B	440	 5% 79% 11% • 9%
1	C	440	 9% 70% 20% • 9%
1	D	440	 9% 69% 22% • 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BTB	D	505	-	-	X	-

2 Entry composition [i](#)

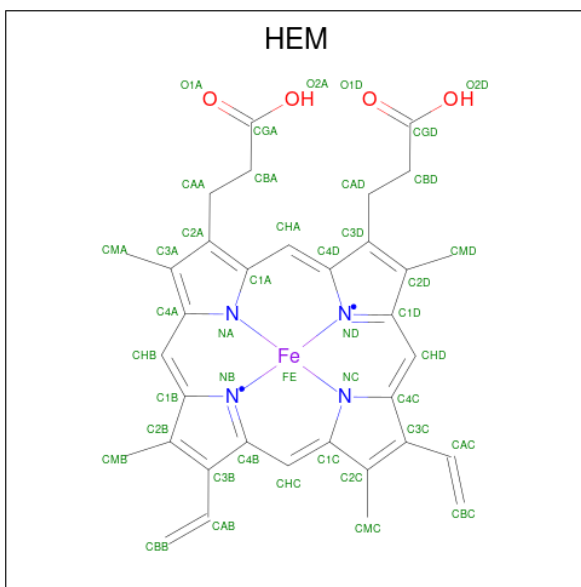
There are 9 unique types of molecules in this entry. The entry contains 13564 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	404	Total 3237	C 2062	N 570	O 589	S 16	0	2	0
1	B	402	Total 3221	C 2051	N 566	O 587	S 17	0	3	0
1	C	401	Total 3206	C 2042	N 563	O 585	S 16	0	1	0
1	D	402	Total 3221	C 2051	N 566	O 587	S 17	0	3	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



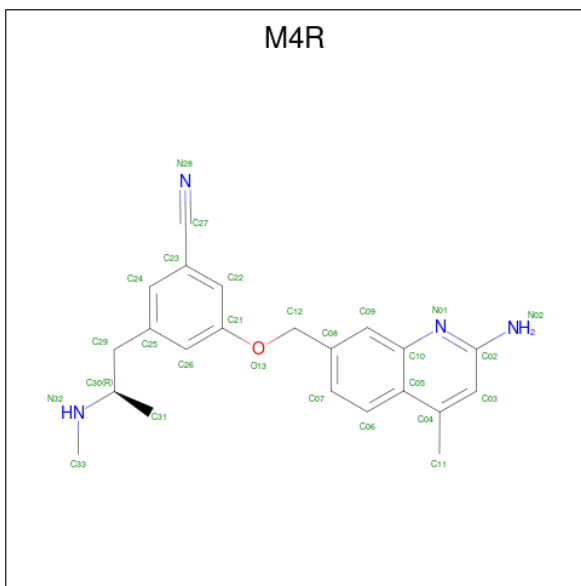
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

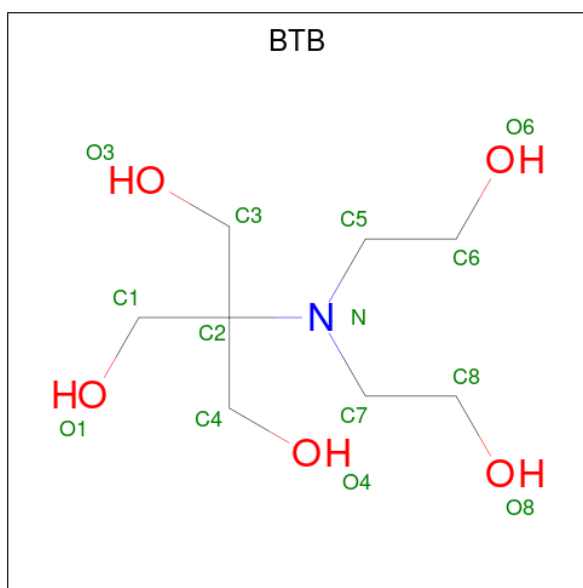
- Molecule 3 is 3-[(2-amino-4-methylquinolin-7-yl)methoxy]-5-[(2R)-2-(methylamino)propyl]benzonitrile (three-letter code: M4R) (formula: C₂₂H₂₄N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	22	4	1		
3	A	1	Total	C	N	O	0	0
			27	22	4	1		
3	B	1	Total	C	N	O	0	0
			27	22	4	1		
3	B	1	Total	C	N	O	0	0
			27	22	4	1		
3	C	1	Total	C	N	O	0	0
			27	22	4	1		
3	C	1	Total	C	N	O	0	0
			27	22	4	1		
3	D	1	Total	C	N	O	0	0
			27	22	4	1		
3	D	1	Total	C	N	O	0	0
			27	22	4	1		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN

E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).

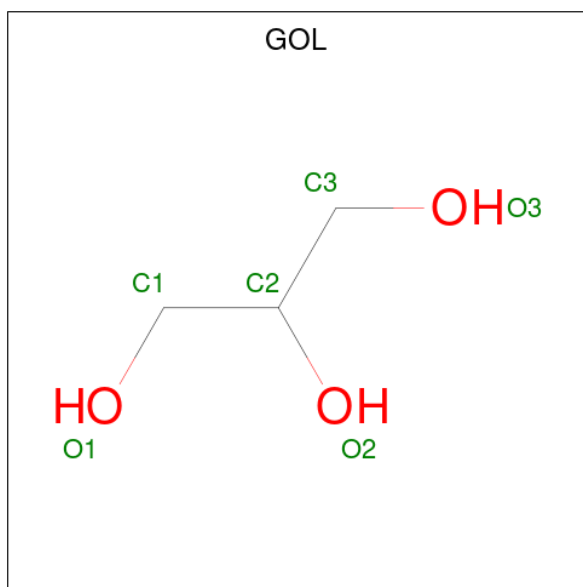


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Zn	0	0
			3	3		
5	C	3	Total	Zn	0	0
			3	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		

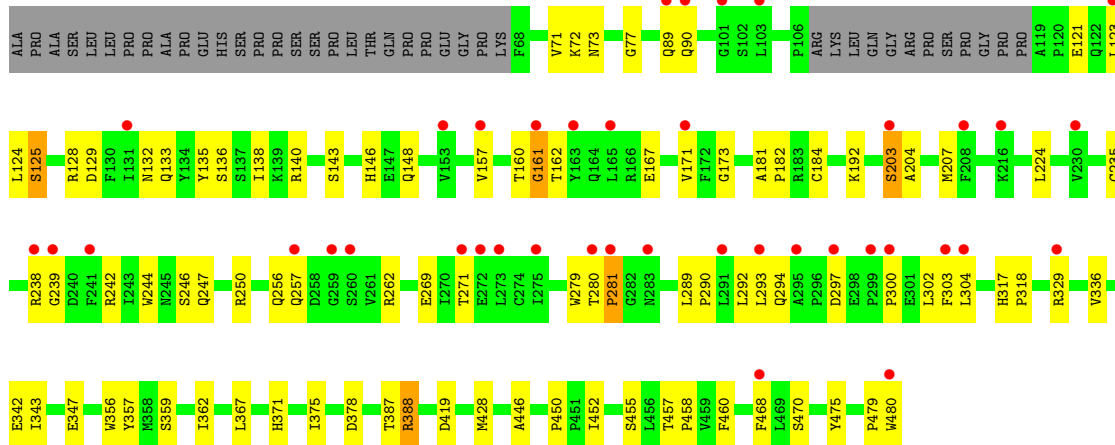
- Molecule 8 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Gd 1 1	0	0
8	B	1	Total Gd 1 1	0	0
8	C	1	Total Gd 1 1	0	0
8	D	1	Total Gd 1 1	0	0

- Molecule 9 is water.

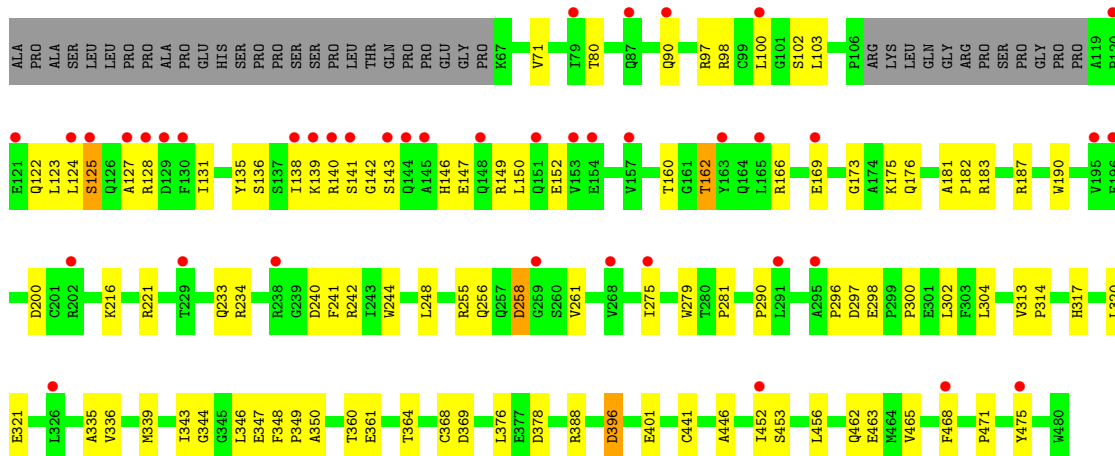
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	29	Total O 29 29	0	0
9	B	34	Total O 34 34	0	0
9	C	29	Total O 29 29	0	0
9	D	19	Total O 19 19	0	0

Chain C: 



• Molecule 1: Nitric oxide synthase, endothelial

Chain D: 



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.53Å 153.95Å 109.83Å 90.00° 90.57° 90.00°	Depositor
Resolution (Å)	38.49 – 2.29 38.64 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.1 (38.49-2.29) 95.3 (38.64-2.29)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.221 , 0.279 0.218 , 0.276	Depositor DCC
R_{free} test set	4169 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtrriage
Anisotropy	0.929	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.298 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13564	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, M4R, HEM, BTB, GOL, GD, ZN

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	A	0.39	0/3335	0.53	0/4543
1	B	0.41	0/3319	0.56	0/4523
1	C	0.40	0/3301	0.56	0/4499
1	D	0.44	0/3319	0.58	1/4523 (0.0%)
All	All	0.41	0/13274	0.56	1/18088 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	ASP	CB-CG-OD1	5.67	123.41	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3237	0	3146	51	1
1	B	3221	0	3126	36	0
1	C	3206	0	3104	53	0
1	D	3221	0	3126	66	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	5	0
2	D	43	0	30	4	0
3	A	54	0	0	1	0
3	B	54	0	0	3	0
3	C	54	0	0	4	0
3	D	54	0	0	4	0
4	A	28	0	36	5	0
4	B	42	0	55	3	0
4	C	28	0	38	4	0
4	D	56	0	76	16	1
5	A	3	0	0	0	0
5	C	3	0	0	0	0
6	A	6	0	8	0	0
6	C	6	0	8	0	0
7	A	1	0	0	0	0
7	B	1	0	0	1	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	29	0	0	2	0
9	B	34	0	0	2	0
9	C	29	0	0	4	0
9	D	19	0	0	3	0
All	All	13564	0	12843	223	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 223 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:B:235[B]:CYS:SG	1:B:238:ARG:NH1	2.52	0.83
2:A:501:HEM:HHA	2:A:501:HEM:HBD2	1.61	0.83
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.68	0.75
1:D:347:GLU:OE2	9:D:601:HOH:O	2.06	0.74
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.71	0.73

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLU:OE1	4:D:505:BTB:O8[2_751]	2.19	0.01

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	A	402/440 (91%)	367 (91%)	31 (8%)	4 (1%)	15 17
1	B	401/440 (91%)	379 (94%)	21 (5%)	1 (0%)	47 58
1	C	398/440 (90%)	365 (92%)	29 (7%)	4 (1%)	15 17
1	D	401/440 (91%)	375 (94%)	23 (6%)	3 (1%)	22 26
All	All	1602/1760 (91%)	1486 (93%)	104 (6%)	12 (1%)	19 26

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ARG
1	C	89	GLN
1	C	161	GLY
1	A	320	LEU
1	B	88	ALA

