



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:22 am BST

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)benzonitrile
Authors : Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on : 2017-01-31
Resolution : 2.29 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

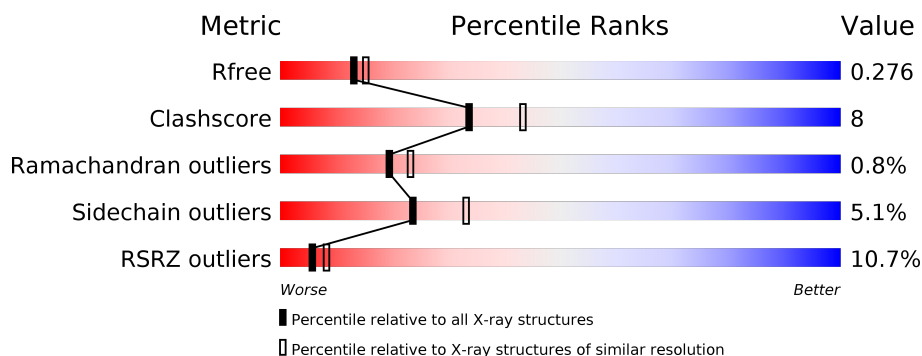
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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

Mol	Chain	Length	Quality of chain
1	A	440	<div> <div>16%</div> <div> <div>70%</div> <div>20%</div> <div>• 8%</div> </div> </div>
1	B	440	<div> <div>5%</div> <div> <div>79%</div> <div>11%</div> <div>• 9%</div> </div> </div>
1	C	440	<div> <div>9%</div> <div> <div>70%</div> <div>20%</div> <div>• 9%</div> </div> </div>
1	D	440	<div> <div>9%</div> <div> <div>69%</div> <div>22%</div> <div>• 9%</div> </div> </div>

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 crite-

ria:

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

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



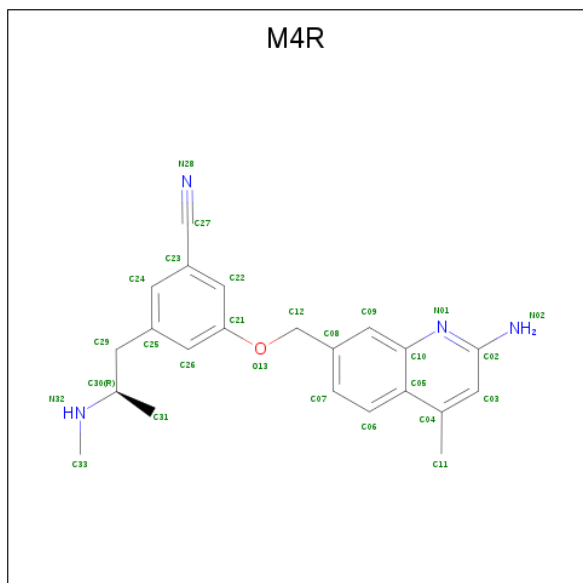
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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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		

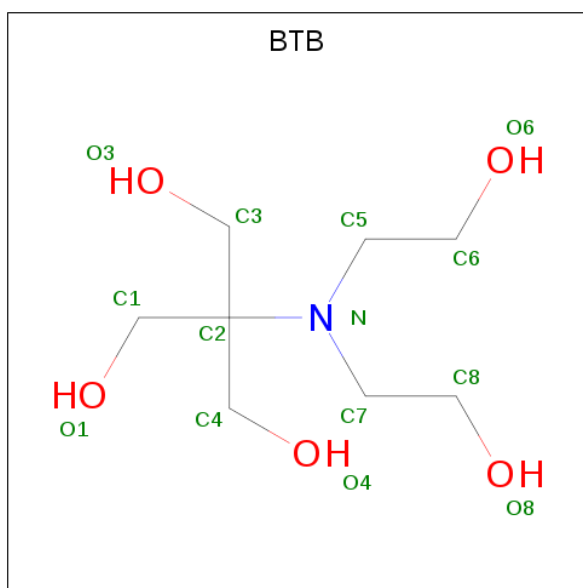
- Molecule 3 is 3-[(2-amino-4-methylquinolin-7-yl)methoxy]-5-[(2R)-2-(methylamino)propyl]benzonitrile (three-letter code: M4R) (formula: C₂₂H₂₄N₄O).



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: $C_8H_{19}NO_5$).



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: $C_3H_8O_3$).



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	B	1	Total	Cl	0	0
			1	1		
7	A	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		
7	C	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	B	1	Total 1	Gd 1	0	0
8	A	1	Total 1	Gd 1	0	0
8	D	1	Total 1	Gd 1	0	0
8	C	1	Total 1	Gd 1	0	0

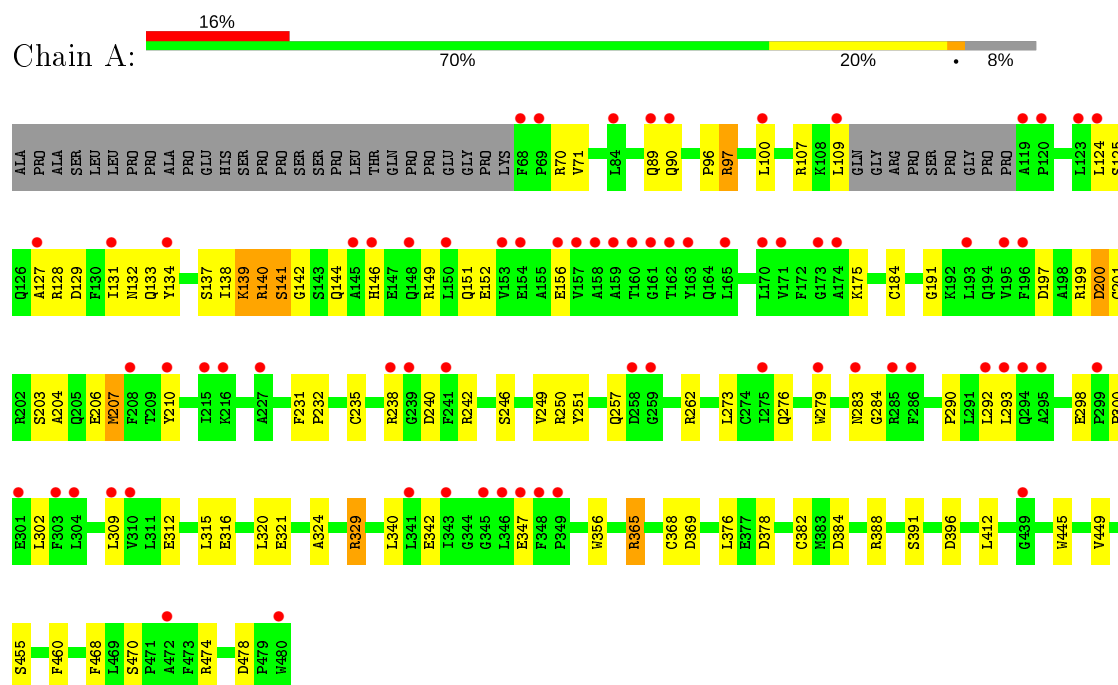
- Molecule 9 is water.

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

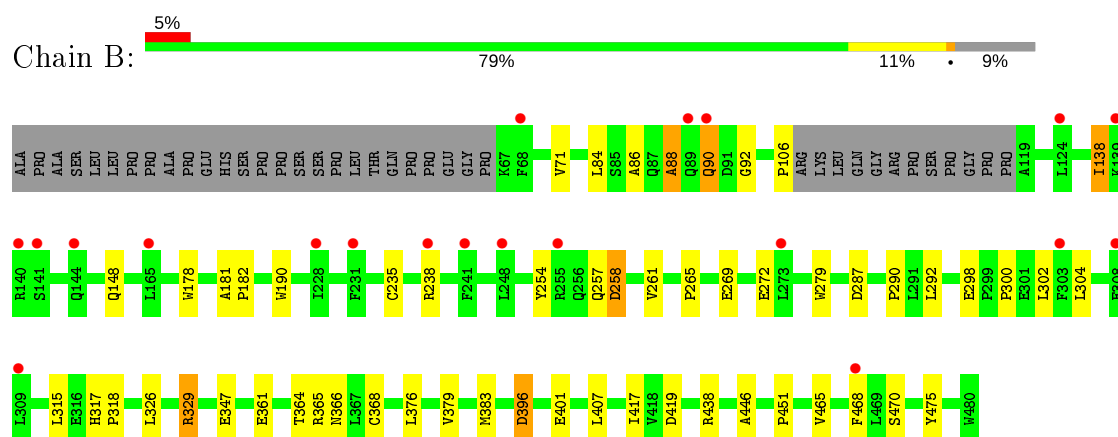
3 Residue-property plots [i](#)

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

- Molecule 1: Nitric oxide synthase, endothelial

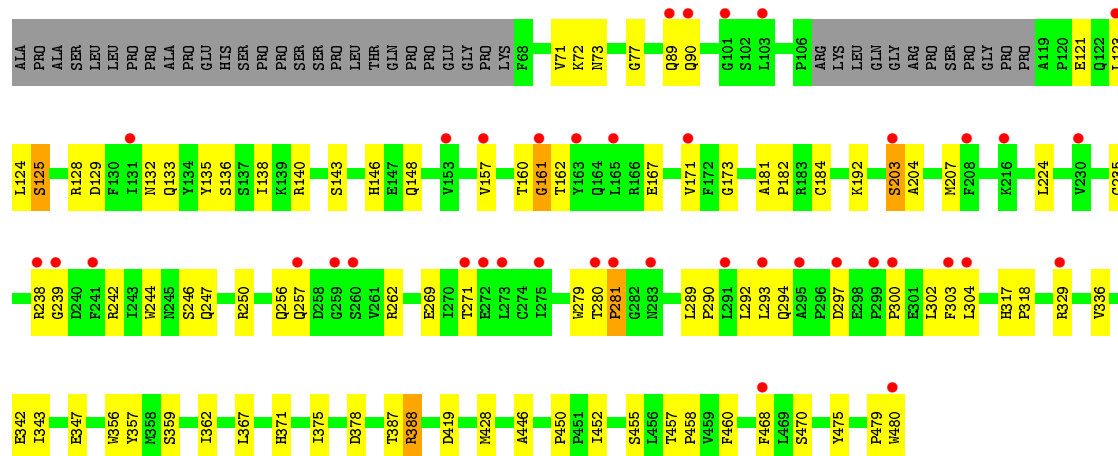


- Molecule 1: Nitric oxide synthase, endothelial



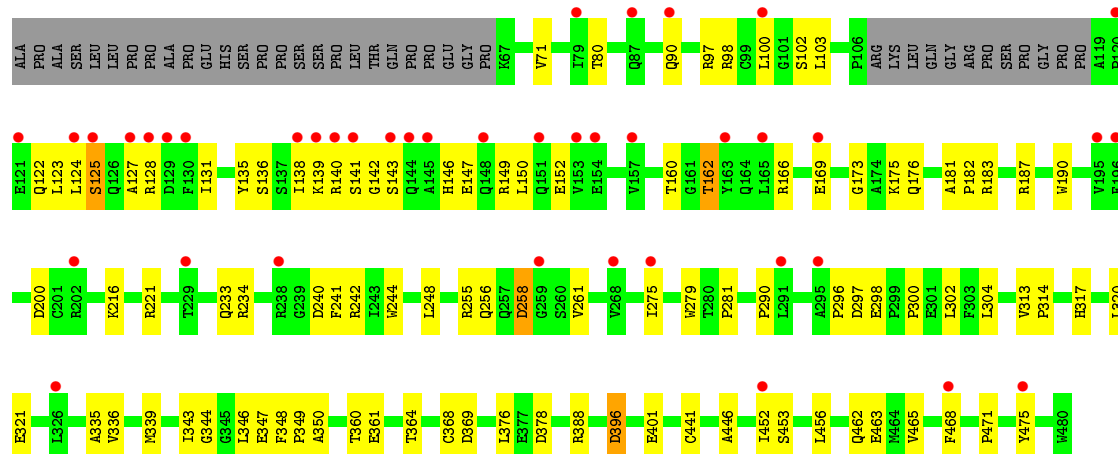
- Molecule 1: Nitric oxide synthase, endothelial

Chain C: 



• Molecule 1: Nitric oxide synthase, endothelial

Chain D: 



4 Data and refinement statistics

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)	Xtriage
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	Xtriage
Anisotropy	0.929	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.298 for h,-k,-l	Xtriage
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

Xtriage'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: GOL, ZN, CL, M4R, GD, BTB, HEM

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.