5.3.2 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 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	A	345/373 (92%)	313 (91%)	32 (9%)	9	10
1	B	344/373 (92%)	334 (97%)	10 (3%)	42	58
1	C	341/373 (91%)	327 (96%)	14 (4%)	30	43
1	D	344/373 (92%)	330 (96%)	14 (4%)	30	43
All	All	1374/1492 (92%)	1304 (95%)	70 (5%)	24	33

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	97	ARG
1	D	124	LEU
1	D	258	ASP
1	A	309	LEU
1	A	302	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 14 are monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	M4R	D	502	-	29,29,29	1.58	1 (3%)	38,40,40	1.17	6 (15%)
6	GOL	A	508	-	5,5,5	0.44	0	5,5,5	0.44	0
4	BTB	D	506	-	13,13,13	0.36	0	7,16,16	0.64	0
3	M4R	B	502	-	29,29,29	1.55	2 (6%)	38,40,40	0.94	3 (7%)
2	HEM	A	501	1	41,50,50	1.94	6 (14%)	45,82,82	2.04	11 (24%)
4	BTB	B	504	8	13,13,13	0.53	0	7,16,16	0.43	0
4	BTB	C	505	-	13,13,13	0.40	0	7,16,16	0.95	0
4	BTB	D	507	-	13,13,13	0.37	0	7,16,16	0.48	0
3	M4R	C	503	-	29,29,29	1.55	2 (6%)	38,40,40	1.27	6 (15%)
3	M4R	D	503	-	29,29,29	1.52	1 (3%)	38,40,40	1.08	2 (5%)
4	BTB	D	504	8	13,13,13	0.53	0	7,16,16	0.48	0
3	M4R	B	503	-	29,29,29	1.52	2 (6%)	38,40,40	0.96	1 (2%)
3	M4R	A	502	-	29,29,29	1.55	2 (6%)	38,40,40	1.02	4 (10%)
6	GOL	C	508	-	5,5,5	0.29	0	5,5,5	0.40	0
4	BTB	C	504	8	13,13,13	0.35	0	7,16,16	0.49	0
4	BTB	A	504	8	13,13,13	0.44	0	7,16,16	1.22	1 (14%)
4	BTB	B	505	-	13,13,13	0.42	0	7,16,16	0.54	0
2	HEM	B	501	1	41,50,50	1.92	7 (17%)	45,82,82	1.88	13 (28%)
4	BTB	B	506	-	13,13,13	0.58	0	7,16,16	0.79	0
4	BTB	D	505	-	13,13,13	0.42	0	7,16,16	0.64	0
4	BTB	A	505	-	13,13,13	0.37	0	7,16,16	0.53	0
3	M4R	C	502	-	29,29,29	1.59	1 (3%)	38,40,40	1.13	3 (7%)
2	HEM	D	501	1	41,50,50	1.94	7 (17%)	45,82,82	2.09	10 (22%)
3	M4R	A	503	-	29,29,29	1.52	2 (6%)	38,40,40	1.25	3 (7%)
2	HEM	C	501	1	41,50,50	1.98	8 (19%)	45,82,82	1.80	9 (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
3	M4R	D	502	-	-	3/13/13/13	0/3/3/3
6	GOL	A	508	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTB	D	506	-	-	8/21/21/21	-
3	M4R	B	502	-	-	5/13/13/13	0/3/3/3
2	HEM	A	501	1	-	6/12/54/54	-
4	BTB	B	504	8	-	3/21/21/21	-
4	BTB	C	505	-	-	3/21/21/21	-
4	BTB	D	507	-	-	8/21/21/21	-
3	M4R	C	503	-	-	8/13/13/13	0/3/3/3
3	M4R	D	503	-	-	5/13/13/13	0/3/3/3
4	BTB	D	504	8	-	4/21/21/21	-
3	M4R	B	503	-	-	8/13/13/13	0/3/3/3
3	M4R	A	502	-	-	3/13/13/13	0/3/3/3
6	GOL	C	508	-	-	4/4/4/4	-
4	BTB	C	504	8	-	4/21/21/21	-
4	BTB	A	504	8	-	8/21/21/21	-
4	BTB	B	505	-	-	7/21/21/21	-
2	HEM	B	501	1	-	6/12/54/54	-
4	BTB	B	506	-	-	3/21/21/21	-
4	BTB	D	505	-	-	4/21/21/21	-
4	BTB	A	505	-	-	6/21/21/21	-
3	M4R	C	502	-	-	7/13/13/13	0/3/3/3
2	HEM	D	501	1	-	4/12/54/54	-
3	M4R	A	503	-	-	3/13/13/13	0/3/3/3
2	HEM	C	501	1	-	2/12/54/54	-

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3D-C2D	8.25	1.54	1.36
2	A	501	HEM	C3D-C2D	8.06	1.53	1.36
2	D	501	HEM	C3D-C2D	7.78	1.53	1.36
2	B	501	HEM	C3D-C2D	7.23	1.52	1.36
3	C	502	M4R	C23-C27	-7.13	1.28	1.44

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C4D-ND-C1D	7.62	112.94	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	C4D-ND-C1D	7.08	112.39	105.07
2	A	501	HEM	C4D-ND-C1D	6.76	112.06	105.07
2	B	501	HEM	C4D-ND-C1D	5.52	110.77	105.07
2	A	501	HEM	CAD-C3D-C4D	5.00	133.40	124.66

There are no chirality outliers.

5 of 124 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2D-C3D-CAD-CBD
2	A	501	HEM	C4D-C3D-CAD-CBD
3	A	503	M4R	C25-C29-C30-C31
3	A	503	M4R	C25-C29-C30-N32
3	B	503	M4R	C25-C29-C30-C31

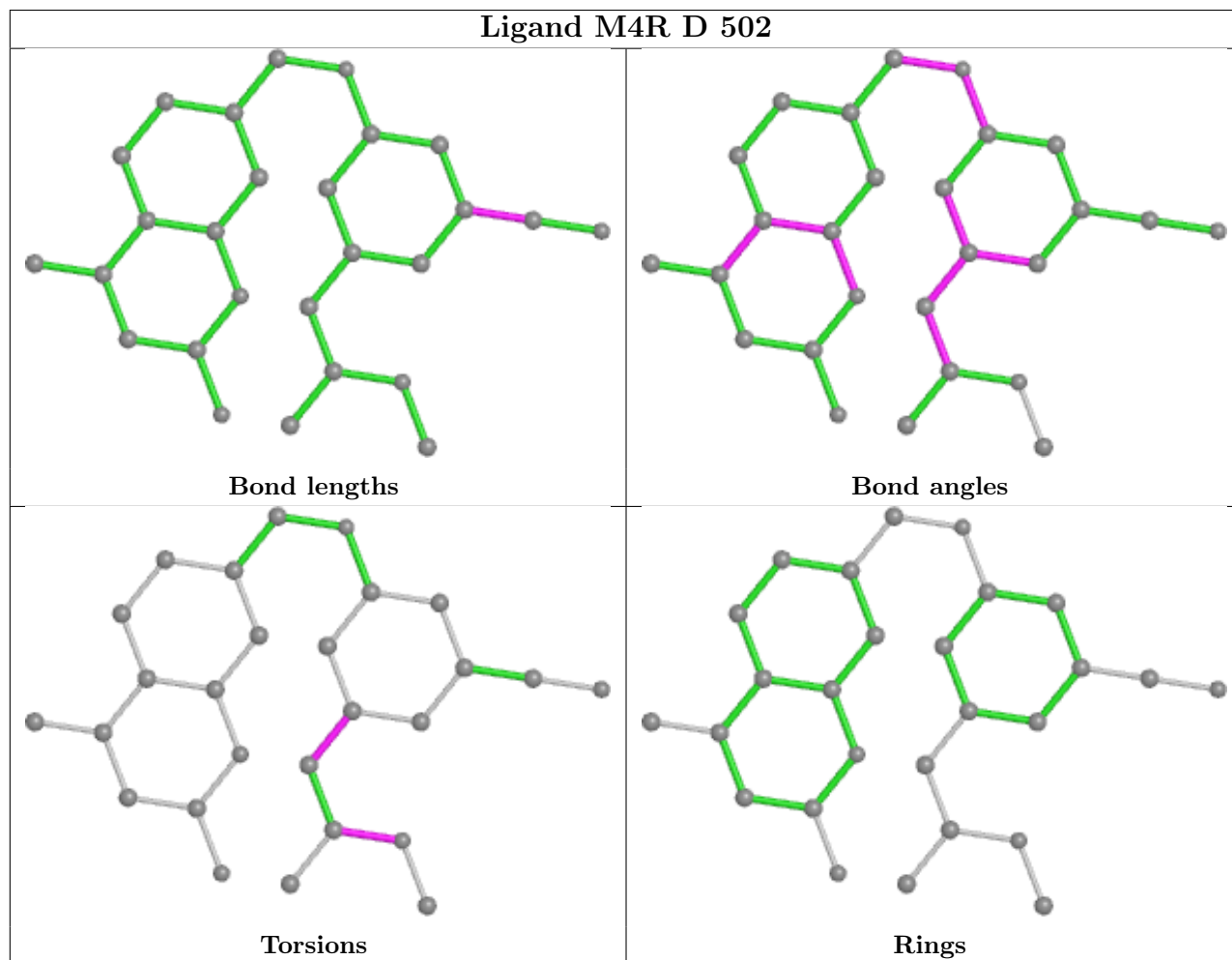
There are no ring outliers.

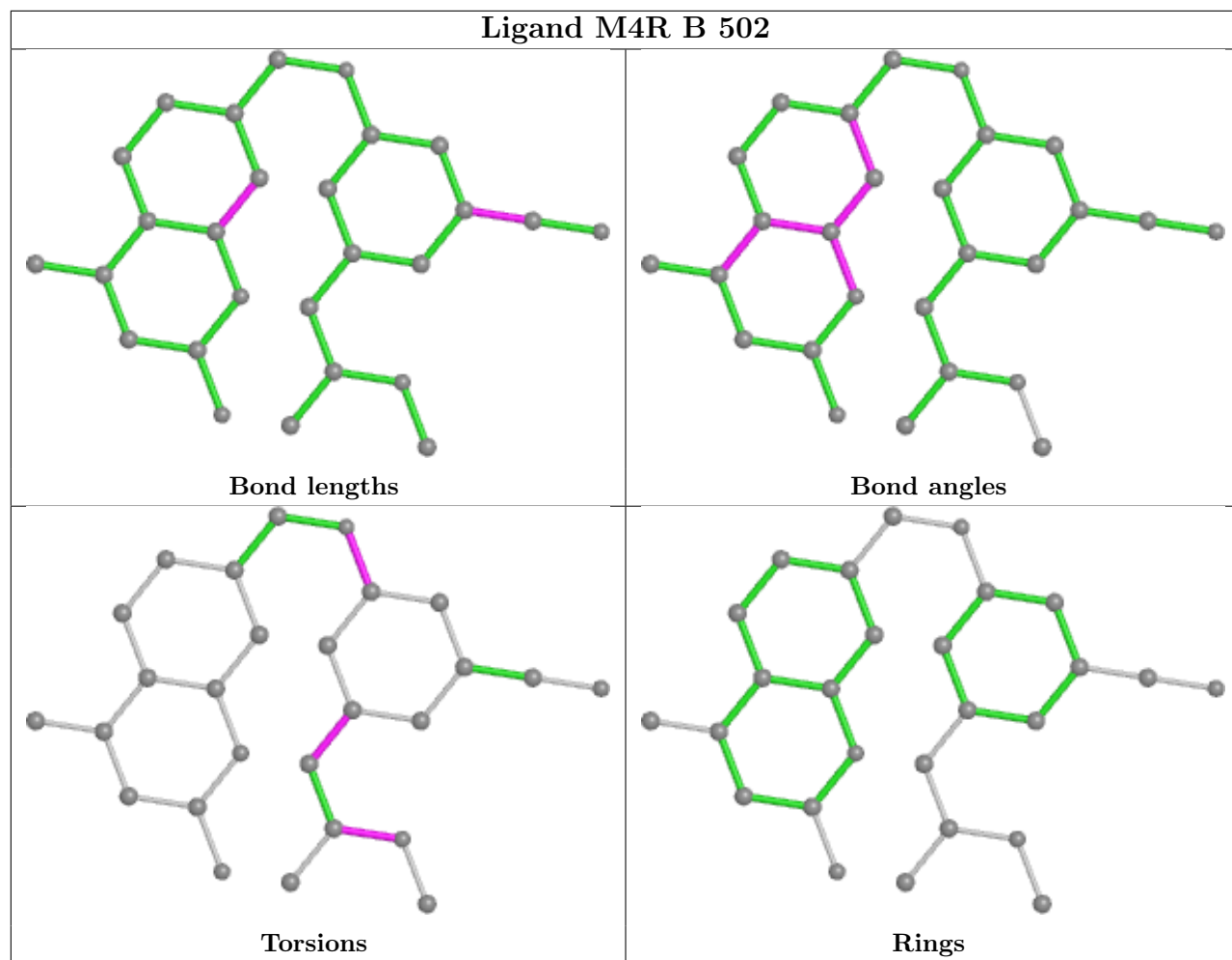
21 monomers are involved in 57 short contacts:

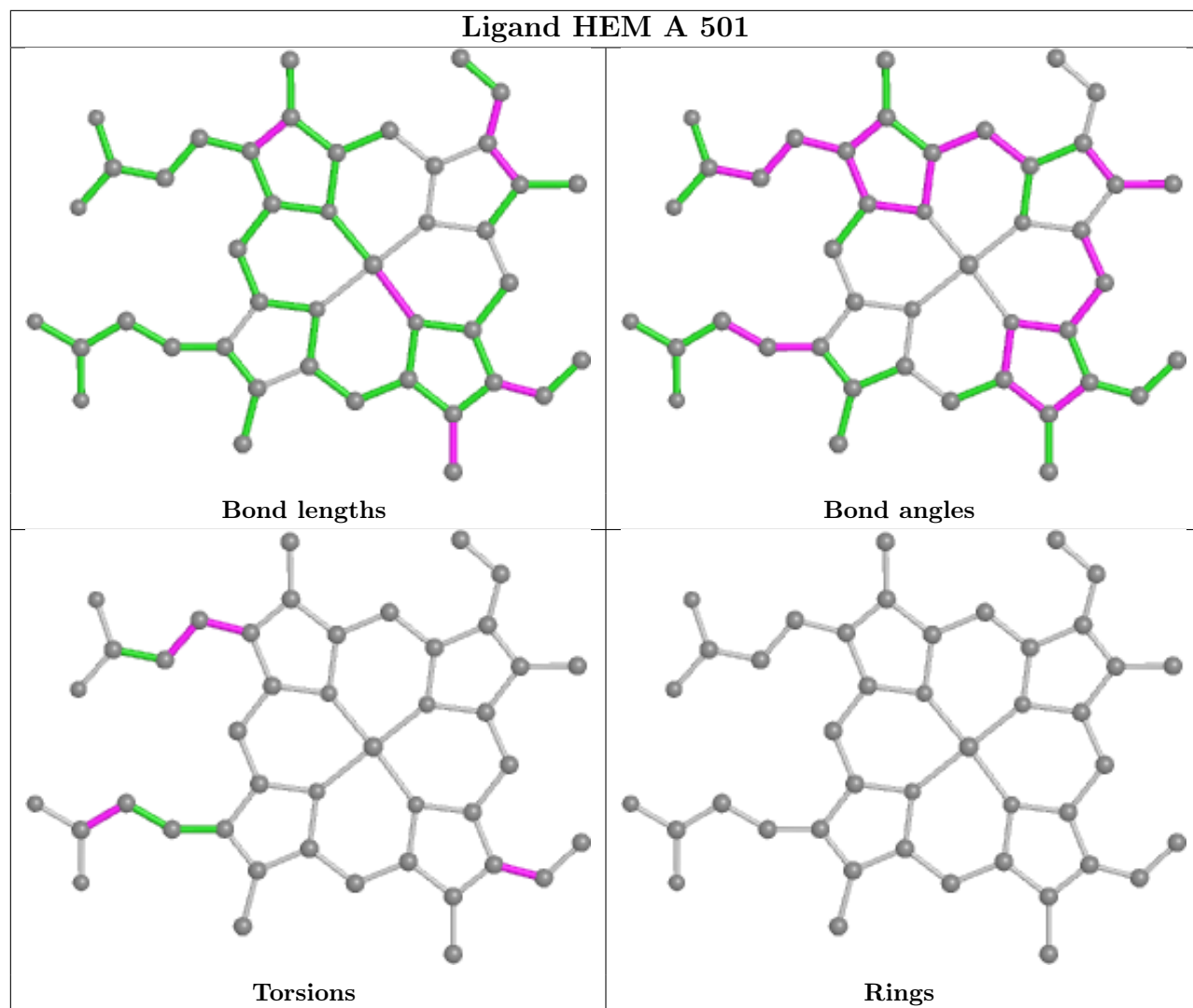
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	M4R	3	0
4	D	506	BTB	4	0
3	B	502	M4R	2	0
2	A	501	HEM	4	0
4	B	504	BTB	2	0
4	C	505	BTB	1	0
4	D	507	BTB	2	0
3	C	503	M4R	1	0
3	D	503	M4R	1	0
4	D	504	BTB	3	0
3	B	503	M4R	1	0
3	A	502	M4R	1	0
4	C	504	BTB	3	0
4	A	504	BTB	3	0
2	B	501	HEM	4	0
4	B	506	BTB	1	0
4	D	505	BTB	7	1
4	A	505	BTB	2	0
3	C	502	M4R	3	0
2	D	501	HEM	4	0
2	C	501	HEM	5	0

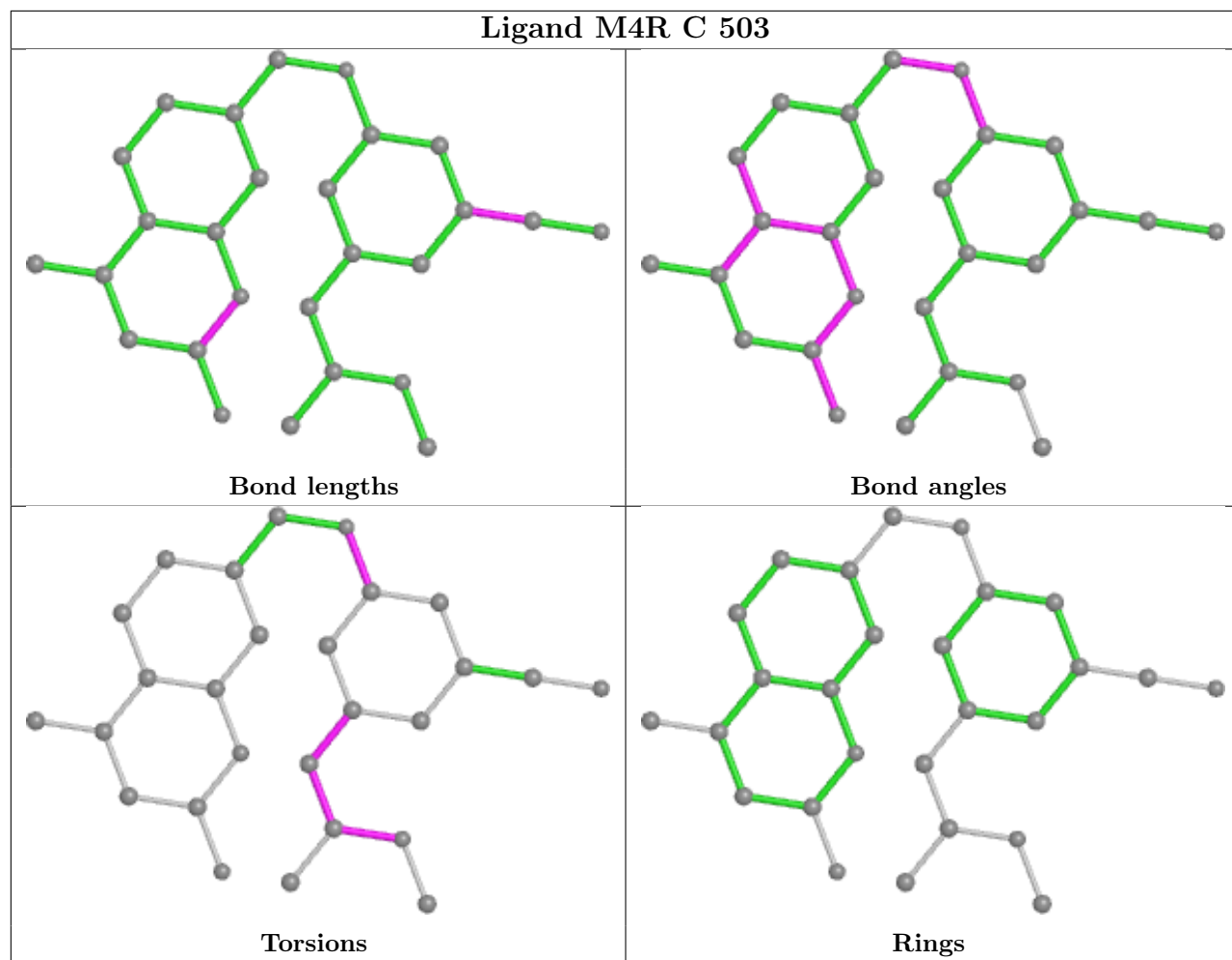
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

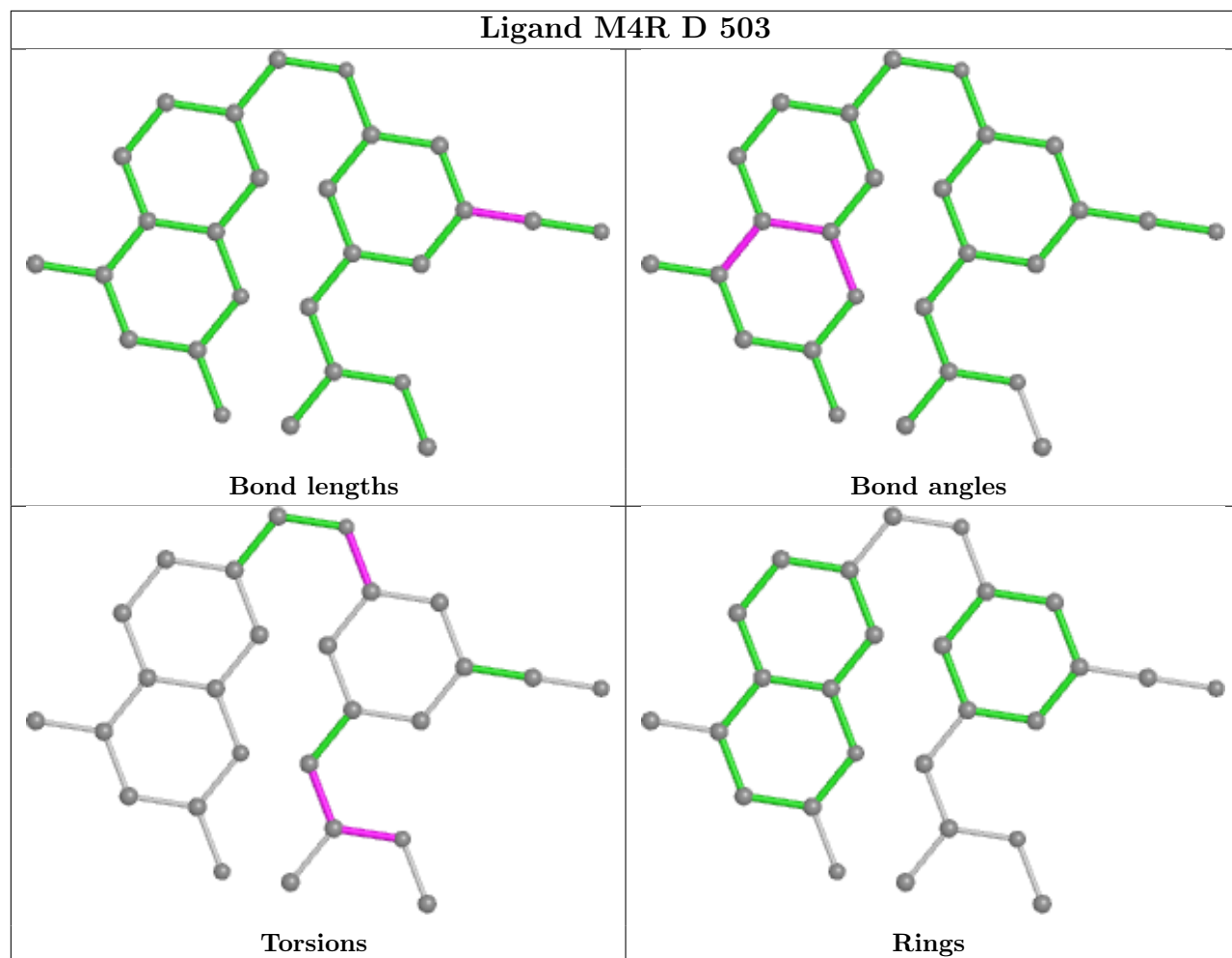
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