All (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:HBD2	2:A:501:HEM:HHA	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
1:C:160:THR:O	1:C:162:THR:N	2.22	0.71
1:A:128:ARG:O	1:A:132:ASN:ND2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:GLU:OE1	9:C:601:HOH:O	2.09	0.71
2:A:501:HEM:HHC	2:A:501:HEM:HBB2	1.73	0.70
1:C:271:THR:HA	1:C:289:LEU:HD21	1.73	0.70
1:C:347:GLU:OE2	9:C:602:HOH:O	2.11	0.68
1:A:347:GLU:OE2	9:A:601:HOH:O	2.10	0.68
1:D:258:ASP:N	1:D:258:ASP:OD1	2.27	0.67
1:C:356:TRP:O	3:C:502:M4R:N02	2.28	0.67
1:C:235:CYS:O	1:C:238:ARG:NH1	2.28	0.67
1:A:378:ASP:OD1	9:A:602:HOH:O	2.13	0.67
1:D:152:GLU:OE1	1:D:166:ARG:NH2	2.28	0.67
1:C:235:CYS:H	1:C:238:ARG:HD3	1.59	0.66
1:D:136:SER:HA	1:D:141[A]:SER:HB2	1.77	0.66
1:C:292:LEU:HD22	1:C:300:PRO:HB2	1.78	0.66
1:A:292:LEU:HD22	1:A:300:PRO:HB2	1.76	0.65
1:A:197:ASP:OD2	1:A:199:ARG:NH2	2.27	0.65
1:C:132:ASN:O	1:C:136:SER:OG	2.14	0.65
1:C:124:LEU:O	1:C:128:ARG:HG2	1.96	0.64
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.79	0.64
1:D:90:GLN:HB3	1:D:468:PHE:CD1	2.34	0.63
1:C:450:PRO:HG2	1:C:457:THR:HG21	1.80	0.62
1:A:97:ARG:HG2	1:B:88:ALA:HB3	1.80	0.62
1:B:446:ALA:O	3:B:503:M4R:N02	2.32	0.62
1:D:200:ASP:OD1	4:D:507:BTB:O8	2.17	0.62
4:B:504:BTB:O6	1:C:378:ASP:OD2	2.18	0.61
2:C:501:HEM:HHC	2:C:501:HEM:HBB2	1.81	0.61
1:B:368:CYS:SG	1:B:376:LEU:HD13	2.41	0.61
2:B:501:HEM:HMC2	2:B:501:HEM:HBC2	1.82	0.61
1:B:347:GLU:OE2	9:B:601:HOH:O	2.16	0.61
1:D:136:SER:HA	1:D:141[B]:SER:HB2	1.81	0.61
1:A:455:SER:HB3	1:B:451:PRO:HB2	1.81	0.60
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.83	0.60
1:A:340:LEU:HD21	1:A:347:GLU:HB3	1.84	0.59
1:B:90:GLN:HB2	1:B:468:PHE:CD1	2.37	0.59
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.85	0.59
1:C:184:CYS:HB2	2:C:501:HEM:ND	2.17	0.59
1:A:200:ASP:OD1	1:A:200:ASP:N	2.35	0.58
1:C:428:MET:HG3	1:C:458:PRO:HB2	1.84	0.58
1:A:347:GLU:OE2	1:A:474:ARG:NH2	2.37	0.58
1:A:96:PRO:O	1:B:92:GLY:N	2.30	0.58
1:C:207:MET:HG2	1:C:293:LEU:HD13	1.86	0.58
1:B:279:TRP:HB2	1:B:302:LEU:HD21	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ALA:O	1:D:131:ILE:HG12	2.05	0.57
1:A:134:TYR:O	1:A:137:SER:OG	2.16	0.56
1:D:343:ILE:O	1:D:346:LEU:N	2.37	0.56
1:A:321:GLU:CD	1:A:321:GLU:H	2.09	0.56
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.88	0.56
1:D:234:ARG:NH1	1:D:347:GLU:OE1	2.39	0.56
1:D:321:GLU:OE1	4:D:504:BTB:O6	2.18	0.56
1:D:462:GLN:NE2	1:D:463:GLU:O	2.32	0.55
1:A:262:ARG:HH21	1:A:284:GLY:HA2	1.72	0.55
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.88	0.55
1:C:244:TRP:NE1	1:C:294:GLN:OE1	2.34	0.55
1:A:251:TYR:OH	1:A:312:GLU:OE2	2.23	0.55
1:B:317:HIS:NE2	1:B:401:GLU:OE1	2.40	0.54
1:C:173:GLY:HA3	1:C:343:ILE:HD13	1.89	0.54
1:D:368:CYS:SG	1:D:376:LEU:HD13	2.48	0.54
1:C:246:SER:HB2	3:C:502:M4R:N28	2.22	0.54
1:B:106:PRO:O	9:B:602:HOH:O	2.18	0.53
1:C:242:ARG:NH2	1:C:479:PRO:HD3	2.23	0.53
1:D:453:SER:HB3	1:D:456:LEU:HD12	1.90	0.53
1:A:175:LYS:NZ	1:A:191:GLY:O	2.41	0.53
1:C:204:ALA:HB1	1:C:303:PHE:HE2	1.74	0.53
1:B:292:LEU:HD22	1:B:300:PRO:HB2	1.91	0.53
1:D:138:ILE:C	1:D:140:ARG:H	2.12	0.52
1:A:455:SER:HA	1:A:460:PHE:CG	2.45	0.52
1:D:298:GLU:CD	4:D:506:BTB:H82	2.30	0.52
1:B:261:VAL:HG11	1:B:265:PRO:HA	1.92	0.52
1:A:142:GLY:HA2	1:A:146:HIS:ND1	2.24	0.52
1:C:129:ASP:O	1:C:133:GLN:HG3	2.09	0.51
1:C:279:TRP:CG	1:C:290:PRO:HG3	2.45	0.51
1:B:254:TYR:OH	1:B:287:ASP:OD2	2.22	0.51
1:D:146:HIS:CD2	1:D:150:LEU:HD11	2.46	0.51
1:A:139:LYS:O	1:A:141:SER:N	2.44	0.51
1:A:388:ARG:HG2	4:A:505:BTB:H62	1.93	0.51
1:C:90:GLN:HB2	1:C:468:PHE:CD1	2.46	0.51
1:A:315:LEU:HG	1:A:329:ARG:HA	1.93	0.50
1:D:241:PHE:CE1	1:D:296:PRO:HD3	2.46	0.50
1:C:367:LEU:HB3	1:C:375:ILE:HD13	1.93	0.50
1:C:138:ILE:HG13	1:C:140:ARG:HG3	1.93	0.50
1:C:73:ASN:O	1:C:77:GLY:N	2.36	0.50
4:D:505:BTB:O1	4:D:505:BTB:O4	2.29	0.50
1:A:100:LEU:HD21	1:B:465:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ARG:HB2	2:D:501:HEM:HAD2	1.94	0.49
1:D:360:THR:HG22	1:D:452:ILE:HD11	1.93	0.49
1:D:317:HIS:NE2	1:D:401:GLU:OE1	2.36	0.49
1:D:242:ARG:HD3	1:D:349:PRO:HB2	1.93	0.49
1:D:339:MET:O	9:D:602:HOH:O	2.20	0.49
1:D:296:PRO:O	1:D:298:GLU:HG2	2.13	0.49
1:C:224:LEU:HD12	1:C:356:TRP:HB3	1.94	0.49
1:A:90:GLN:HB2	1:A:468:PHE:CD1	2.47	0.48
1:C:279:TRP:HB2	1:C:302:LEU:HD21	1.95	0.48
1:C:135:TYR:O	1:C:140:ARG:N	2.37	0.48
1:D:173:GLY:HA3	1:D:343:ILE:HD13	1.94	0.48
1:C:475:TYR:OH	2:C:501:HEM:O1D	2.25	0.48
1:A:445:TRP:CZ2	1:A:449:VAL:HG21	2.49	0.47
1:A:365:ARG:O	1:A:369:ASP:HB2	2.14	0.47
1:B:396:ASP:N	1:B:396:ASP:OD1	2.47	0.47
4:D:506:BTB:H41	4:D:506:BTB:H71	1.41	0.47
4:A:504:BTB:H71	4:A:504:BTB:H42	1.58	0.47
1:B:84:LEU:HB2	1:B:438:ARG:O	2.15	0.47
1:B:257:GLN:NE2	1:B:258:ASP:OD1	2.49	0.46
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.96	0.46
1:B:315:LEU:HG	1:B:329:ARG:HA	1.96	0.46
1:D:146:HIS:CE1	1:D:150:LEU:HD11	2.49	0.46
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.51	0.46
1:A:262:ARG:NH2	1:A:284:GLY:HA2	2.29	0.46
4:D:507:BTB:H51	4:D:507:BTB:H41	1.63	0.46
1:C:167:GLU:O	1:C:171:VAL:HG23	2.16	0.46
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.51	0.46
1:A:207:MET:HE2	1:A:293:LEU:HB3	1.98	0.46
4:D:505:BTB:H11	4:D:505:BTB:H52	1.34	0.46
1:D:135:TYR:OH	1:D:149:ARG:HB3	2.16	0.46
1:A:125:SER:HA	1:A:128:ARG:HE	1.80	0.45
4:C:504:BTB:H52	4:C:504:BTB:H31	1.78	0.45
1:A:231:PHE:HB3	1:A:232:PRO:HD2	1.98	0.45
1:C:455:SER:HA	1:C:460:PHE:CG	2.51	0.45
1:D:139:LYS:C	1:D:141[A]:SER:H	2.19	0.45
1:D:255:ARG:HG3	1:D:261:VAL:HG22	1.98	0.45
1:D:139:LYS:C	1:D:141[B]:SER:H	2.19	0.45
1:A:356:TRP:O	3:A:502:M4R:N02	2.50	0.45
1:D:361:GLU:OE2	3:D:502:M4R:N02	2.49	0.45
1:B:181:ALA:HA	1:B:182:PRO:HD3	1.80	0.45
1:B:364:THR:O	1:B:368:CYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:505:BTB:H71	4:D:505:BTB:H42	1.55	0.45
1:A:316[B]:GLU:HG2	1:A:324:ALA:HB2	1.98	0.45
1:D:446:ALA:O	3:D:503:M4R:N02	2.50	0.45
1:A:201:CYS:SG	1:A:206:GLU:HB3	2.57	0.45
1:A:273:LEU:HA	1:A:276:GLN:HG2	1.99	0.45
1:D:336:VAL:HG21	3:D:502:M4R:C07	2.46	0.45
1:A:388:ARG:HG2	4:A:505:BTB:C6	2.46	0.44
1:B:475:TYR:OH	2:B:501:HEM:O1D	2.25	0.44
1:D:176:GLN:HB3	1:D:471:PRO:HD2	2.00	0.44
4:D:506:BTB:H62	9:D:619:HOH:O	2.17	0.44
1:B:257:GLN:H	1:B:257:GLN:CD	2.20	0.44
1:C:247:GLN:HB2	1:C:250:ARG:HG2	2.00	0.44
1:D:364:THR:O	1:D:368:CYS:HB2	2.17	0.44
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.53	0.44
1:B:379:VAL:O	1:B:383:MET:HG3	2.17	0.44
1:C:342:GLU:OE1	9:C:602:HOH:O	2.21	0.44
1:C:359:SER:OG	1:C:419:ASP:HA	2.18	0.44
1:A:184:CYS:HB2	2:A:501:HEM:ND	2.31	0.44
1:B:138:ILE:HG12	1:B:138:ILE:H	1.59	0.44
1:D:244:TRP:CZ2	1:D:300:PRO:HG3	2.53	0.44
4:D:506:BTB:H11	4:D:506:BTB:H52	1.40	0.44
1:C:203:SER:OG	1:C:204:ALA:N	2.50	0.44
1:D:240:ASP:HB3	1:D:349:PRO:HG3	1.99	0.44
1:D:125:SER:OG	4:D:505:BTB:H31	2.17	0.44
1:C:446:ALA:O	3:C:503:M4R:N02	2.51	0.44
1:D:100:LEU:HB3	1:D:103:LEU:HD22	2.00	0.44
1:D:248:LEU:HB2	1:D:335:ALA:HB3	1.99	0.44
4:D:504:BTB:H52	4:D:504:BTB:O1	2.17	0.44
1:B:326:LEU:HD12	4:C:504:BTB:H11	2.00	0.43
1:C:124:LEU:HD23	1:C:124:LEU:HA	1.91	0.43
1:C:239:GLY:HA3	1:C:297:ASP:N	2.32	0.43
1:A:388:ARG:NH1	1:C:257:GLN:OE1	2.43	0.43
1:D:149:ARG:HA	1:D:152:GLU:HB3	2.00	0.43
1:C:121:GLU:O	1:C:125:SER:OG	2.36	0.43
1:D:396:ASP:N	1:D:396:ASP:OD1	2.44	0.43
1:A:238:ARG:H	1:A:238:ARG:HH11	1.66	0.43
1:A:368:CYS:SG	1:A:376:LEU:HD13	2.59	0.43
4:C:505:BTB:H52	4:C:505:BTB:H42	1.63	0.43
1:D:255:ARG:HG2	1:D:256:GLN:O	2.18	0.43
1:D:313:VAL:HA	1:D:314:PRO:HD2	1.89	0.43
1:D:122:GLN:NE2	4:D:505:BTB:O8	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ALA:O	1:A:207:MET:HB2	2.19	0.43
1:D:146:HIS:NE2	1:D:150:LEU:HD21	2.34	0.43
1:D:475:TYR:HD1	3:D:502:M4R:C27	2.32	0.43
1:C:143:SER:O	1:C:146:HIS:HB3	2.19	0.42
1:A:127:ALA:O	1:A:131:ILE:HG12	2.20	0.42
1:A:388:ARG:HH12	1:C:257:GLN:CD	2.20	0.42
4:C:504:BTB:H42	4:C:504:BTB:H71	1.76	0.42
1:D:122:GLN:HE22	4:D:505:BTB:HO8	1.64	0.42
1:A:279:TRP:CE2	1:A:290:PRO:HD3	2.54	0.42
1:A:97:ARG:HH12	1:B:86:ALA:C	2.23	0.42
1:D:142:GLY:HA2	1:D:146:HIS:ND1	2.33	0.42
1:B:365:ARG:HD2	1:B:366:ASN:OD1	2.19	0.42
1:B:365:ARG:NH1	7:B:507:CL:CL	2.88	0.42
1:D:71:VAL:HG11	1:D:465:VAL:HG23	2.01	0.42
1:D:181:ALA:HA	1:D:182:PRO:HD3	1.81	0.42
1:C:157:VAL:HG13	1:C:161:GLY:O	2.20	0.42
1:D:160:THR:OG1	1:D:162:THR:O	2.25	0.42
4:B:506:BTB:H31	1:C:388:ARG:HD3	2.02	0.41
1:D:123:LEU:HA	1:D:123:LEU:HD12	1.90	0.41
1:C:72:LYS:NZ	9:C:604:HOH:O	2.52	0.41
1:D:317:HIS:HB3	1:D:320:LEU:HB2	2.01	0.41
1:B:407:LEU:HD21	1:B:419:ASP:HB3	2.02	0.41
1:C:336:VAL:HG21	3:C:502:M4R:C07	2.51	0.41
1:A:246:SER:OG	1:A:250:ARG:HD2	2.20	0.41
1:D:122:GLN:NE2	4:D:505:BTB:H61	2.35	0.41
1:A:376:LEU:HD12	1:A:376:LEU:HA	1.93	0.41
1:D:241:PHE:O	1:D:350:ALA:HB2	2.21	0.41
1:A:342:GLU:OE2	1:A:474:ARG:NH1	2.54	0.41
1:B:269:GLU:O	1:B:272:GLU:HB2	2.20	0.41
1:D:90:GLN:HB3	1:D:468:PHE:HD1	1.84	0.41
4:B:504:BTB:H71	4:B:504:BTB:H42	1.89	0.41
2:B:501:HEM:HBA2	3:B:502:M4R:C12	2.50	0.41
1:C:280:THR:HA	1:C:281:PRO:HD2	1.68	0.41
1:A:382:CYS:O	4:A:504:BTB:H42	2.21	0.41
1:B:361:GLU:OE2	3:B:502:M4R:N02	2.54	0.41
1:C:269:GLU:OE2	1:C:480:TRP:NE1	2.49	0.41
1:D:233:GLN:H	1:D:233:GLN:HG2	1.72	0.41
1:D:187:ARG:NH1	1:D:441:CYS:SG	2.94	0.41
1:C:181:ALA:HA	1:C:182:PRO:HD3	1.85	0.40
1:A:152:GLU:O	1:A:156:GLU:HB2	2.22	0.40
1:B:84:LEU:HD22	1:B:438:ARG:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:SER:O	1:D:147:GLU:HG2	2.21	0.40
4:D:504:BTB:H42	4:D:504:BTB:H71	1.73	0.40
1:A:249:VAL:O	1:A:250:ARG:HG2	2.22	0.40
1:A:384:ASP:OD1	4:A:504:BTB:O4	2.29	0.40
1:C:184:CYS:HB2	2:C:501:HEM:C4D	2.56	0.40
1:D:175:LYS:HB3	1:D:190:TRP:CE3	2.57	0.40
1:D:348:PHE:HA	1:D:349:PRO:HD2	1.89	0.40
1:A:445:TRP:CE2	1:A:449:VAL:HG21	2.56	0.40
1:C:357:TYR:CD2	1:C:362:ILE:HD11	2.56	0.40
1:D:279:TRP:HB2	1:D:302:LEU:HD21	2.03	0.40
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.37	0.40

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

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

All (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
1	C	203	SER
1	D	102	SER
1	A	144	GLN
1	A	283	ASN
1	D	344	GLY
1	C	281	PRO
1	D	221	ARG

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	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

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	71	VAL
1	A	89	GLN
1	A	97	ARG
1	A	107	ARG
1	A	109	LEU
1	A	124	LEU
1	A	129	ASP
1	A	133	GLN
1	A	138	ILE

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Mol	Chain	Res	Type
1	A	139	LYS
1	A	140	ARG
1	A	141	SER
1	A	149	ARG
1	A	151	GLN
1	A	200	ASP
1	A	203	SER
1	A	207	MET
1	A	210	TYR
1	A	235	CYS
1	A	240	ASP
1	A	242	ARG
1	A	257	GLN
1	A	302	LEU
1	A	309	LEU
1	A	329	ARG
1	A	365	ARG
1	A	391	SER
1	A	396	ASP
1	A	412	LEU
1	A	470	SER
1	A	478	ASP
1	B	71	VAL
1	B	90	GLN
1	B	138	ILE
1	B	148	GLN
1	B	258	ASP
1	B	298	GLU
1	B	329	ARG
1	B	396	ASP
1	B	417	ILE
1	B	470	SER
1	C	71	VAL
1	C	123	LEU
1	C	125	SER
1	C	148	GLN
1	C	192	LYS
1	C	256	GLN
1	C	262	ARG
1	C	304	LEU
1	C	329	ARG
1	C	371	HIS

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Mol	Chain	Res	Type
1	C	387	THR
1	C	388	ARG
1	C	452	ILE
1	C	470	SER
1	D	80	THR
1	D	97	ARG
1	D	98	ARG
1	D	124	LEU
1	D	125	SER
1	D	128	ARG
1	D	162	THR
1	D	169	GLU
1	D	216	LYS
1	D	258	ASP
1	D	297	ASP
1	D	378	ASP
1	D	388	ARG
1	D	396	ASP

Some 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 carbohydrates 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	B	502	-	29,29,29	1.55	2 (6%)	38,40,40	0.94	3 (7%)
3	M4R	D	503	-	29,29,29	1.52	1 (3%)	38,40,40	1.08	2 (5%)
3	M4R	B	503	-	29,29,29	1.52	2 (6%)	38,40,40	0.96	1 (2%)
4	BTB	C	504	8	13,13,13	0.35	0	7,16,16	0.49	0
2	HEM	C	501	1	27,50,50	2.08	6 (22%)	17,82,82	1.77	4 (23%)
4	BTB	A	505	-	13,13,13	0.37	0	7,16,16	0.53	0
4	BTB	C	505	-	13,13,13	0.40	0	7,16,16	0.95	0
6	GOL	A	508	-	5,5,5	0.44	0	5,5,5	0.44	0
3	M4R	D	502	-	29,29,29	1.58	1 (3%)	38,40,40	1.17	6 (15%)
3	M4R	C	502	-	29,29,29	1.59	1 (3%)	38,40,40	1.13	3 (7%)
3	M4R	C	503	-	29,29,29	1.55	2 (6%)	38,40,40	1.27	6 (15%)
2	HEM	B	501	1	27,50,50	2.11	5 (18%)	17,82,82	1.95	6 (35%)
4	BTB	D	504	8	13,13,13	0.53	0	7,16,16	0.48	0
4	BTB	D	506	-	13,13,13	0.36	0	7,16,16	0.64	0
4	BTB	B	506	-	13,13,13	0.58	0	7,16,16	0.79	0
3	M4R	A	502	-	29,29,29	1.55	2 (6%)	38,40,40	1.02	4 (10%)
4	BTB	D	505	-	13,13,13	0.42	0	7,16,16	0.64	0
6	GOL	C	508	-	5,5,5	0.29	0	5,5,5	0.40	0
2	HEM	D	501	1	27,50,50	2.08	6 (22%)	17,82,82	1.94	5 (29%)
4	BTB	B	504	8	13,13,13	0.53	0	7,16,16	0.43	0
2	HEM	A	501	1	27,50,50	2.14	5 (18%)	17,82,82	1.54	3 (17%)
4	BTB	D	507	-	13,13,13	0.37	0	7,16,16	0.48	0
3	M4R	A	503	-	29,29,29	1.52	2 (6%)	38,40,40	1.25	3 (7%)
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

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	B	502	-	-	5/13/13/13	0/3/3/3
3	M4R	D	503	-	-	5/13/13/13	0/3/3/3
3	M4R	B	503	-	-	8/13/13/13	0/3/3/3
4	BTB	C	504	8	-	4/21/21/21	-
2	HEM	C	501	1	-	0/6/54/54	-
4	BTB	A	505	-	-	6/21/21/21	-
4	BTB	C	505	-	-	3/21/21/21	-
6	GOL	A	508	-	-	2/4/4/4	-
3	M4R	D	502	-	-	3/13/13/13	0/3/3/3
3	M4R	C	502	-	-	7/13/13/13	0/3/3/3
3	M4R	C	503	-	-	8/13/13/13	0/3/3/3
2	HEM	B	501	1	-	1/6/54/54	-
4	BTB	D	504	8	-	4/21/21/21	-
4	BTB	D	506	-	-	8/21/21/21	-
4	BTB	B	506	-	-	3/21/21/21	-
3	M4R	A	502	-	-	3/13/13/13	0/3/3/3
4	BTB	D	505	-	-	4/21/21/21	-
6	GOL	C	508	-	-	4/4/4/4	-
2	HEM	D	501	1	-	0/6/54/54	-
4	BTB	B	504	8	-	3/21/21/21	-
2	HEM	A	501	1	-	3/6/54/54	-
4	BTB	D	507	-	-	8/21/21/21	-
3	M4R	A	503	-	-	3/13/13/13	0/3/3/3
4	BTB	A	504	8	-	8/21/21/21	-
4	BTB	B	505	-	-	7/21/21/21	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	M4R	C23-C27	-7.13	1.28	1.44
3	D	502	M4R	C23-C27	-7.01	1.29	1.44
3	B	502	M4R	C23-C27	-6.89	1.29	1.44
3	A	502	M4R	C23-C27	-6.84	1.29	1.44
3	A	503	M4R	C23-C27	-6.76	1.29	1.44
3	C	503	M4R	C23-C27	-6.75	1.29	1.44
3	D	503	M4R	C23-C27	-6.71	1.29	1.44
3	B	503	M4R	C23-C27	-6.45	1.30	1.44
2	C	501	HEM	C3D-C2D	5.60	1.54	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3D-C2D	5.47	1.53	1.37
2	D	501	HEM	C3D-C2D	5.27	1.53	1.37
2	B	501	HEM	C3D-C2D	4.88	1.52	1.37
2	A	501	HEM	C3B-C2B	-4.57	1.34	1.40
2	B	501	HEM	C3B-C2B	-4.42	1.34	1.40
2	C	501	HEM	C3B-C2B	-4.13	1.34	1.40
2	B	501	HEM	C3C-CAC	3.97	1.55	1.47
2	D	501	HEM	C3B-C2B	-3.93	1.34	1.40
2	D	501	HEM	C3C-CAC	3.89	1.55	1.47
2	B	501	HEM	C3C-C2C	-3.86	1.35	1.40
2	A	501	HEM	C3C-CAC	3.85	1.55	1.47
2	B	501	HEM	C3B-CAB	3.74	1.55	1.47
2	C	501	HEM	C3B-CAB	3.59	1.55	1.47
2	D	501	HEM	C3B-CAB	3.51	1.55	1.47
2	C	501	HEM	C3C-CAC	3.48	1.54	1.47
2	D	501	HEM	C3C-C2C	-3.47	1.35	1.40
2	A	501	HEM	C3B-CAB	3.40	1.54	1.47
2	A	501	HEM	C3C-C2C	-3.27	1.35	1.40
2	C	501	HEM	C3C-C2C	-2.89	1.36	1.40
3	C	503	M4R	C02-N01	2.41	1.36	1.33
2	D	501	HEM	CMA-C3A	2.39	1.56	1.51
3	B	503	M4R	C09-C10	-2.32	1.38	1.41
3	A	503	M4R	C02-N01	2.26	1.36	1.33
3	A	502	M4R	C05-C10	-2.18	1.38	1.42
2	C	501	HEM	CMC-C2C	2.10	1.56	1.51
3	B	502	M4R	C09-C10	-2.02	1.38	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	CAD-CBD-CGD	-4.82	104.58	112.67
2	D	501	HEM	CAD-CBD-CGD	-4.68	104.81	112.67
3	A	503	M4R	C04-C05-C10	3.70	120.02	118.01
2	D	501	HEM	CBA-CAA-C2A	-3.70	105.67	112.49
2	C	501	HEM	CBD-CAD-C3D	-3.51	106.01	112.48
3	C	503	M4R	C04-C05-C10	3.44	119.88	118.01
3	C	502	M4R	C04-C05-C10	3.19	119.74	118.01
3	D	503	M4R	C05-C10-N01	-3.15	119.47	122.81
2	B	501	HEM	C1D-C2D-C3D	-2.94	104.95	107.00
2	C	501	HEM	C1D-C2D-C3D	-2.89	104.98	107.00
2	A	501	HEM	CBA-CAA-C2A	-2.88	107.18	112.49
3	C	502	M4R	C05-C10-N01	-2.85	119.79	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	CMC-C2C-C3C	2.83	129.97	124.68
3	D	502	M4R	C04-C05-C10	2.83	119.54	118.01
2	B	501	HEM	CAA-CBA-CGA	-2.80	107.97	112.67
4	A	504	BTB	O3-C3-C2	-2.78	103.81	111.44
3	D	502	M4R	C05-C10-N01	-2.78	119.87	122.81
3	C	503	M4R	N02-C02-N01	2.77	120.55	118.26
3	A	503	M4R	C05-C10-N01	-2.77	119.87	122.81
3	D	502	M4R	C12-O13-C21	2.62	124.12	117.65
3	B	503	M4R	C12-C08-C09	-2.62	115.49	121.22
3	C	503	M4R	C05-C10-N01	-2.59	120.06	122.81
3	D	503	M4R	C04-C05-C10	2.53	119.38	118.01
3	B	502	M4R	C04-C05-C10	2.50	119.36	118.01
2	B	501	HEM	CBA-CAA-C2A	-2.46	107.95	112.49
3	A	502	M4R	C05-C10-N01	-2.45	120.21	122.81
2	A	501	HEM	CMC-C2C-C3C	2.45	129.26	124.68
2	D	501	HEM	CMB-C2B-C3B	2.41	129.19	124.68
3	A	502	M4R	N02-C02-N01	2.40	120.25	118.26
2	D	501	HEM	CMC-C2C-C3C	2.27	128.93	124.68
3	D	502	M4R	C25-C29-C30	2.22	117.36	113.39
2	C	501	HEM	CBA-CAA-C2A	-2.18	108.47	112.49
3	A	503	M4R	C06-C05-C04	-2.16	119.53	123.66
3	C	502	M4R	C29-C25-C26	2.16	124.14	120.44
3	C	503	M4R	C06-C05-C04	-2.15	119.55	123.66
2	B	501	HEM	CMA-C3A-C4A	-2.15	125.16	128.46
3	A	502	M4R	C04-C05-C10	2.15	119.17	118.01
3	A	502	M4R	C03-C04-C05	2.13	119.87	117.78
3	B	502	M4R	C08-C09-C10	-2.10	119.23	121.08
2	D	501	HEM	C1D-C2D-C3D	-2.09	105.54	107.00
3	D	502	M4R	C29-C25-C26	2.06	123.97	120.44
3	B	502	M4R	C05-C10-N01	-2.05	120.63	122.81
2	B	501	HEM	CMC-C2C-C3C	2.05	128.51	124.68
2	A	501	HEM	CAD-CBD-CGD	-2.02	109.28	112.67
3	C	503	M4R	C12-O13-C21	2.01	122.61	117.65
3	C	503	M4R	C06-C05-C10	2.01	120.57	118.33
3	D	502	M4R	C29-C25-C24	-2.00	117.00	120.44

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	M4R	C25-C29-C30-C31
4	C	504	BTB	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	C	504	BTB	O1-C1-C2-C4
4	C	504	BTB	O1-C1-C2-N
4	A	505	BTB	C3-C2-C4-O4
4	C	505	BTB	O1-C1-C2-C3
4	C	505	BTB	O1-C1-C2-C4
4	C	505	BTB	O1-C1-C2-N
3	C	503	M4R	C25-C29-C30-C31
3	C	503	M4R	C25-C29-C30-N32
2	B	501	HEM	C3D-CAD-CBD-CGD
4	D	504	BTB	O1-C1-C2-C4
4	D	504	BTB	O1-C1-C2-N
4	D	506	BTB	C1-C2-C4-O4
4	D	506	BTB	C3-C2-C4-O4
4	B	506	BTB	C1-C2-C3-O3
4	B	506	BTB	C4-C2-C3-O3
4	B	506	BTB	N-C2-C3-O3
4	D	505	BTB	O1-C1-C2-C3
6	C	508	GOL	O1-C1-C2-C3
4	B	504	BTB	O1-C1-C2-C4
2	A	501	HEM	C2D-C3D-CAD-CBD
2	A	501	HEM	C4D-C3D-CAD-CBD
2	A	501	HEM	C3D-CAD-CBD-CGD
4	D	507	BTB	O1-C1-C2-C3
4	D	507	BTB	O1-C1-C2-C4
4	D	507	BTB	O1-C1-C2-N
4	D	507	BTB	C1-C2-C3-O3
4	D	507	BTB	C4-C2-C3-O3
4	D	507	BTB	N-C2-C3-O3
3	A	503	M4R	C25-C29-C30-C31
3	A	503	M4R	C25-C29-C30-N32
4	A	504	BTB	O1-C1-C2-C3
4	A	504	BTB	O1-C1-C2-C4
4	A	504	BTB	O1-C1-C2-N
4	A	504	BTB	C4-C2-C3-O3
4	A	504	BTB	N-C2-C3-O3
4	B	505	BTB	C1-C2-C3-O3
4	B	505	BTB	C4-C2-C3-O3
4	B	505	BTB	N-C2-C3-O3
4	B	505	BTB	C1-C2-C4-O4
4	B	505	BTB	C3-C2-C4-O4
4	B	505	BTB	N-C2-C4-O4
4	D	504	BTB	N-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
3	B	503	M4R	C22-C21-O13-C12
3	B	503	M4R	C26-C21-O13-C12
3	A	502	M4R	C26-C21-O13-C12
4	C	504	BTB	N-C5-C6-O6
3	A	502	M4R	C22-C21-O13-C12
3	B	502	M4R	C26-C21-O13-C12
3	C	502	M4R	C22-C21-O13-C12
3	B	502	M4R	C22-C21-O13-C12
4	A	504	BTB	N-C5-C6-O6
3	C	502	M4R	C26-C21-O13-C12
6	A	508	GOL	O1-C1-C2-C3
6	C	508	GOL	O1-C1-C2-O2
3	D	503	M4R	C31-C30-N32-C33
4	A	504	BTB	N-C7-C8-O8
3	B	503	M4R	C25-C29-C30-N32
3	B	502	M4R	C29-C30-N32-C33
3	D	503	M4R	C29-C30-N32-C33
3	B	503	M4R	C29-C30-N32-C33
3	D	502	M4R	C29-C30-N32-C33
3	D	502	M4R	C24-C25-C29-C30
3	D	502	M4R	C26-C25-C29-C30
6	A	508	GOL	O1-C1-C2-O2
3	C	502	M4R	C26-C25-C29-C30
3	C	502	M4R	C24-C25-C29-C30
3	C	503	M4R	C22-C21-O13-C12
4	A	505	BTB	N-C7-C8-O8
3	C	503	M4R	C26-C21-O13-C12
4	D	506	BTB	N-C5-C6-O6
3	D	503	M4R	C22-C21-O13-C12
4	D	507	BTB	N-C7-C8-O8
3	B	502	M4R	C24-C25-C29-C30
3	B	502	M4R	C26-C25-C29-C30
3	A	502	M4R	C31-C30-N32-C33
3	C	502	M4R	C08-C12-O13-C21
3	D	503	M4R	C26-C21-O13-C12
4	B	505	BTB	N-C5-C6-O6
6	C	508	GOL	O2-C2-C3-O3
4	D	504	BTB	O1-C1-C2-C3
4	D	505	BTB	O1-C1-C2-C4
4	B	504	BTB	O1-C1-C2-C3
4	A	504	BTB	C1-C2-C3-O3
3	C	503	M4R	C24-C25-C29-C30