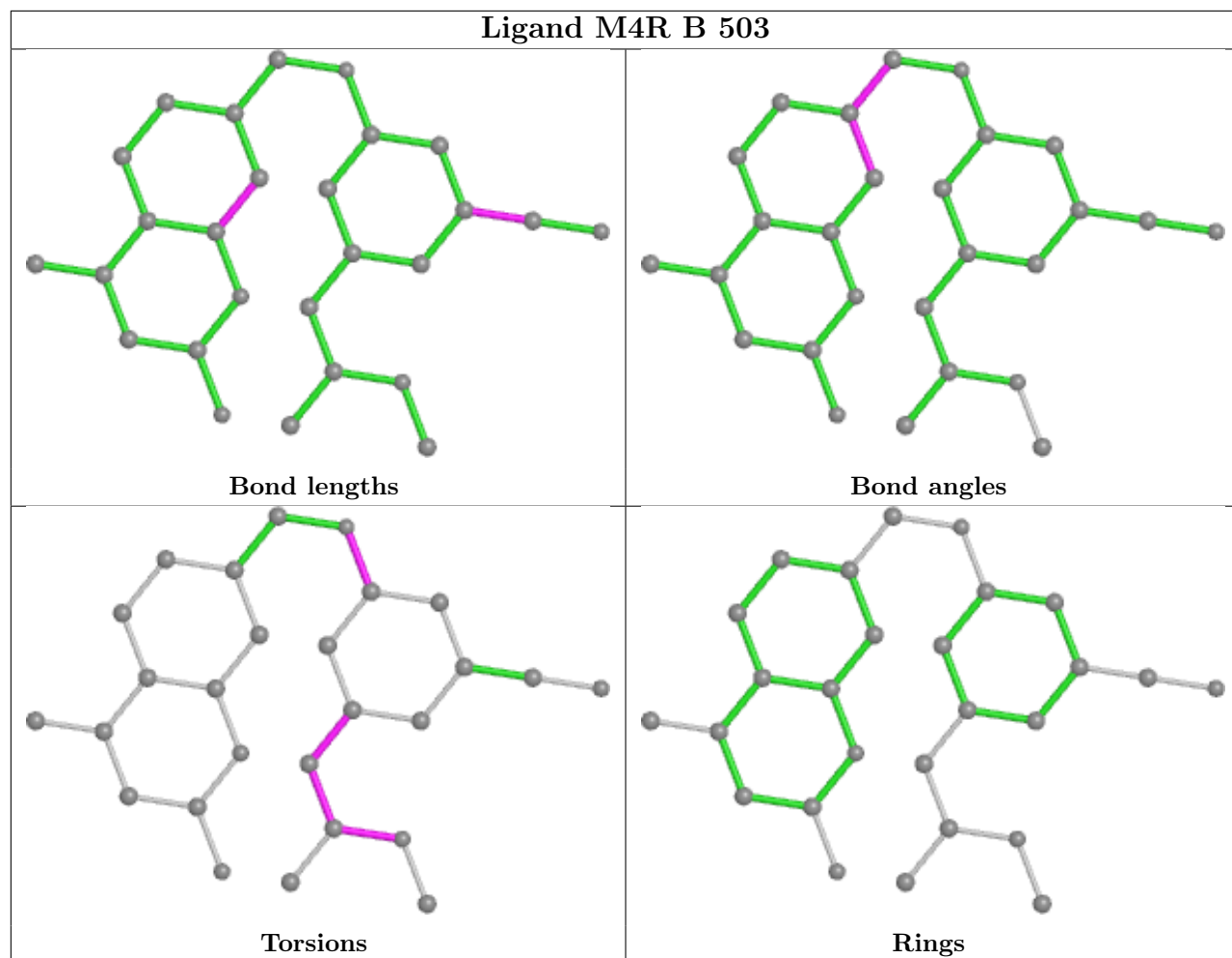


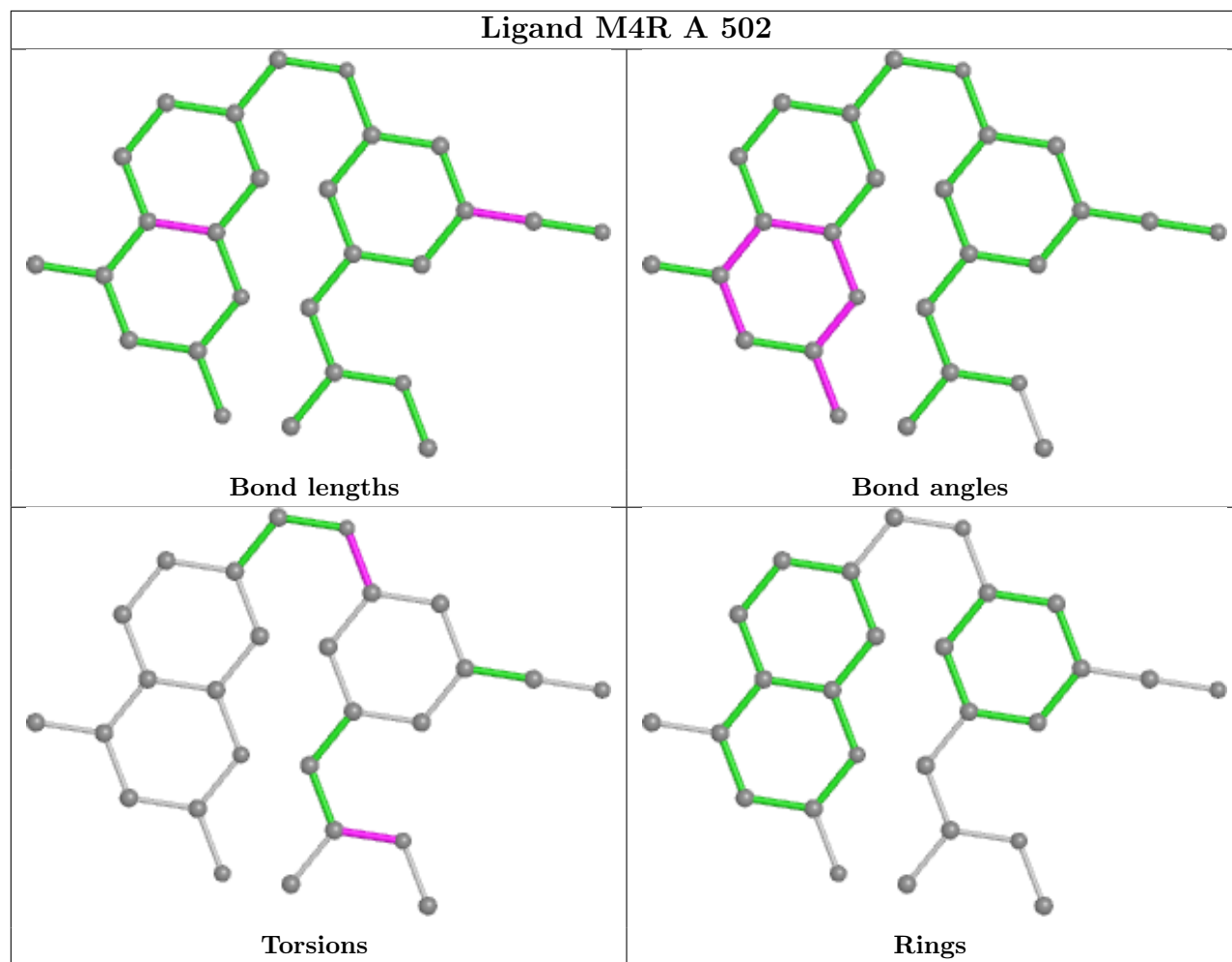


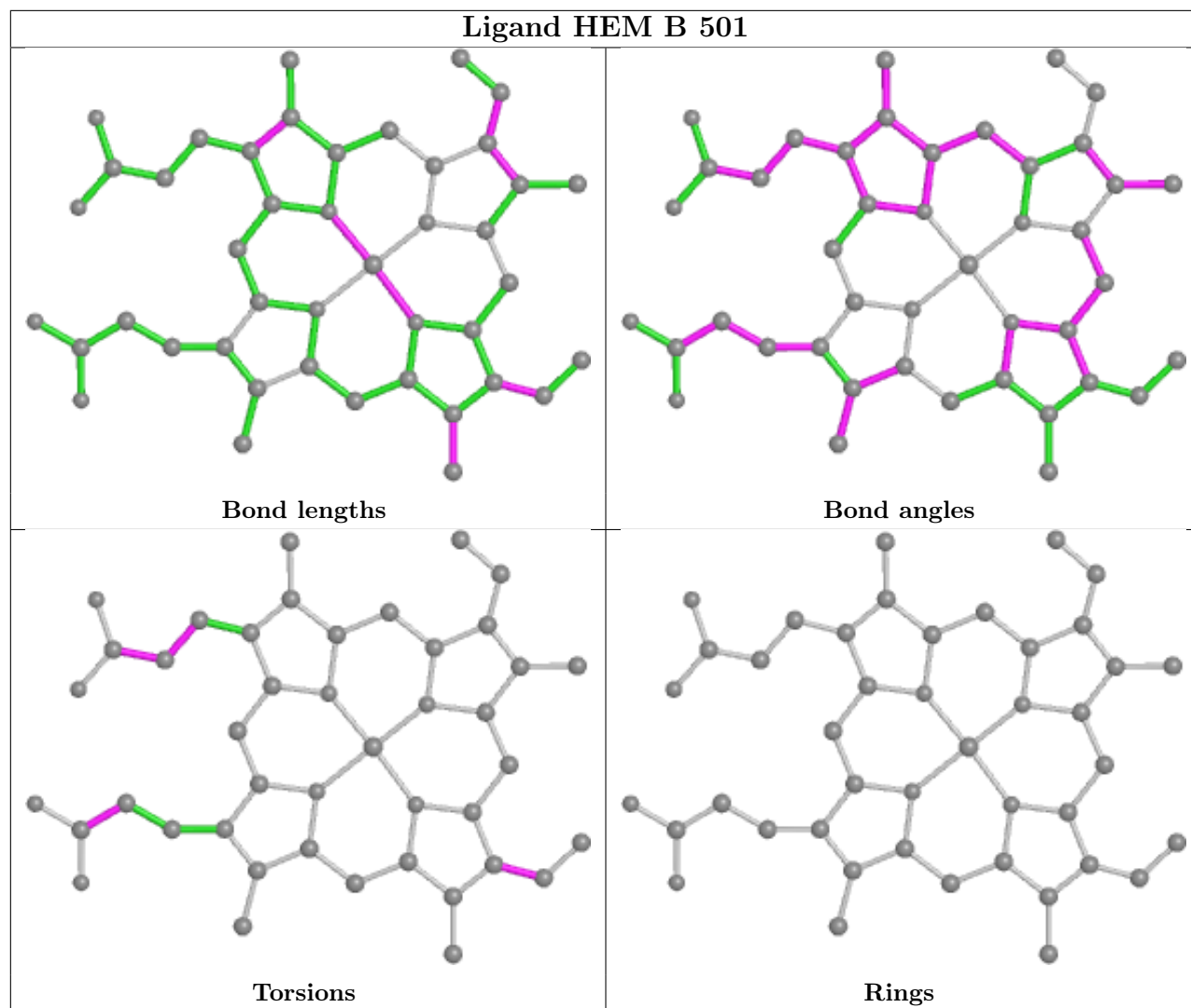


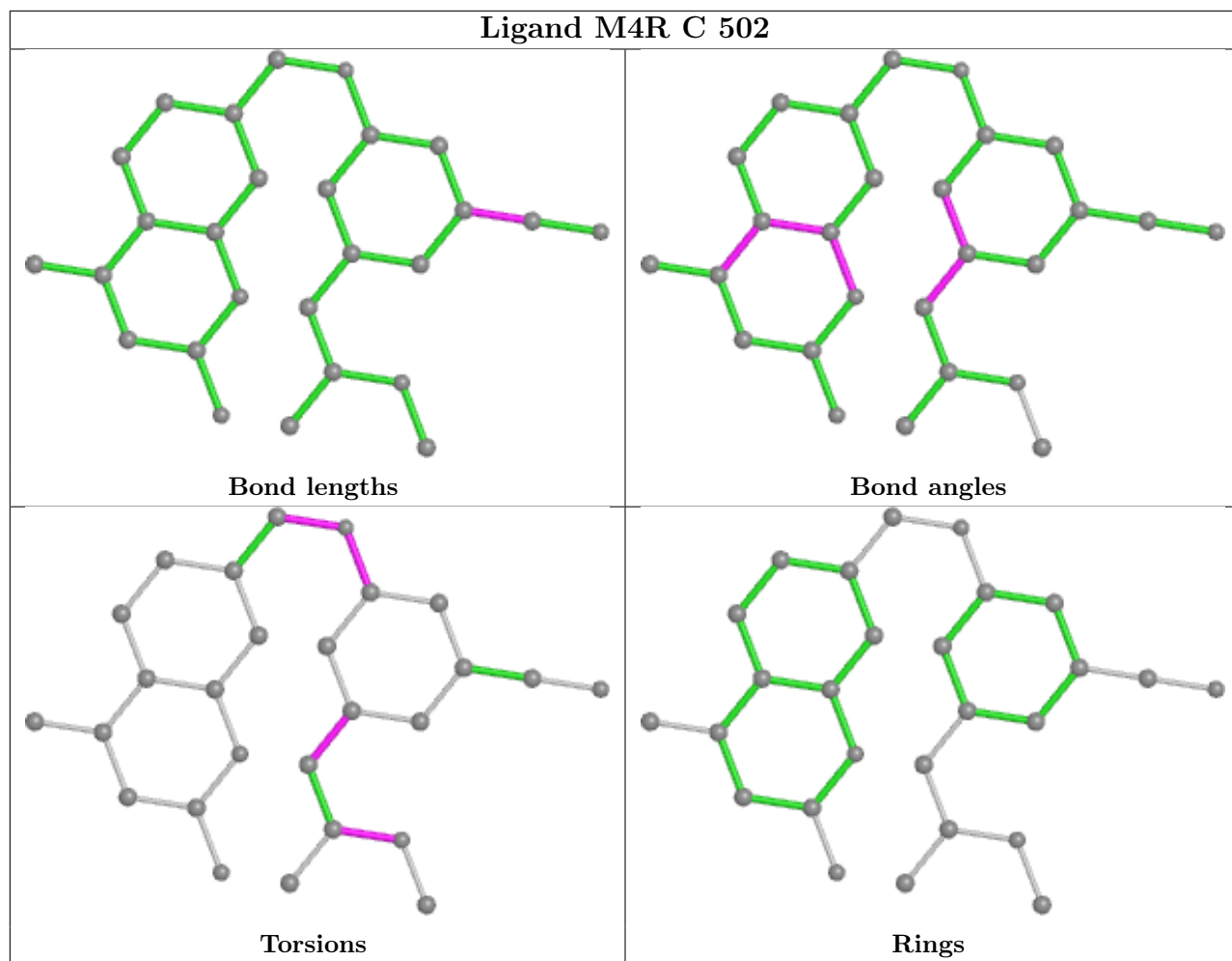


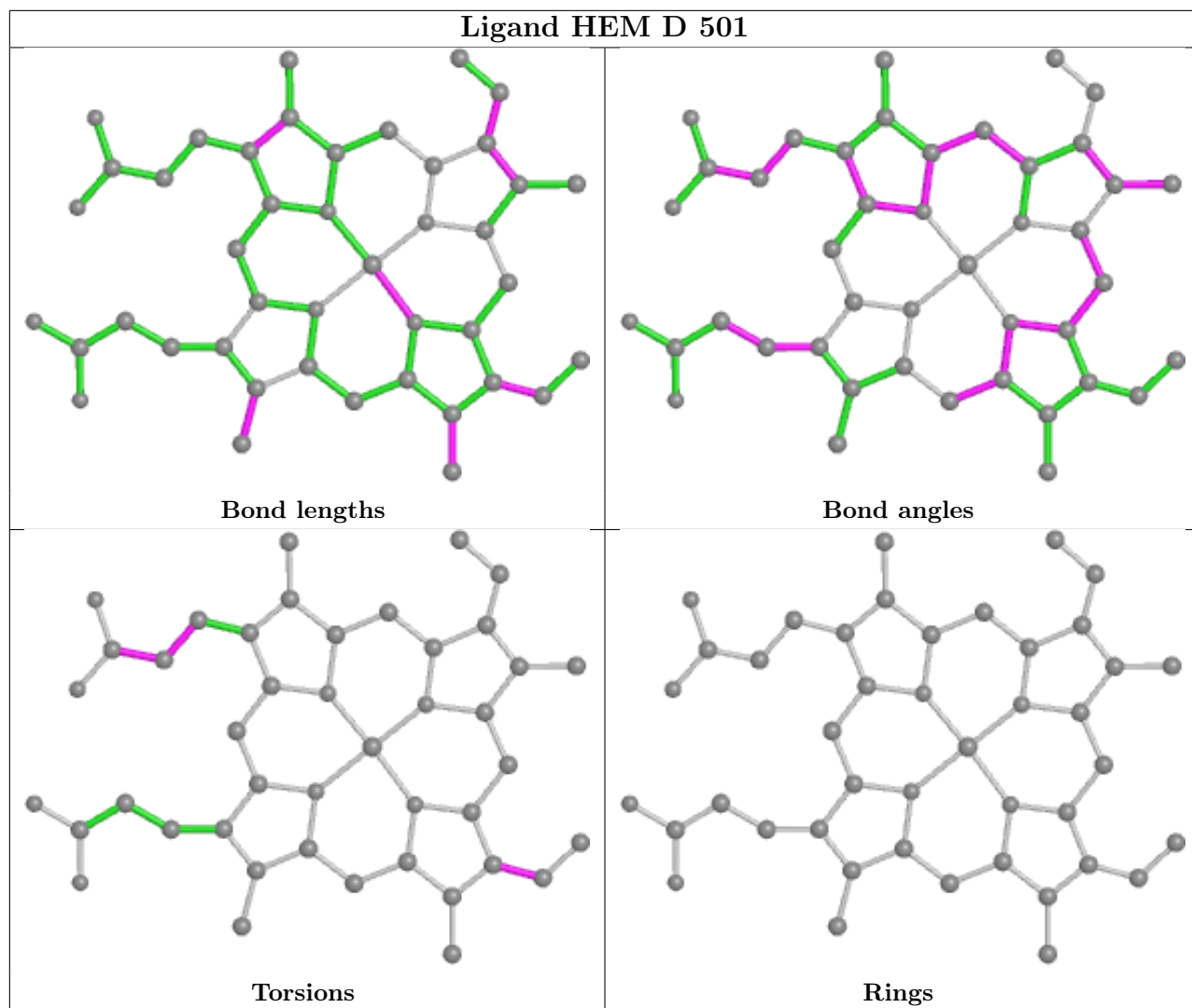


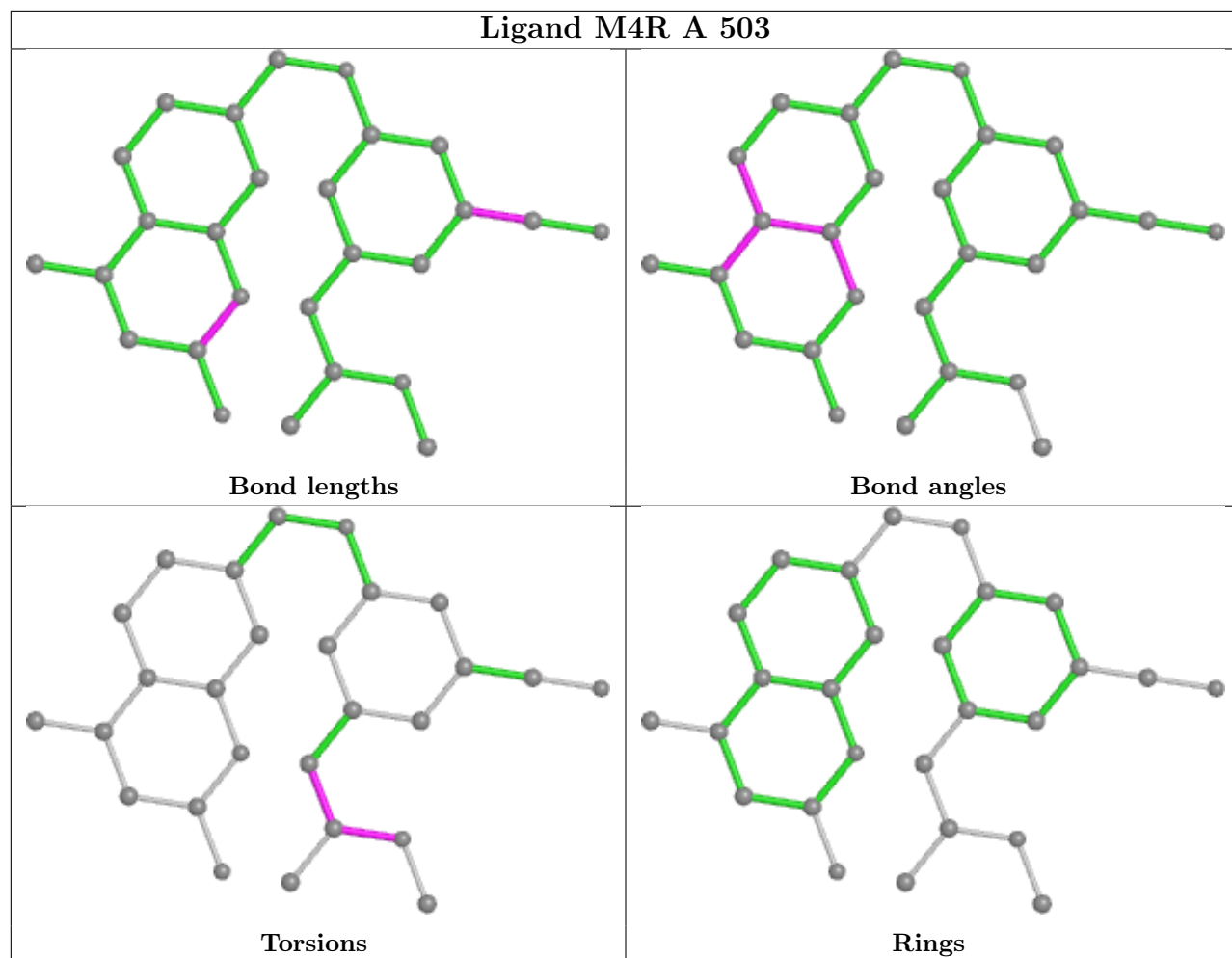


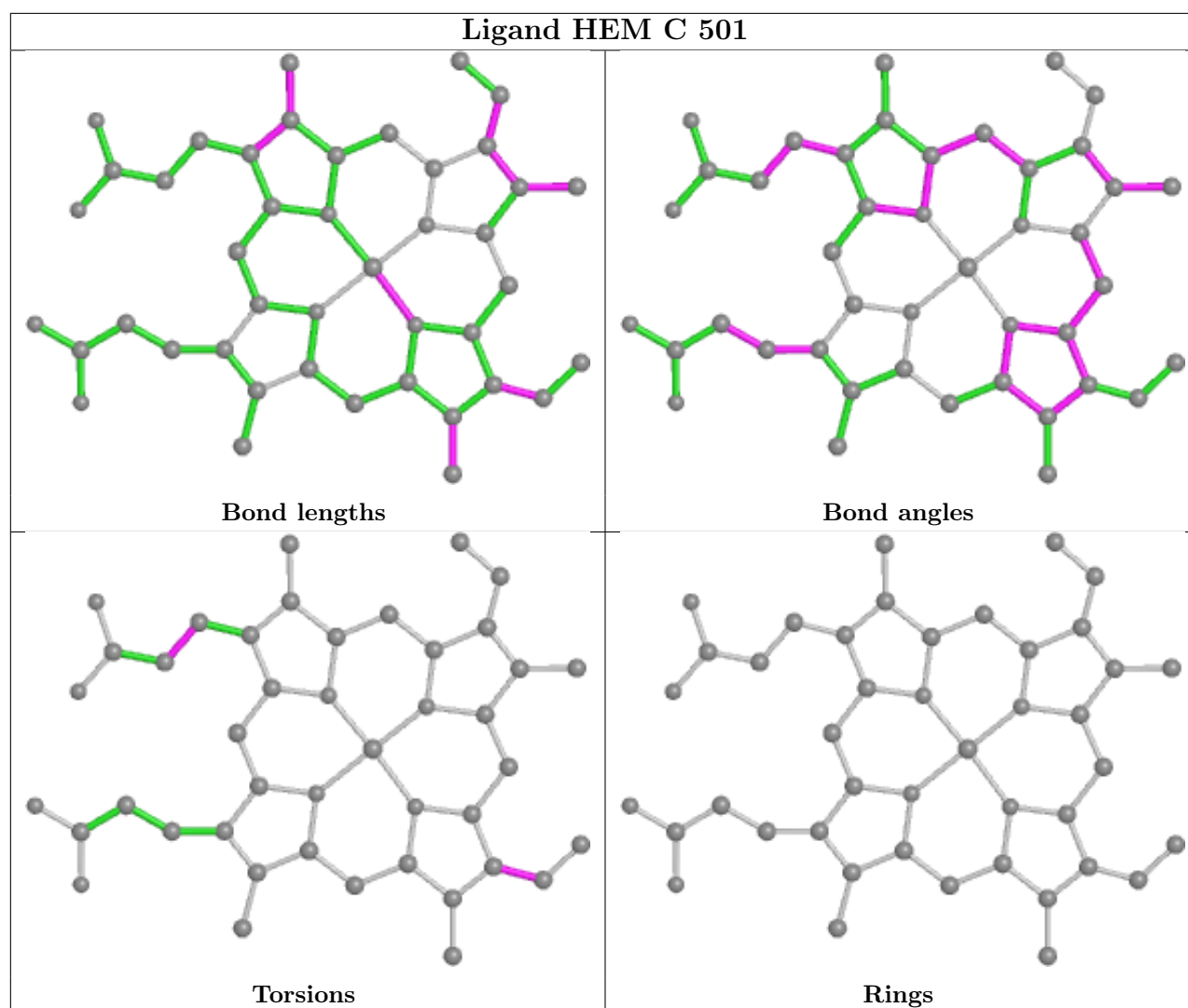












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/440 (91%)	1.05	71 (17%) 1 1	39, 70, 121, 159	0
1	B	402/440 (91%)	0.57	20 (4%) 28 35	35, 58, 99, 141	0
1	C	401/440 (91%)	0.72	40 (9%) 7 10	39, 60, 111, 147	0
1	D	402/440 (91%)	0.75	41 (10%) 6 9	36, 56, 114, 140	0
All	All	1609/1760 (91%)	0.77	172 (10%) 6 8	35, 61, 114, 159	0

The worst 5 of 172 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	PHE	9.1
1	C	239	GLY	9.0
1	A	304	LEU	8.6
1	D	157	VAL	8.0
1	A	241	PHE	7.4

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](#)

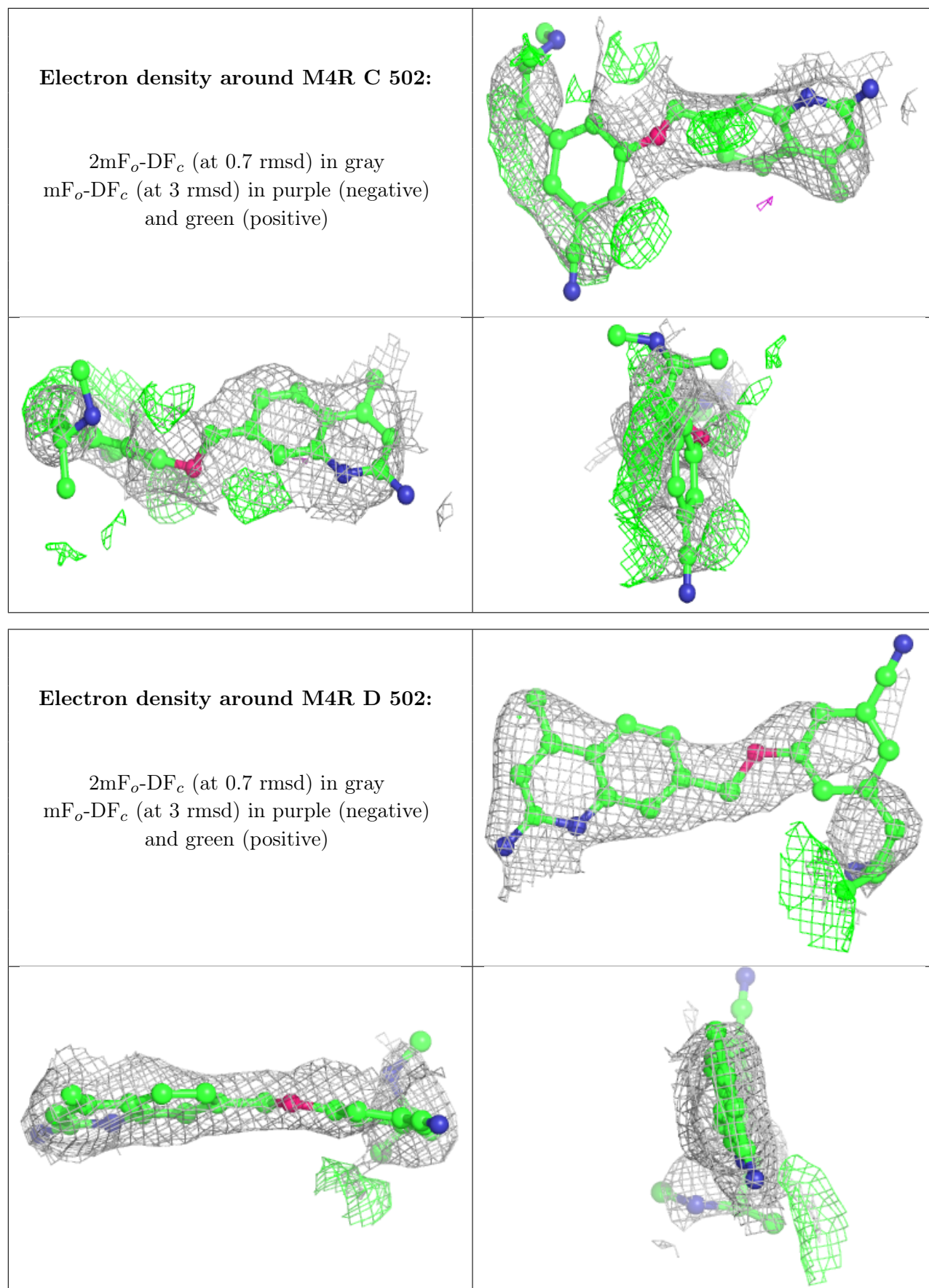
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