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Mol	Chain	Res	Type	Atoms
3	C	503	M4R	C29-C30-N32-C33
4	A	505	BTB	N-C2-C4-O4
4	D	506	BTB	N-C2-C4-O4
4	D	506	BTB	C1-C2-N-C5
4	D	506	BTB	C1-C2-N-C7
4	D	506	BTB	C3-C2-N-C5
4	D	506	BTB	C4-C2-N-C7
4	D	505	BTB	O1-C1-C2-N
4	B	504	BTB	O1-C1-C2-N
4	D	507	BTB	N-C2-C4-O4
3	C	503	M4R	C26-C25-C29-C30
4	D	505	BTB	N-C5-C6-O6
3	B	503	M4R	C24-C25-C29-C30
3	A	503	M4R	C29-C30-N32-C33
3	B	503	M4R	C31-C30-N32-C33
3	C	502	M4R	C31-C30-N32-C33
3	D	503	M4R	C25-C29-C30-N32
3	B	503	M4R	C26-C25-C29-C30
6	C	508	GOL	C1-C2-C3-O3
4	A	505	BTB	O1-C1-C2-C3
4	A	505	BTB	O1-C1-C2-C4
4	A	505	BTB	C1-C2-C4-O4
3	C	503	M4R	C31-C30-N32-C33
3	C	502	M4R	C29-C30-N32-C33

There are no ring outliers.

21 monomers are involved in 57 short contacts:

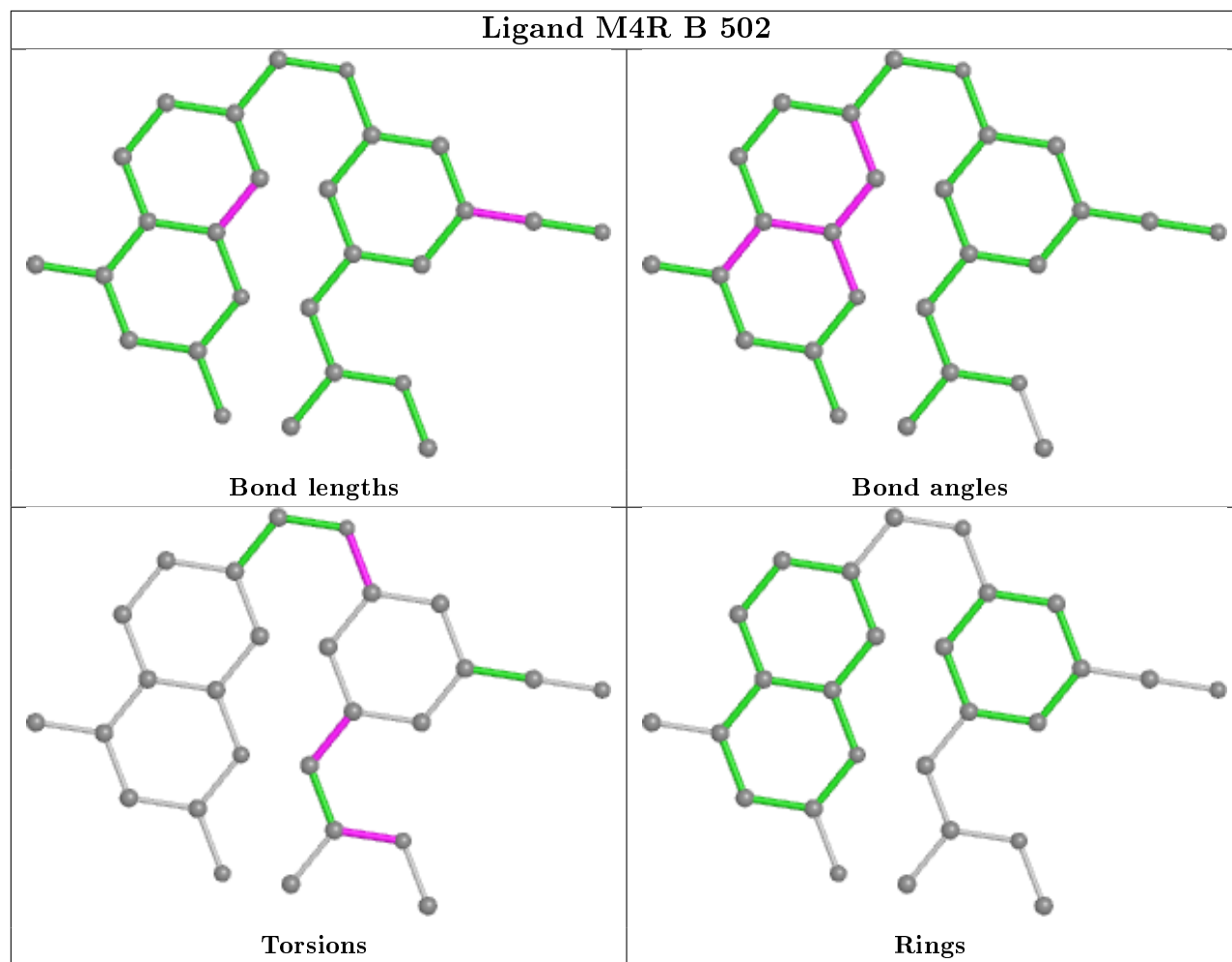
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	M4R	2	0
3	D	503	M4R	1	0
3	B	503	M4R	1	0
4	C	504	BTB	3	0
2	C	501	HEM	5	0
4	A	505	BTB	2	0
4	C	505	BTB	1	0
3	D	502	M4R	3	0
3	C	502	M4R	3	0
3	C	503	M4R	1	0
2	B	501	HEM	4	0
4	D	504	BTB	3	0
4	D	506	BTB	4	0

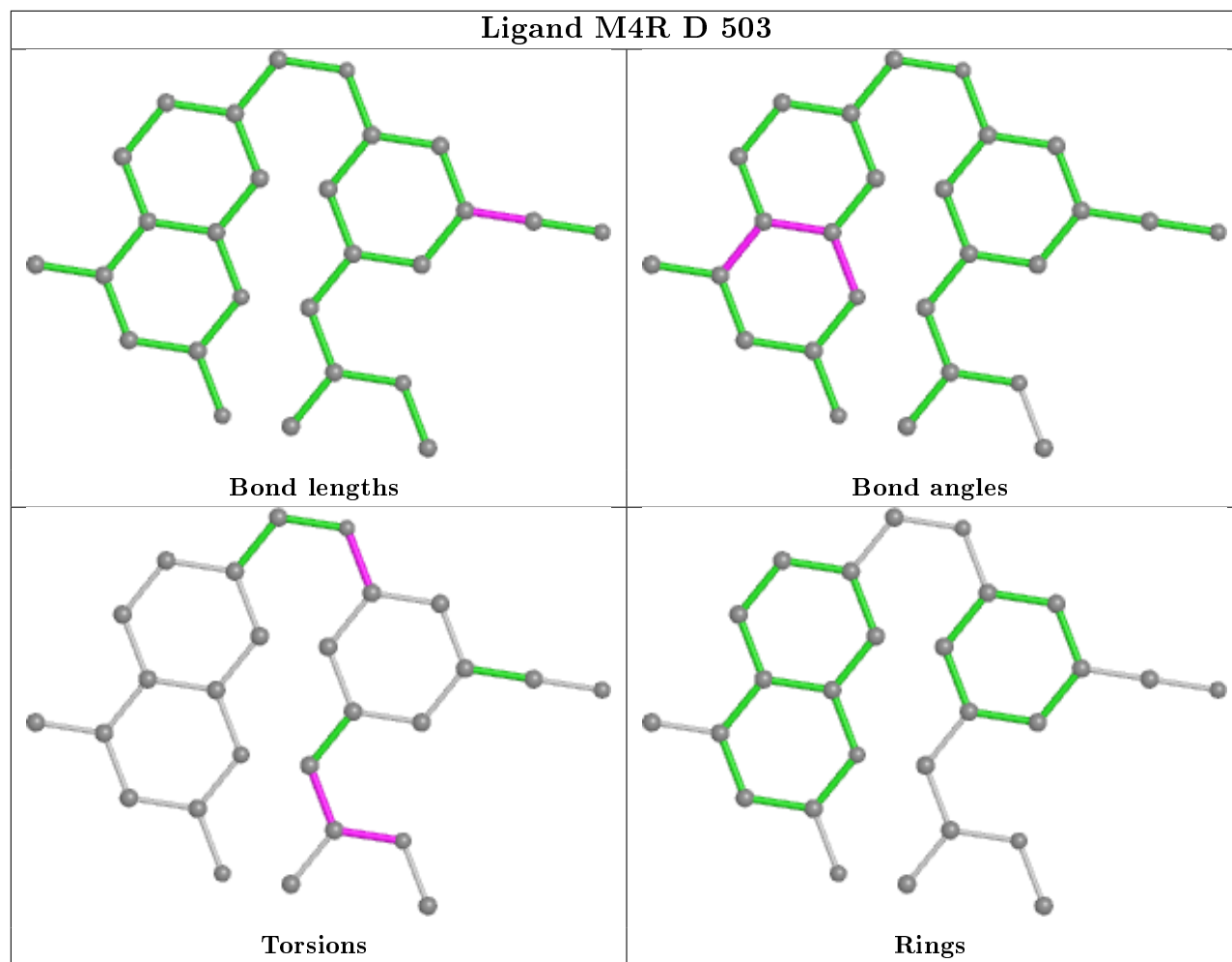
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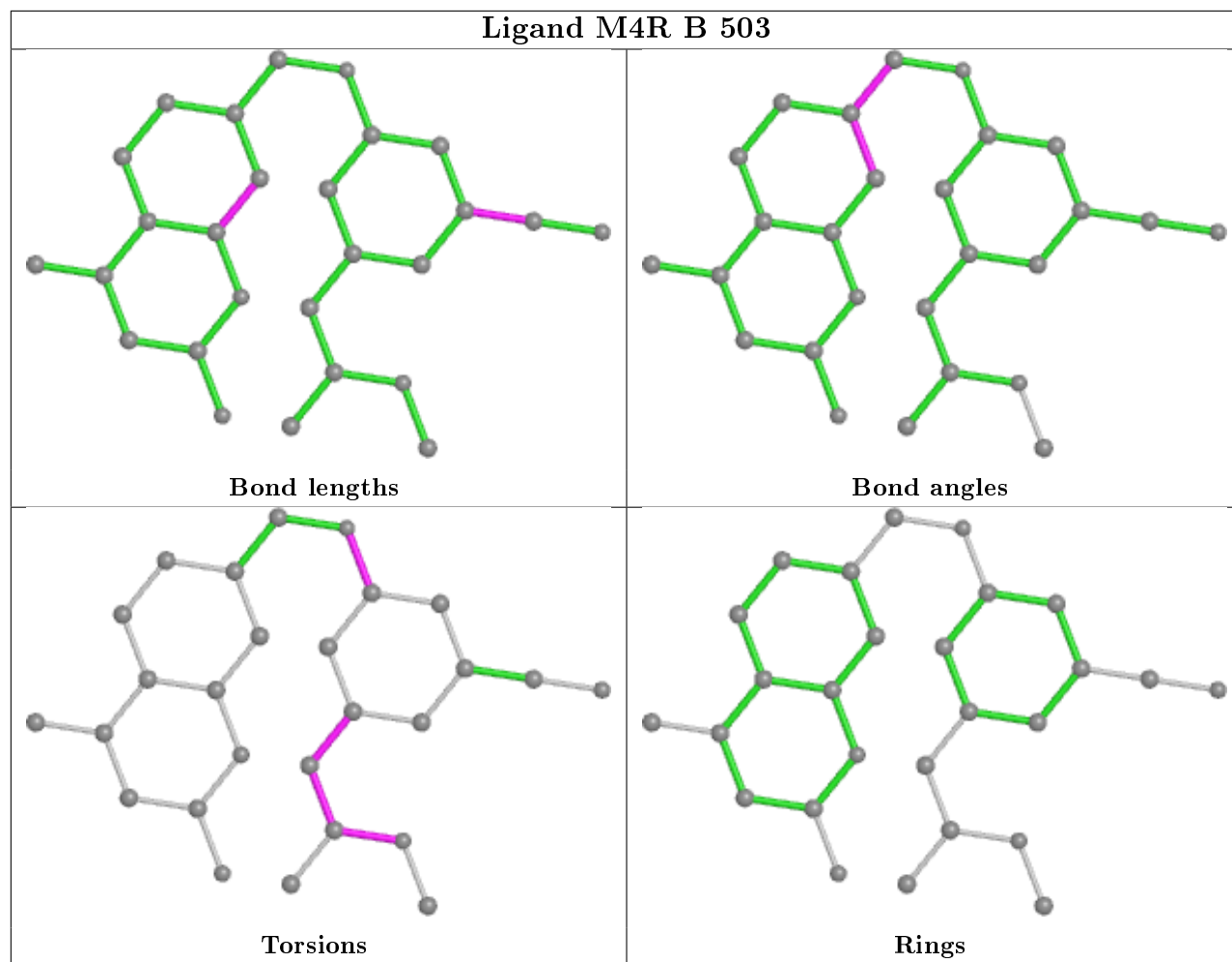
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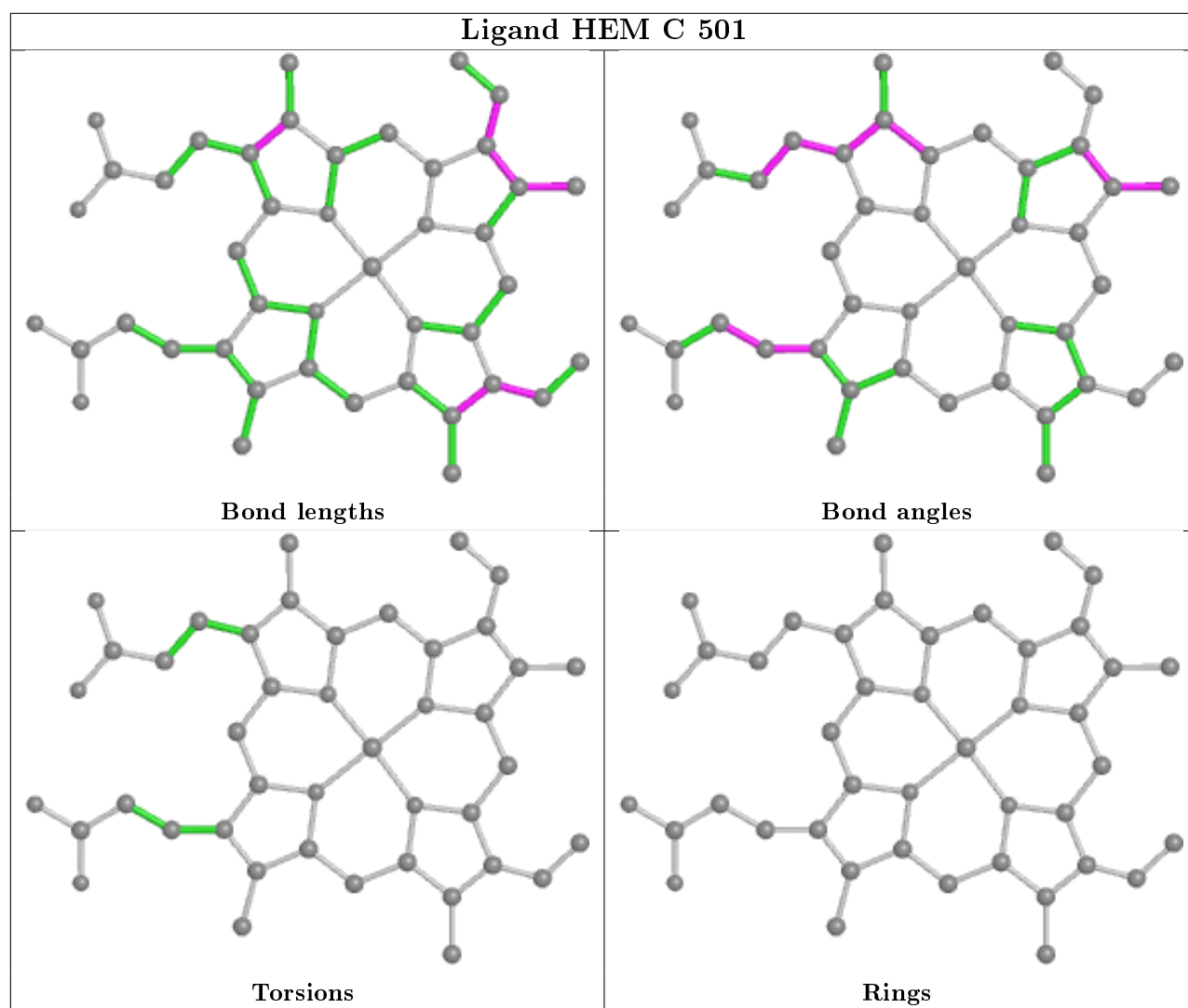
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	506	BTB	1	0
3	A	502	M4R	1	0
4	D	505	BTB	7	1
2	D	501	HEM	4	0
4	B	504	BTB	2	0
2	A	501	HEM	4	0
4	D	507	BTB	2	0
4	A	504	BTB	3	0

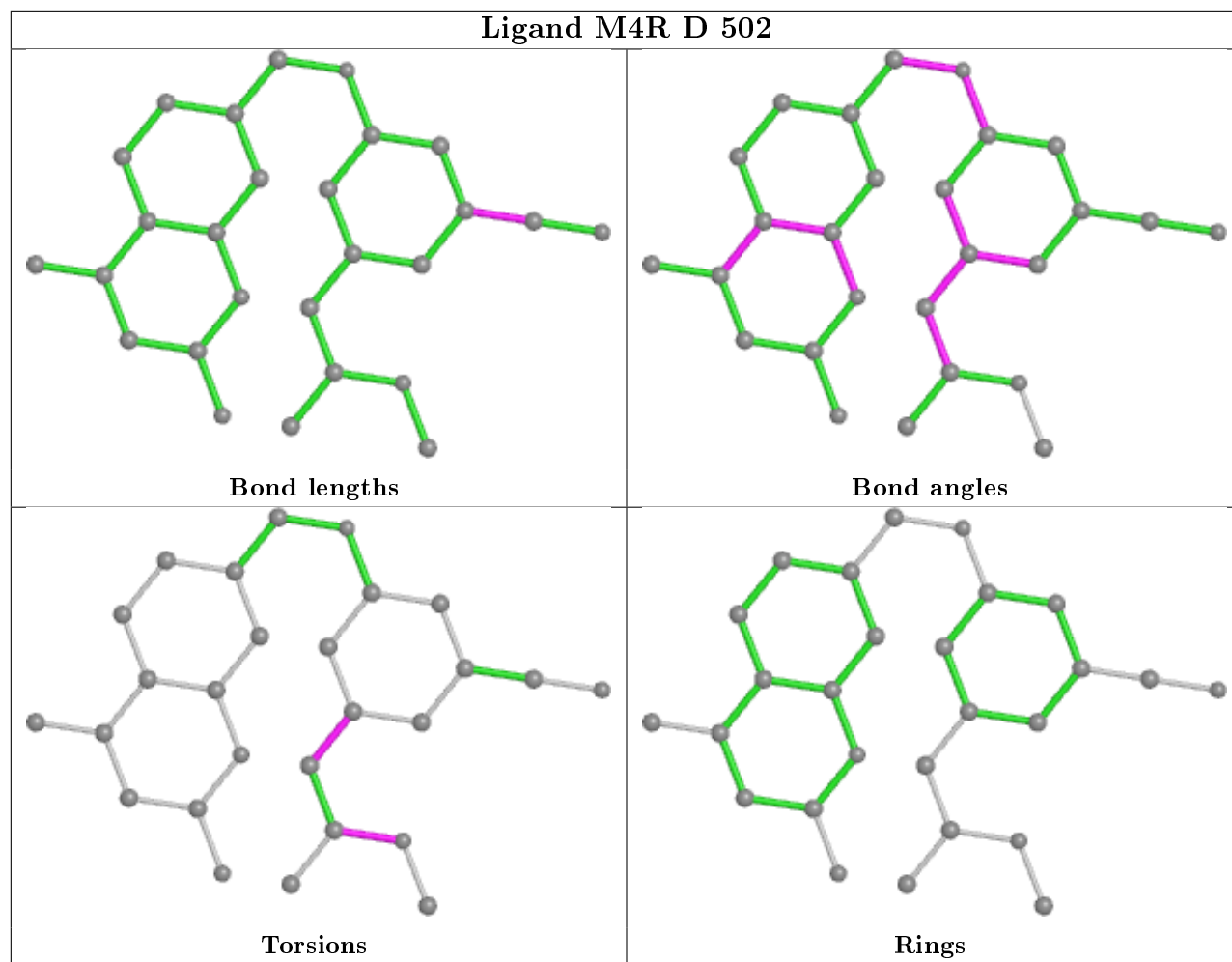
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