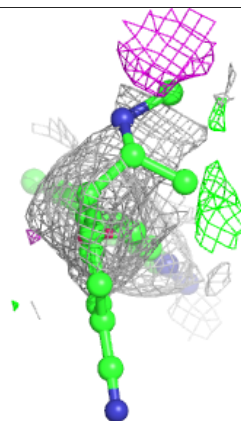
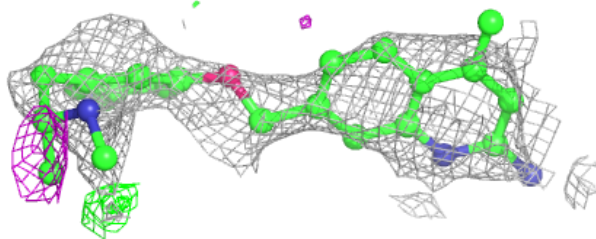
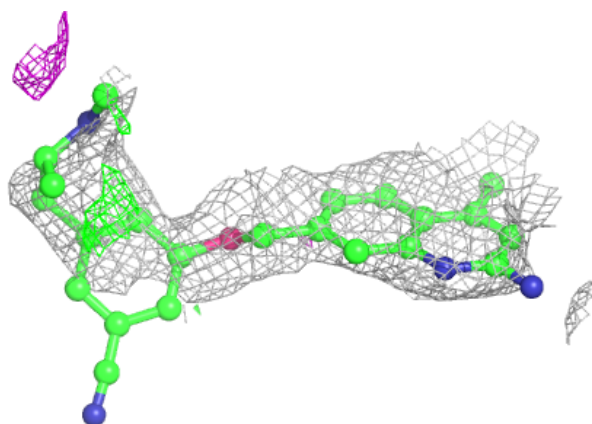
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	M4R	C	502	27/27	0.66	0.30	116,126,135,136	0
8	GD	A	510	1/1	0.69	0.12	171,171,171,171	0
4	BTB	D	506	14/14	0.72	0.29	100,103,107,107	0
4	BTB	D	504	14/14	0.72	0.29	53,88,93,95	0
4	BTB	B	505	14/14	0.74	0.27	83,95,103,105	0
4	BTB	A	505	14/14	0.75	0.17	98,103,107,107	0
3	M4R	D	502	27/27	0.80	0.26	69,89,109,111	0
3	M4R	A	502	27/27	0.83	0.30	92,106,121,121	0
4	BTB	B	506	14/14	0.84	0.24	98,104,107,110	0
3	M4R	B	502	27/27	0.85	0.24	59,94,116,119	0
4	BTB	D	505	14/14	0.85	0.19	107,111,113,114	0
4	BTB	C	505	14/14	0.86	0.24	76,88,91,91	0
5	ZN	C	511	1/1	0.87	0.12	55,55,55,55	1
3	M4R	B	503	27/27	0.88	0.21	41,56,85,94	0
3	M4R	A	503	27/27	0.88	0.21	43,61,88,90	0
6	GOL	C	508	6/6	0.89	0.32	71,80,87,89	0