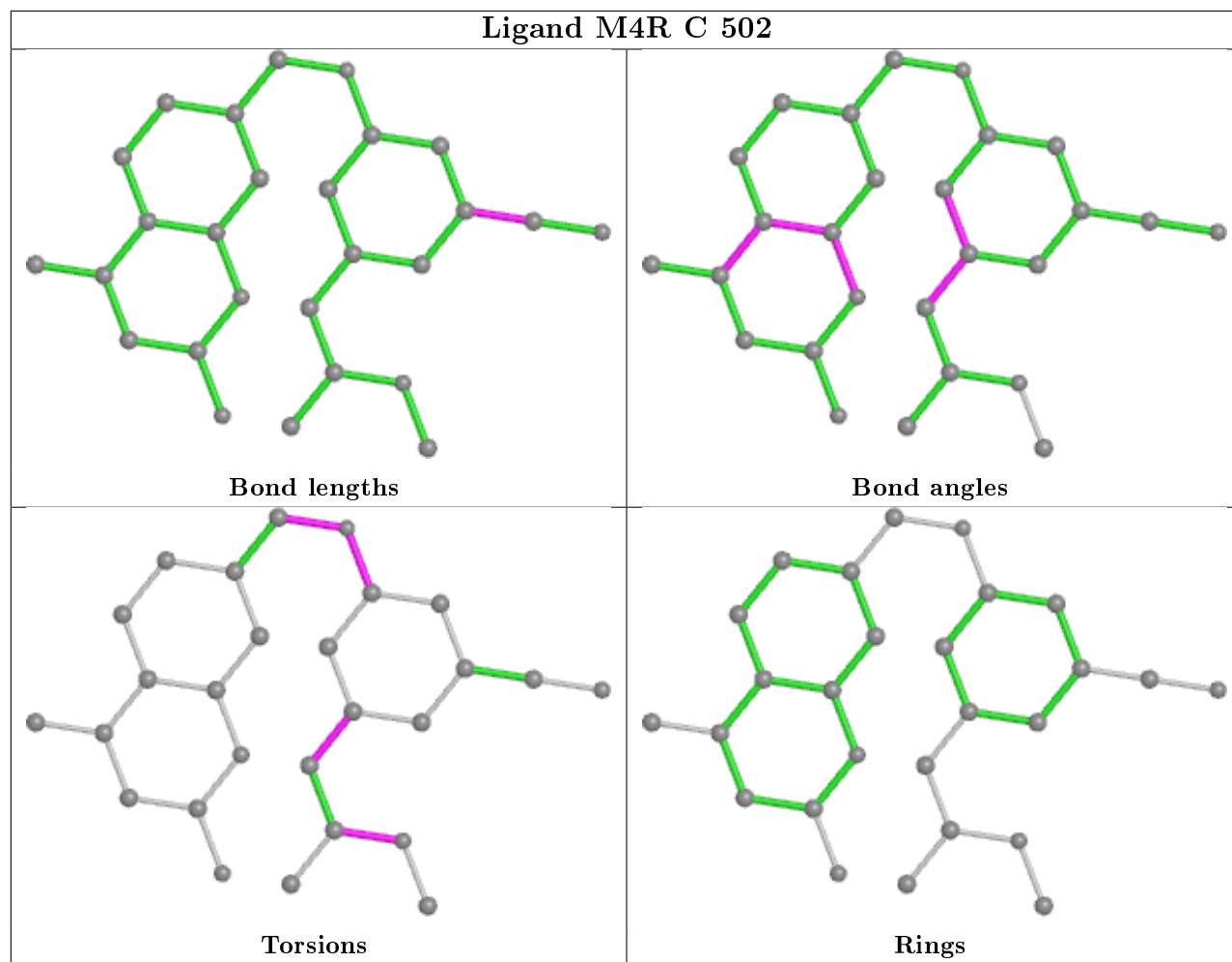


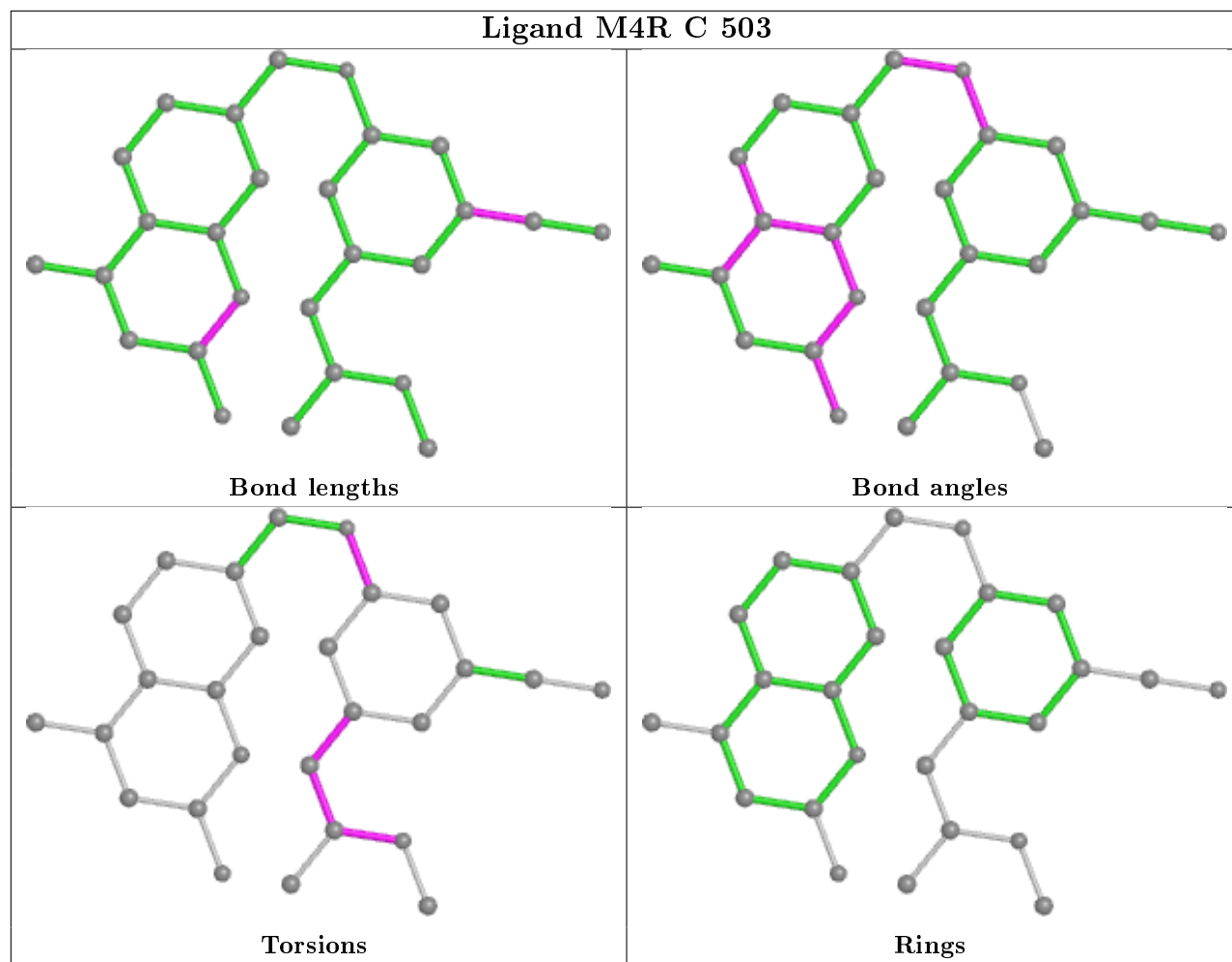


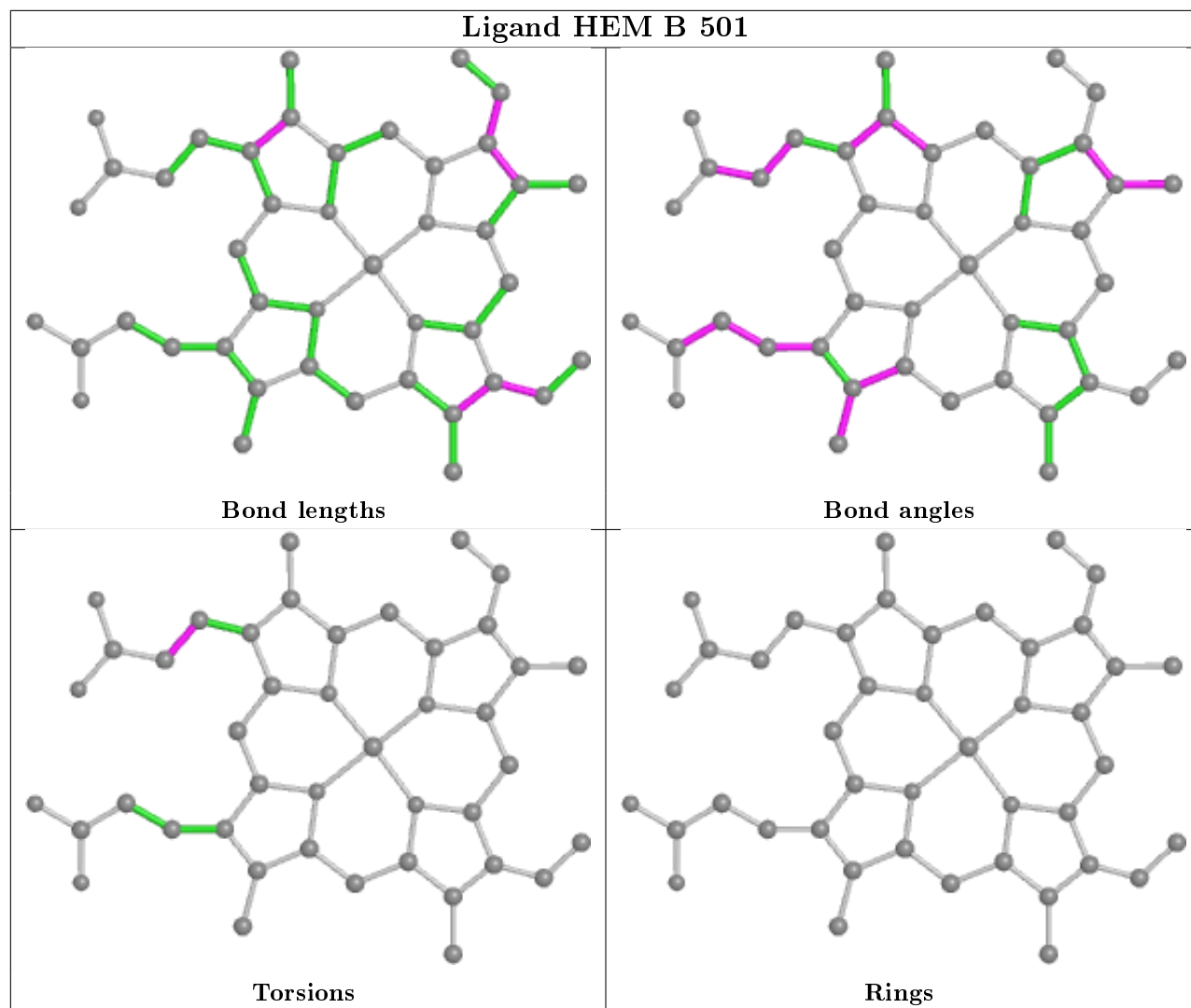


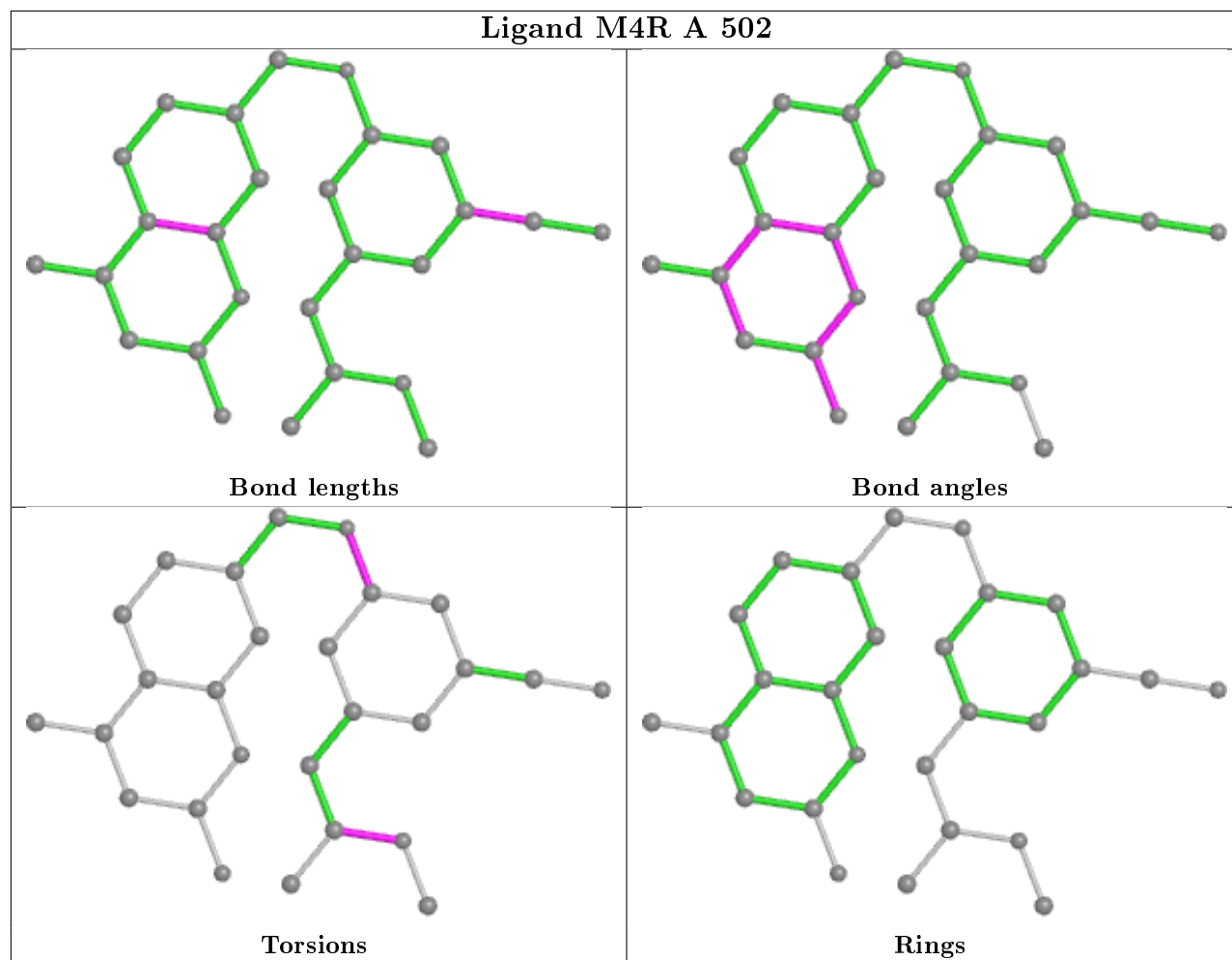


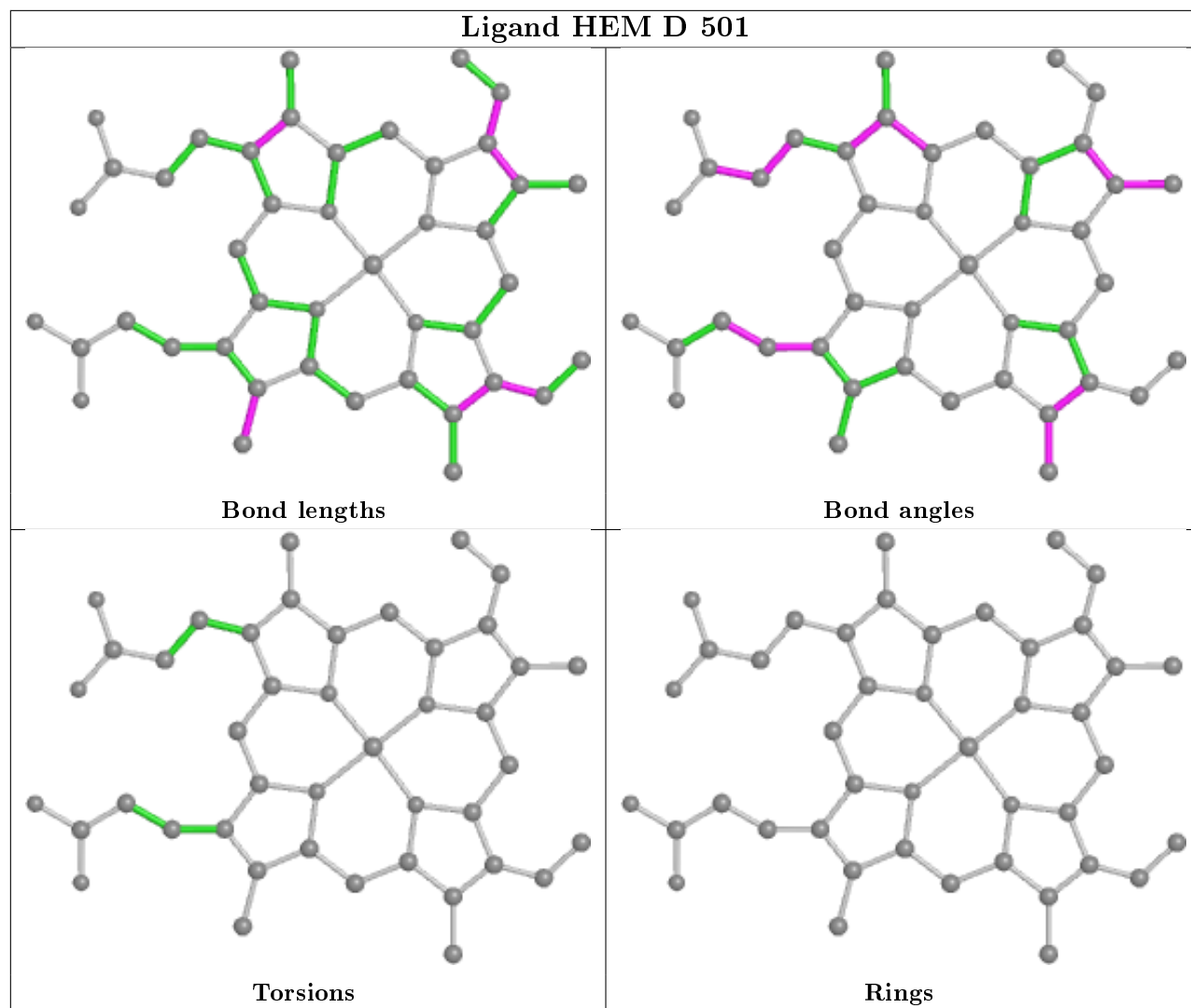


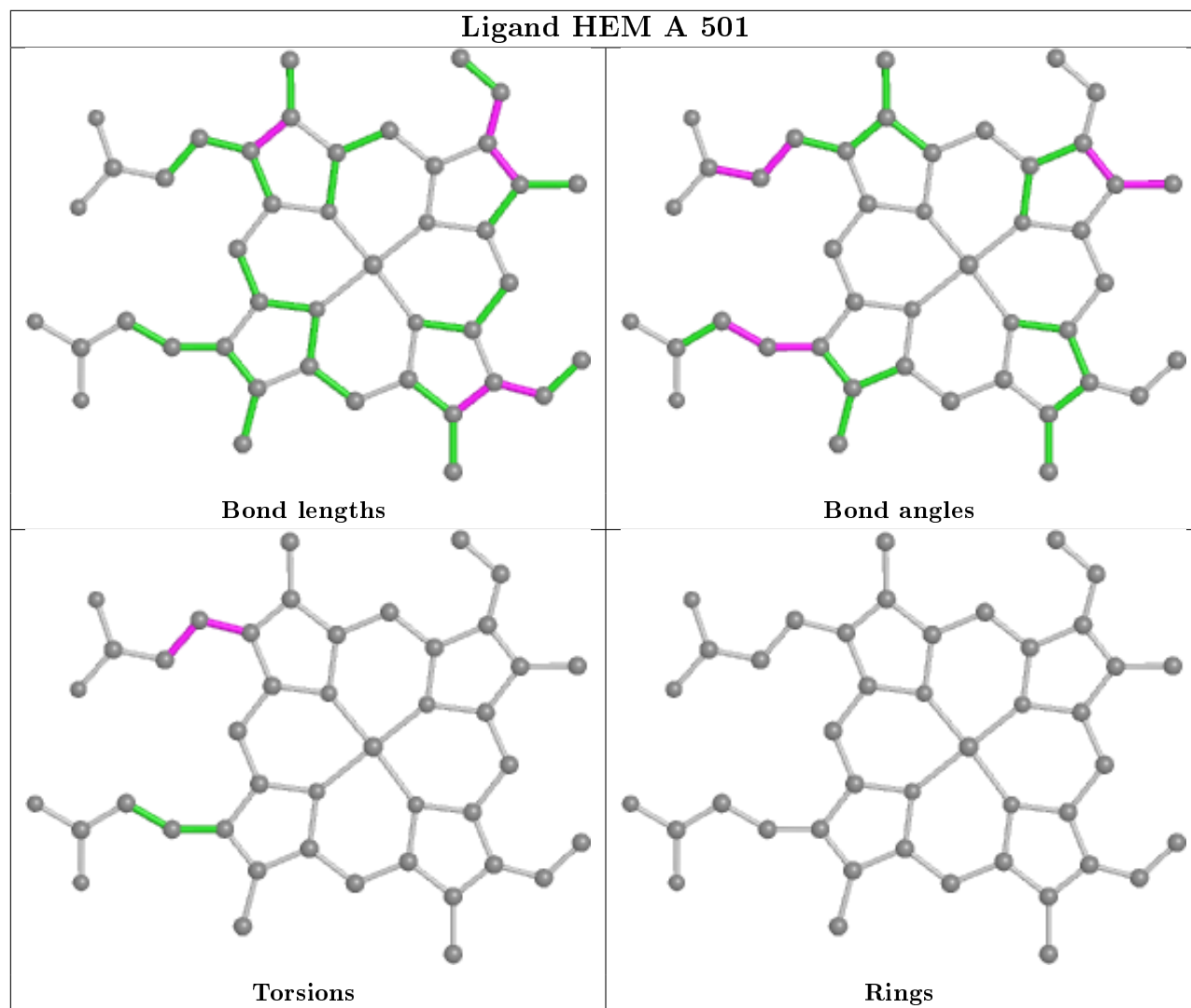


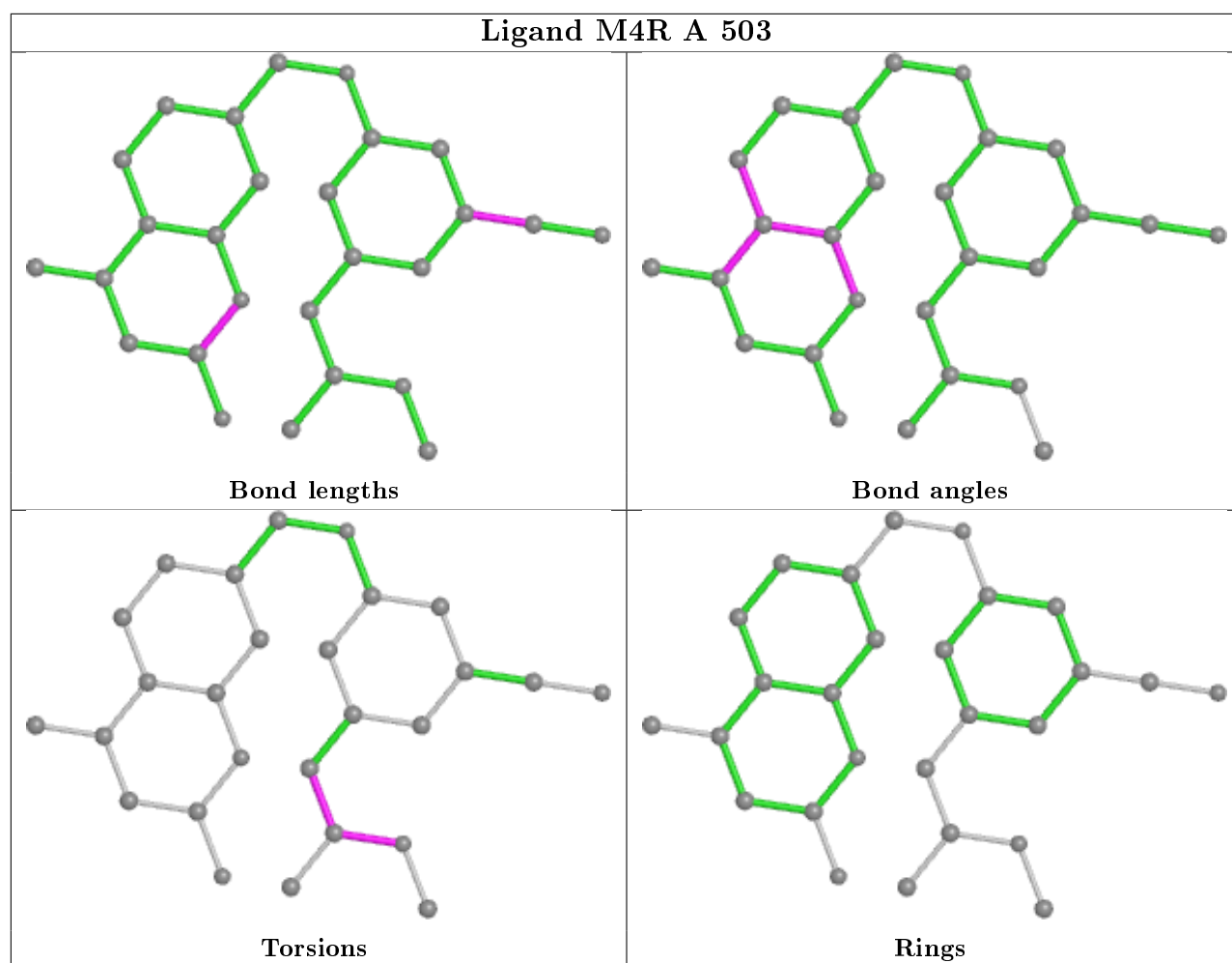












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	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, 141	0
All	All	1609/1760 (91%)	0.77	172 (10%) 6 8	35, 61, 114, 159	0

All (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
1	A	346	LEU	6.7
1	A	158	ALA	6.4
1	D	138	ILE	6.4
1	A	165	LEU	6.1
1	C	300	PRO	5.8
1	D	143	SER	5.5
1	A	161	GLY	5.5
1	A	68	PHE	5.2
1	A	275	ILE	4.8
1	B	89	GLN	4.8
1	D	139	LYS	4.7
1	C	299	PRO	4.7
1	A	301	GLU	4.7
1	A	109	LEU	4.6
1	B	144	GLN	4.6
1	A	174	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	196	PHE	4.5
1	A	292	LEU	4.4
1	A	163	TYR	4.3
1	B	140	ARG	4.3
1	C	259	GLY	4.1
1	D	154	GLU	4.1
1	D	124	LEU	4.1
1	C	238	ARG	4.0
1	D	259	GLY	3.9
1	A	153	VAL	3.9
1	C	89	GLN	3.9
1	C	297	ASP	3.8
1	D	145	ALA	3.8
1	A	259	GLY	3.7
1	A	293	LEU	3.7
1	D	169	GLU	3.7
1	A	171	VAL	3.7
1	B	255	ARG	3.7
1	A	159	ALA	3.6
1	A	131	ILE	3.6
1	B	241	PHE	3.5
1	D	140	ARG	3.5
1	D	153	VAL	3.5
1	A	90	GLN	3.5
1	A	295	ALA	3.4
1	C	271	THR	3.4
1	D	163	TYR	3.4
1	D	125	SER	3.4
1	C	275	ILE	3.3
1	C	304	LEU	3.3
1	D	130	PHE	3.3
1	D	144	GLN	3.2
1	A	162	THR	3.2
1	C	468	PHE	3.2
1	A	472	ALA	3.2
1	A	123	LEU	3.2
1	A	309	LEU	3.2
1	A	157	VAL	3.1
1	D	141[A]	SER	3.1
1	A	480	TRP	3.1
1	D	129	ASP	3.1
1	A	145	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	248	LEU	3.1
1	A	120	PRO	3.1
1	C	103	LEU	3.1
1	C	273	LEU	3.0
1	A	227	ALA	3.0
1	B	468	PHE	3.0
1	A	84	LEU	3.0
1	A	124	LEU	3.0
1	D	90	GLN	3.0
1	A	150	LEU	3.0
1	C	216	LYS	3.0
1	A	134	TYR	2.9
1	A	173	GLY	2.9
1	B	238	ARG	2.9
1	A	195	VAL	2.9
1	D	468	PHE	2.9
1	A	294	GLN	2.9
1	B	124	LEU	2.9
1	A	208	PHE	2.8
1	C	241	PHE	2.8
1	D	238	ARG	2.8
1	B	90	GLN	2.8
1	C	260	SER	2.8
1	C	281	PRO	2.8
1	D	121	GLU	2.8
1	D	196	PHE	2.8
1	D	87	GLN	2.8
1	C	171	VAL	2.8
1	A	238	ARG	2.8
1	C	272	GLU	2.8
1	A	216	LYS	2.7
1	D	275	ILE	2.7
1	A	341	LEU	2.7
1	A	343	ILE	2.7
1	C	283	ASN	2.7
1	C	293	LEU	2.7
1	A	170	LEU	2.7
1	D	120	PRO	2.6
1	C	153	VAL	2.6
1	C	303	PHE	2.6
1	D	128	ARG	2.6
1	A	69	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	123	LEU	2.5
1	A	285	ARG	2.5
1	B	141[A]	SER	2.5
1	A	349	PRO	2.5
1	A	286	PHE	2.5
1	D	165	LEU	2.5
1	D	268	VAL	2.5
1	A	258	ASP	2.5
1	D	79	ILE	2.5
1	B	165	LEU	2.5
1	A	146	HIS	2.5
1	A	160	THR	2.5
1	D	148	GLN	2.5
1	A	119	ALA	2.4
1	D	151	GLN	2.4
1	D	295	ALA	2.4
1	C	208	PHE	2.4
1	A	156	GLU	2.4
1	B	228	ILE	2.4
1	B	68	PHE	2.4
1	A	279	TRP	2.4
1	A	193	LEU	2.4
1	C	161	GLY	2.3
1	C	291	LEU	2.3
1	C	230	VAL	2.3
1	A	239	GLY	2.3
1	C	257	GLN	2.3
1	C	280	THR	2.3
1	D	475	TYR	2.3
1	D	202	ARG	2.3
1	B	303	PHE	2.3
1	D	195	VAL	2.3
1	B	139	LYS	2.3
1	B	308	GLU	2.2
1	A	210	TYR	2.2
1	A	283	ASN	2.2
1	A	148	GLN	2.2
1	C	157	VAL	2.2
1	C	329	ARG	2.2
1	B	273	LEU	2.2
1	D	229	THR	2.2
1	A	89	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	90	GLN	2.2
1	C	131	ILE	2.1
1	B	309	LEU	2.1
1	C	203	SER	2.1
1	C	101	GLY	2.1
1	A	299	PRO	2.1
1	C	165	LEU	2.1
1	A	100	LEU	2.1
1	C	163	TYR	2.1
1	C	295	ALA	2.1
1	A	348	PHE	2.1
1	C	480	TRP	2.1
1	D	127	ALA	2.1
1	A	310	VAL	2.1
1	A	215	ILE	2.1
1	D	291	LEU	2.1
1	A	154	GLU	2.1
1	D	326	LEU	2.0
1	A	345	GLY	2.0
1	B	231	PHE	2.0
1	D	100	LEU	2.0
1	A	127	ALA	2.0
1	A	347	GLU	2.0
1	D	452	ILE	2.0
1	A	439	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

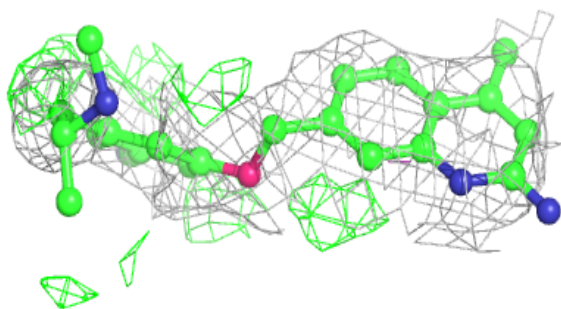
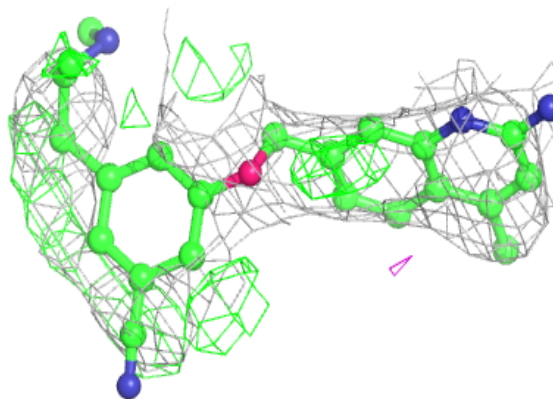
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\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	A	503	27/27	0.88	0.21	43,61,88,90	0
3	M4R	B	503	27/27	0.88	0.21	41,56,85,94	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
6	GOL	A	508	6/6	0.92	0.27	77,87,89,91	0
4	BTB	C	504	14/14	0.92	0.27	95,107,111,112	0
3	M4R	C	503	27/27	0.93	0.24	49,69,92,93	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
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	B	507	1/1	0.95	0.06	47,47,47,47	0
7	CL	D	509	1/1	0.95	0.09	48,48,48,48	0
7	CL	C	509	1/1	0.96	0.05	64,64,64,64	0
2	HEM	C	501	43/43	0.96	0.18	41,54,75,88	0
8	GD	C	510	1/1	0.96	0.19	117,117,117,117	0
2	HEM	A	501	43/43	0.96	0.18	46,56,79,91	0
5	ZN	C	506	1/1	0.96	0.15	50,50,50,50	0
5	ZN	C	507	1/1	0.97	0.12	57,57,57,57	0
2	HEM	B	501	43/43	0.97	0.19	36,46,68,84	0
2	HEM	D	501	43/43	0.97	0.18	32,54,77,86	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

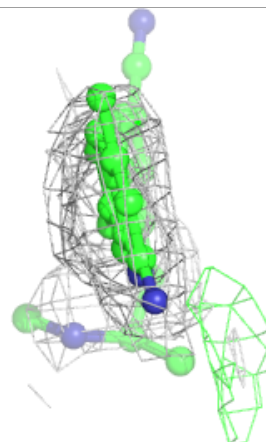
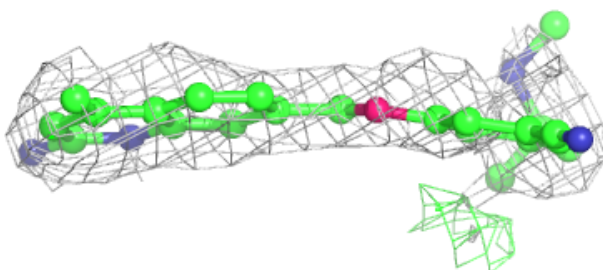
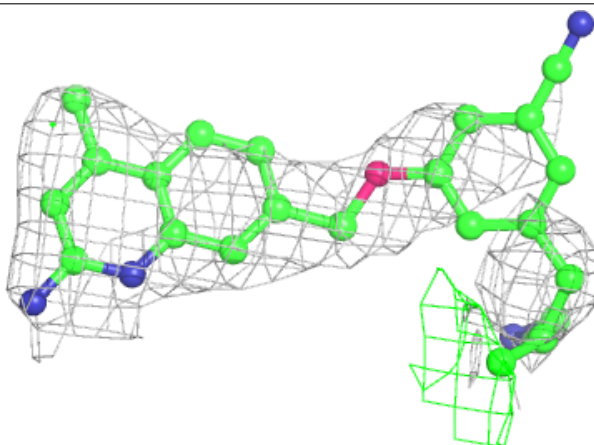
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around M4R C 502:

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

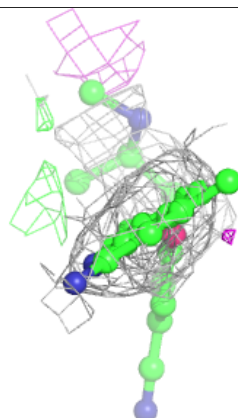
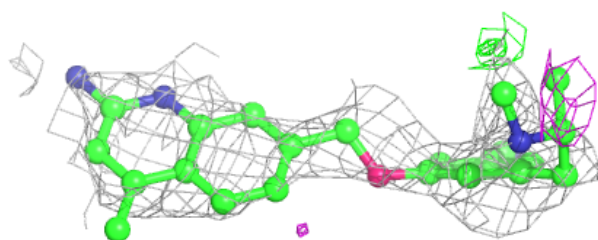
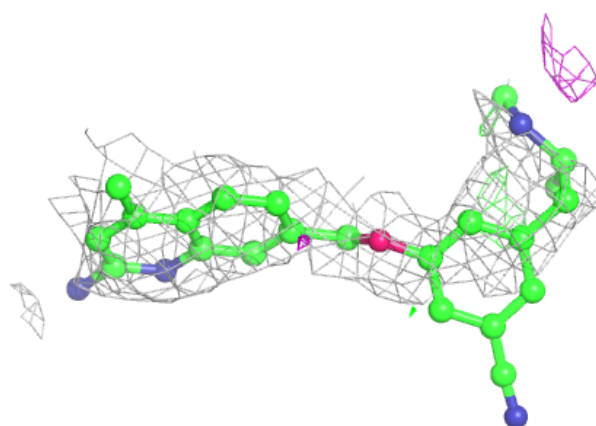
**Electron density around M4R D 502:**