4	BTB	D	507	14/14	0.91	0.19	86,96,100,102	0
4	BTB	C	504	14/14	0.92	0.27	95,107,111,112	0
6	GOL	A	508	6/6	0.92	0.27	77,87,89,91	0
5	ZN	A	506	1/1	0.93	0.20	54,54,54,54	0
3	M4R	D	503	27/27	0.93	0.17	35,55,70,72	0
4	BTB	A	504	14/14	0.93	0.21	37,83,86,87	0
3	M4R	C	503	27/27	0.93	0.24	49,69,92,93	0
4	BTB	B	504	14/14	0.93	0.20	55,67,78,81	0
7	CL	A	509	1/1	0.94	0.13	71,71,71,71	0
7	CL	D	509	1/1	0.95	0.09	48,48,48,48	0
7	CL	B	507	1/1	0.95	0.06	47,47,47,47	0
2	HEM	C	501	43/43	0.96	0.18	41,54,75,88	0
7	CL	C	509	1/1	0.96	0.05	64,64,64,64	0
5	ZN	C	506	1/1	0.96	0.15	50,50,50,50	0
2	HEM	A	501	43/43	0.96	0.18	46,56,79,91	0
8	GD	C	510	1/1	0.96	0.19	117,117,117,117	0
2	HEM	D	501	43/43	0.97	0.18	32,54,77,86	0
2	HEM	B	501	43/43	0.97	0.19	36,46,68,84	0
5	ZN	C	507	1/1	0.97	0.12	57,57,57,57	0
8	GD	B	508	1/1	0.98	0.23	62,62,62,62	0
5	ZN	A	511	1/1	0.98	0.17	64,64,64,64	0
5	ZN	A	507	1/1	0.99	0.16	53,53,53,53	0
8	GD	D	508	1/1	0.99	0.21	59,59,59,59	0

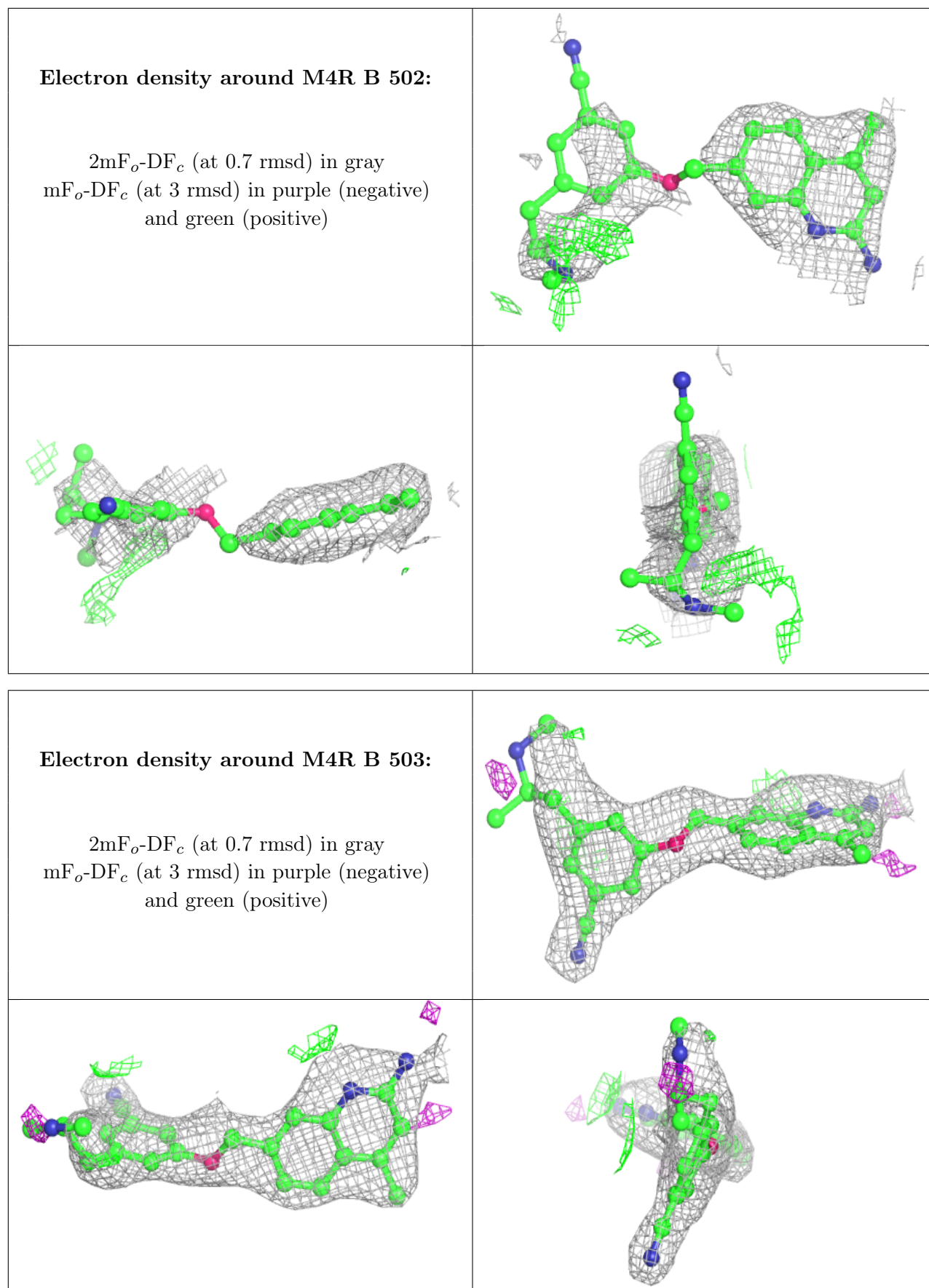
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around M4R A 502:

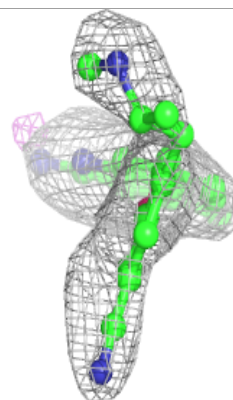
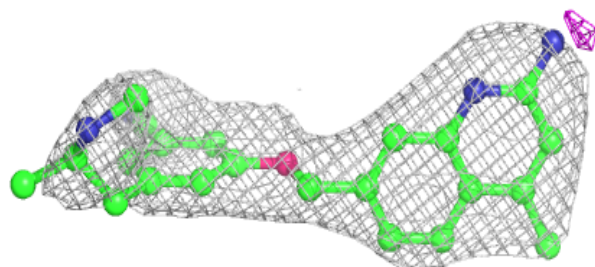
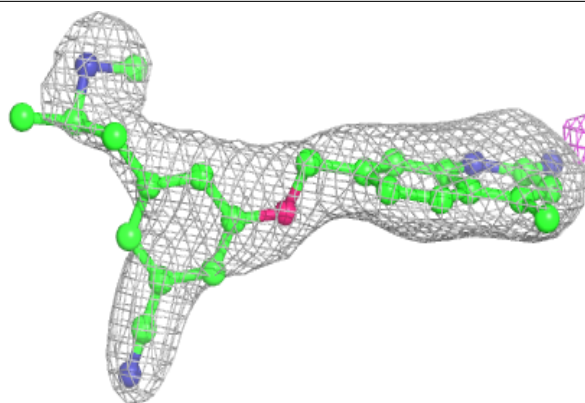
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



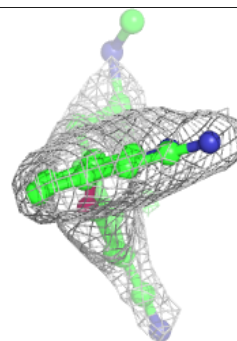
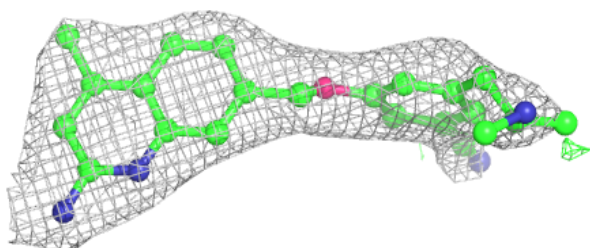
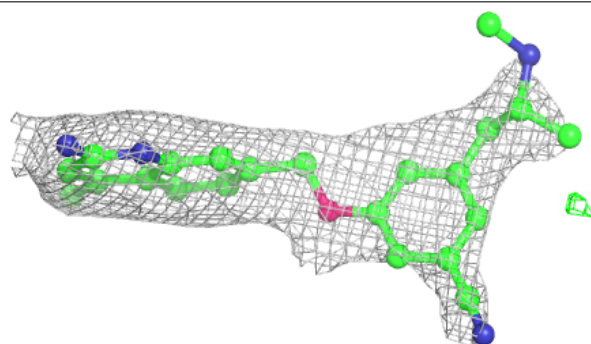


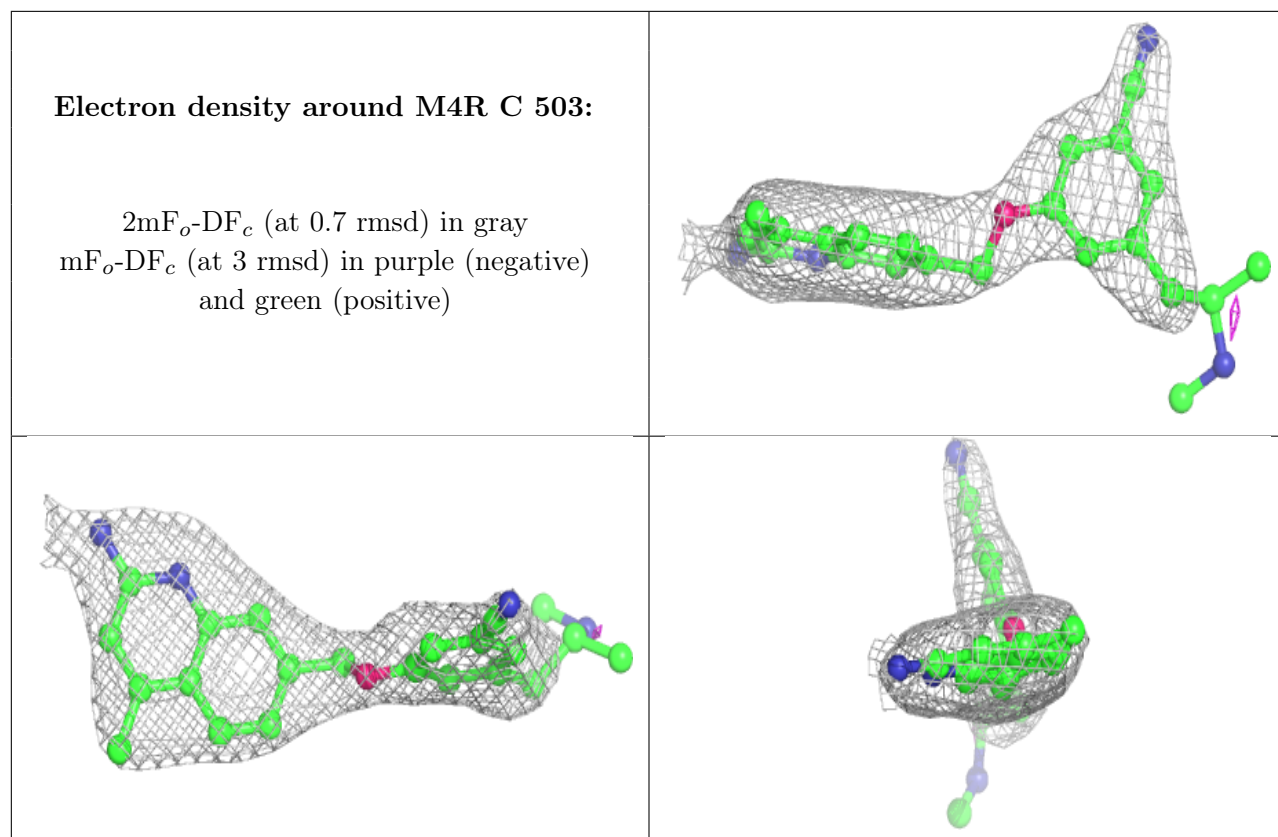
Electron density around M4R A 503:

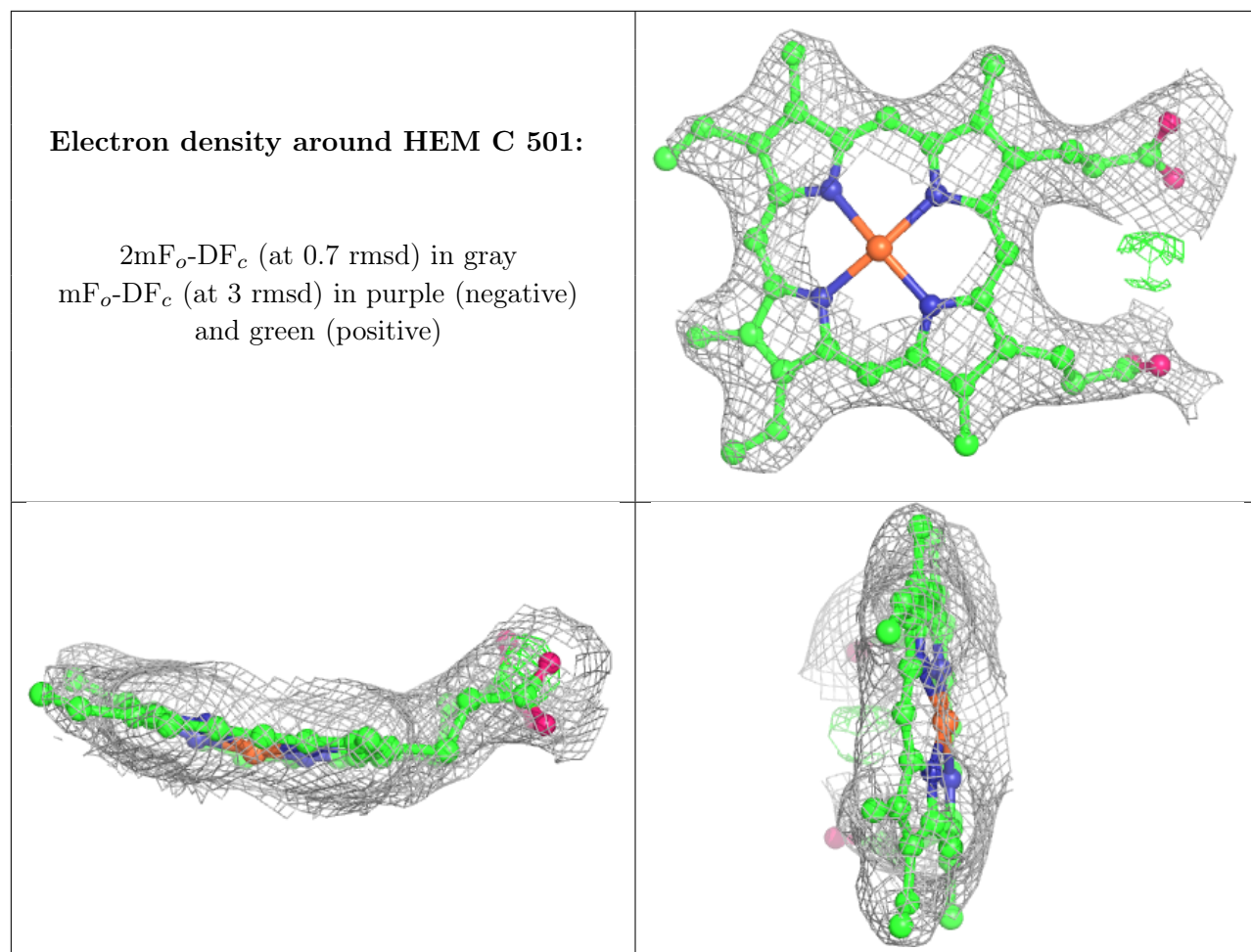
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

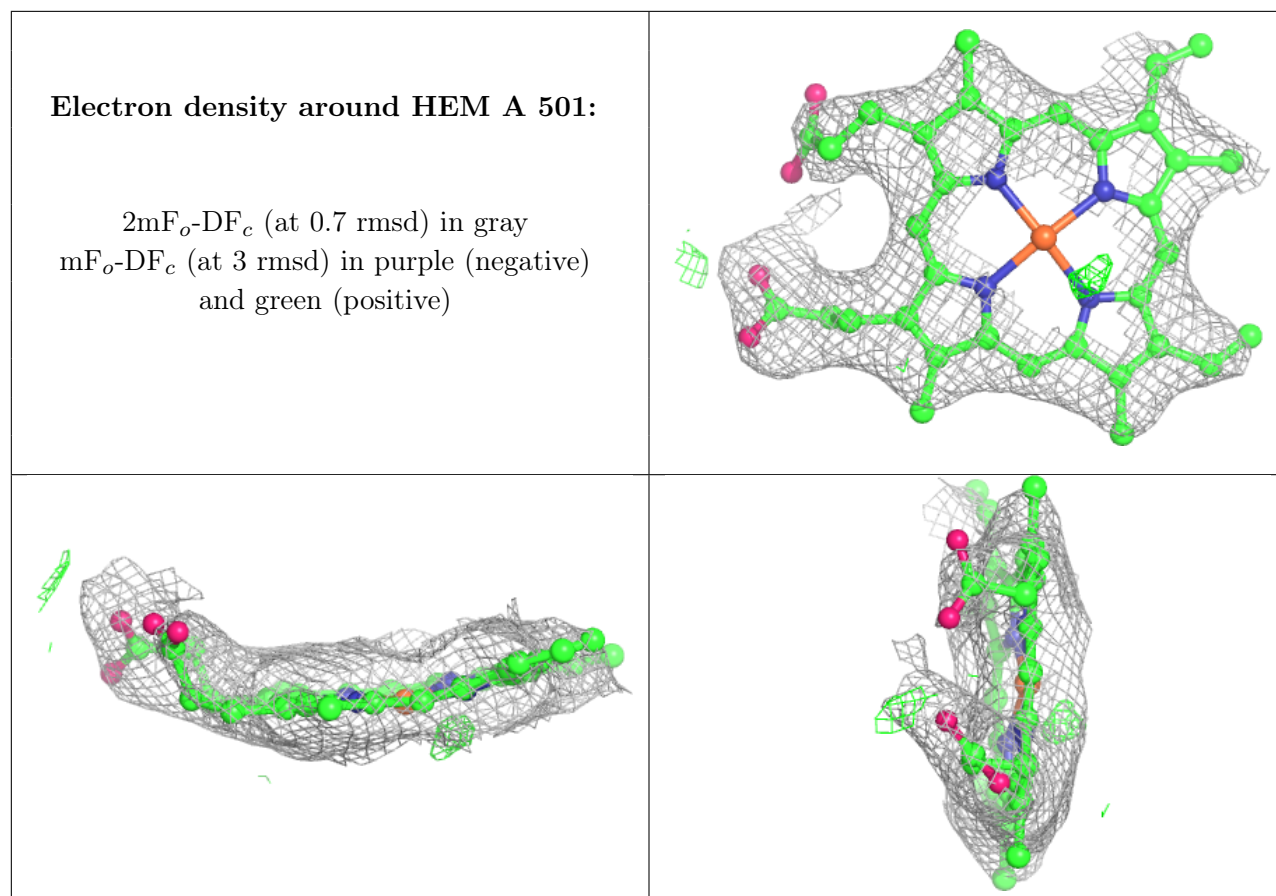
**Electron density around M4R D 503:**

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



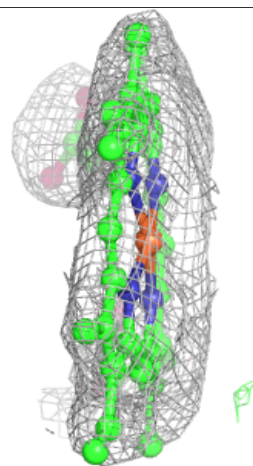
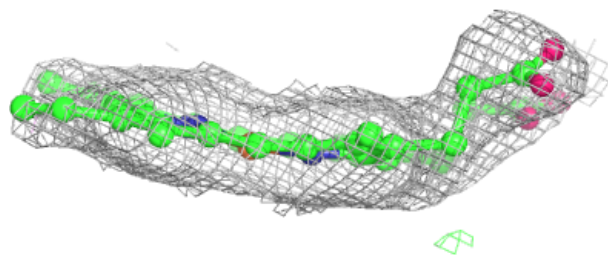
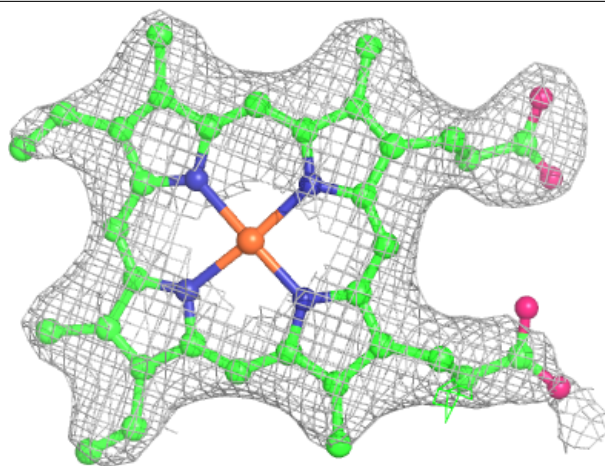


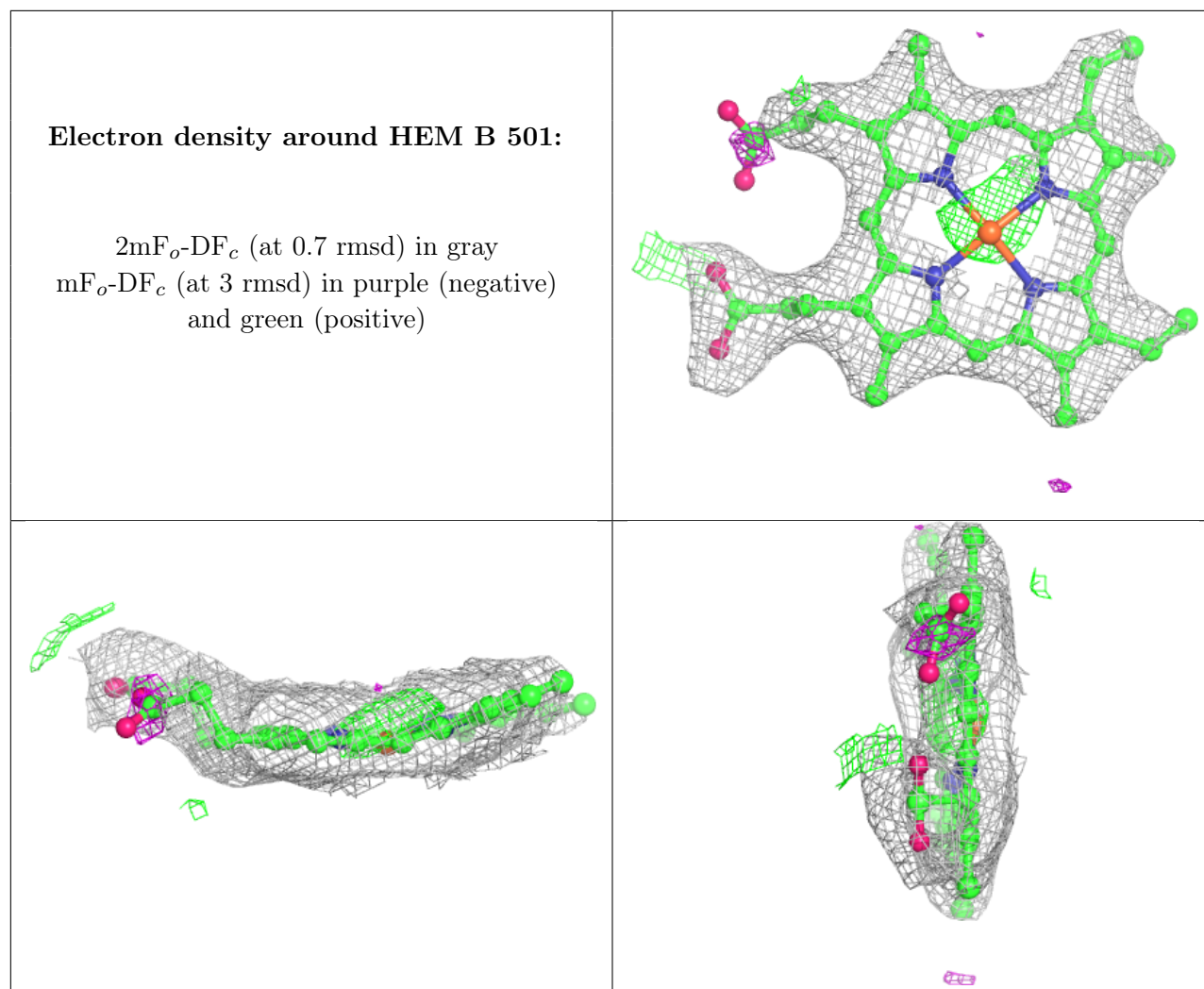




Electron density around HEM D 501:

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





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.