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



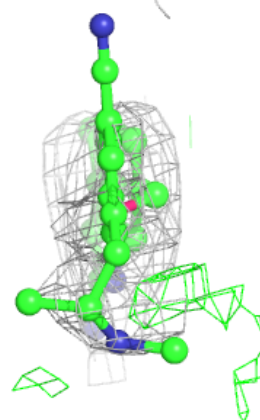
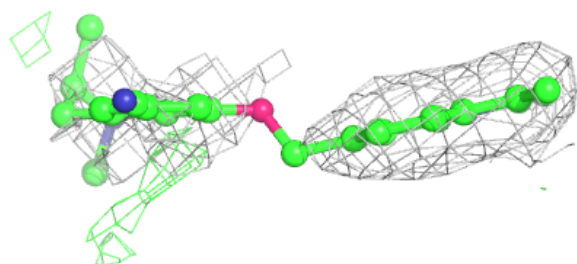
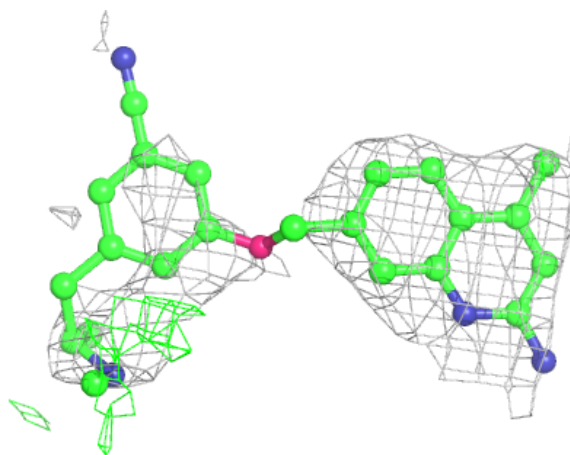
Electron density around M4R A 502:

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



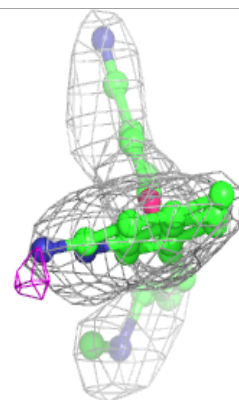
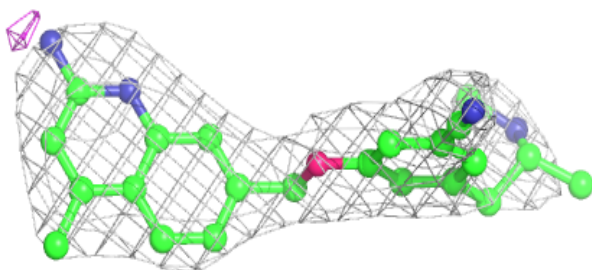
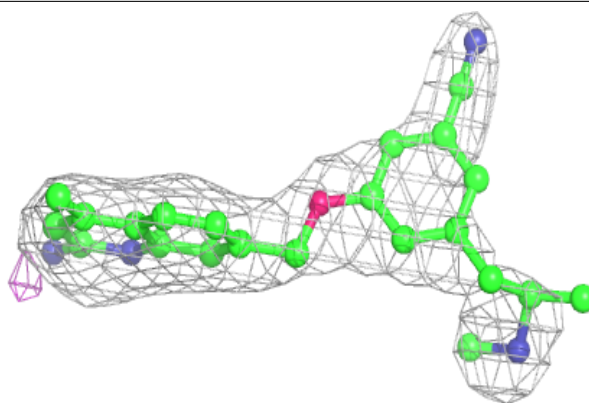
Electron density around M4R B 502:

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

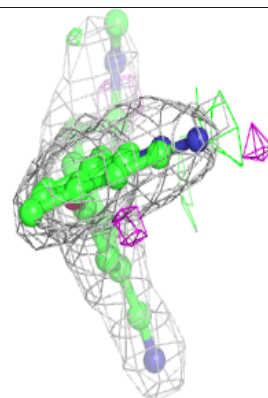
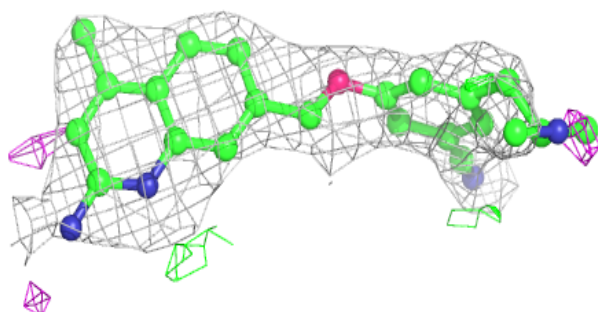
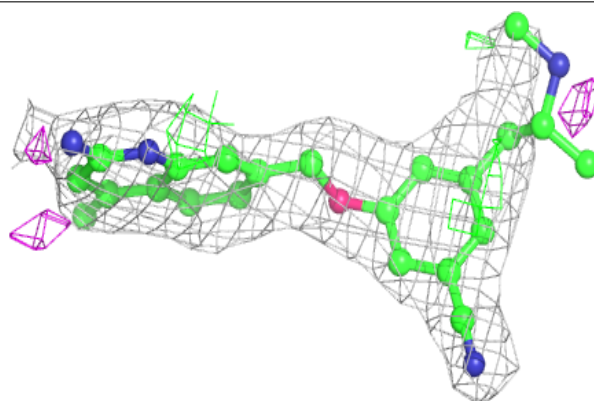


Electron density around M4R A 503:

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

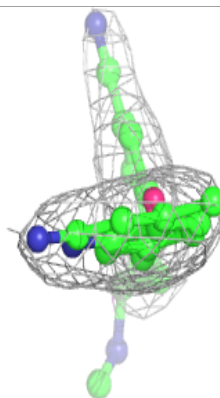
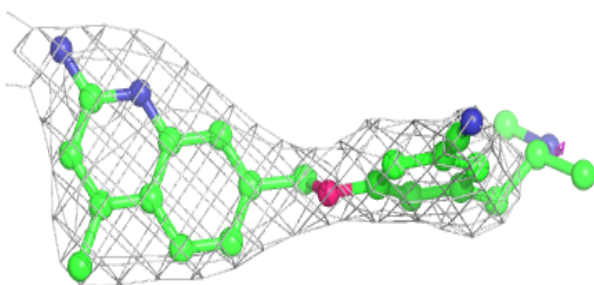
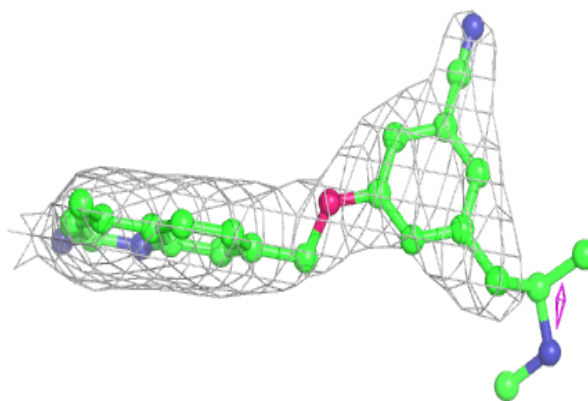
**Electron density around M4R B 503:**

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

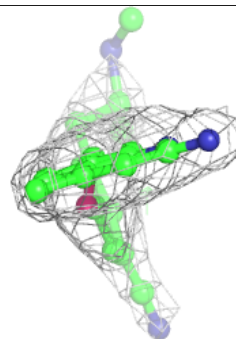
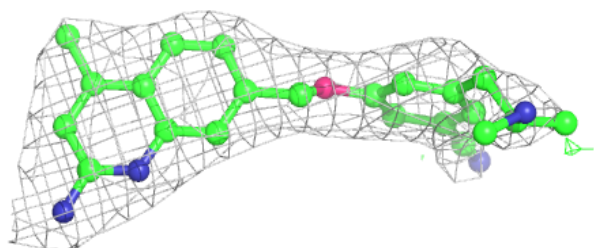
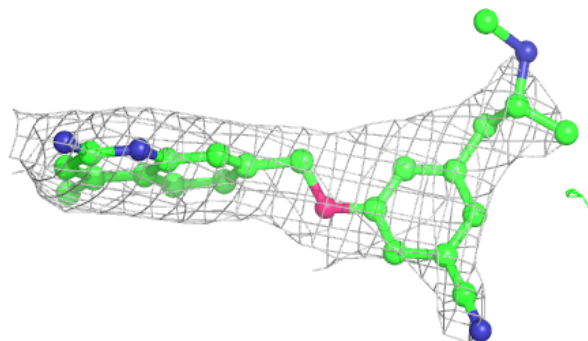


Electron density around M4R C 503:

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

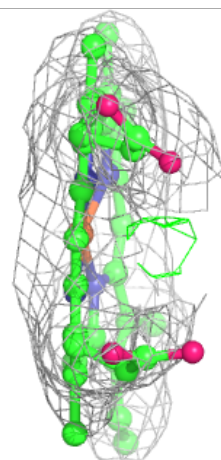
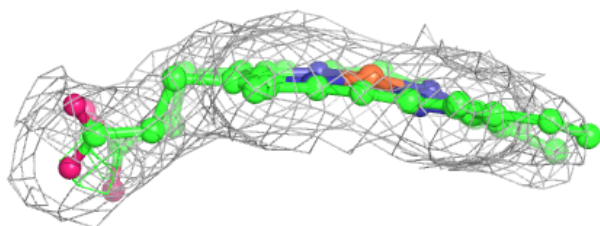
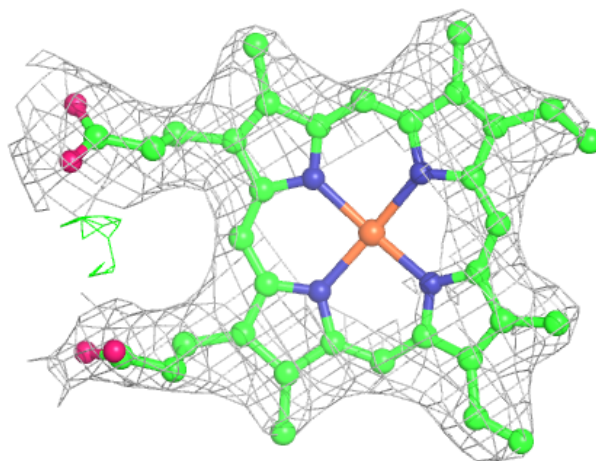
**Electron density around M4R D 503:**

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



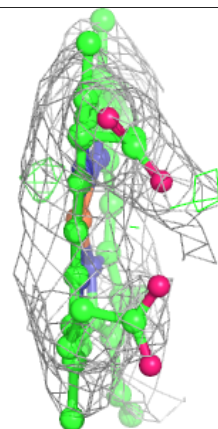
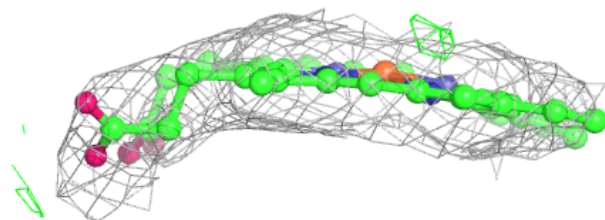
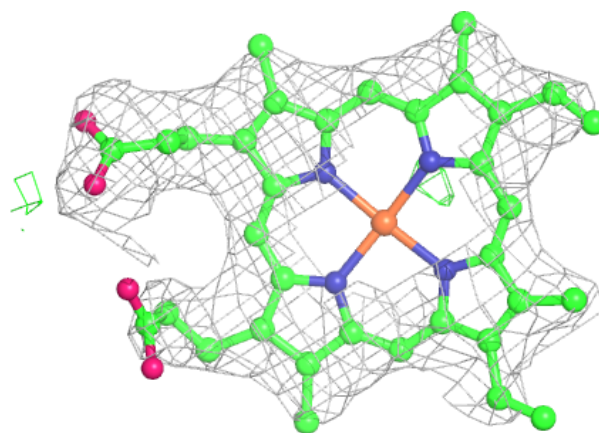
Electron density around HEM C 501:

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



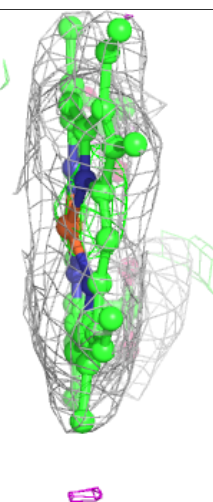
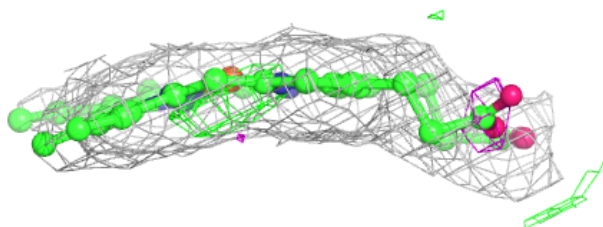
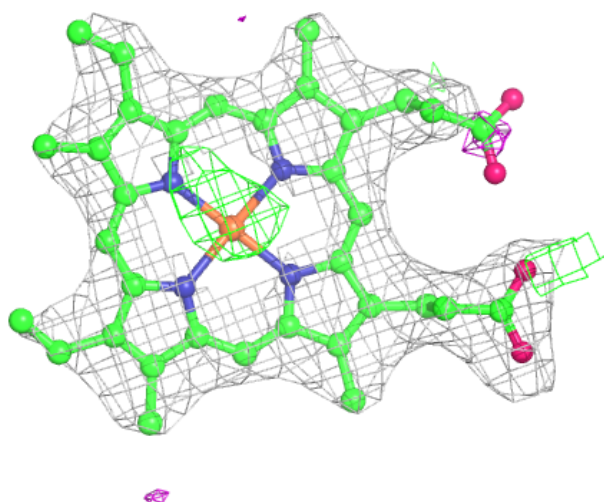
Electron density around HEM A 501:

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



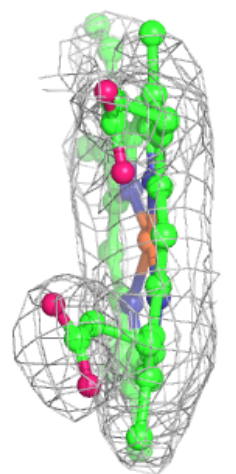
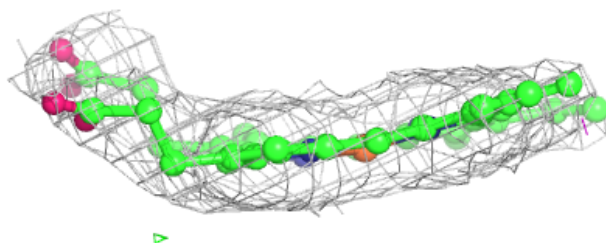
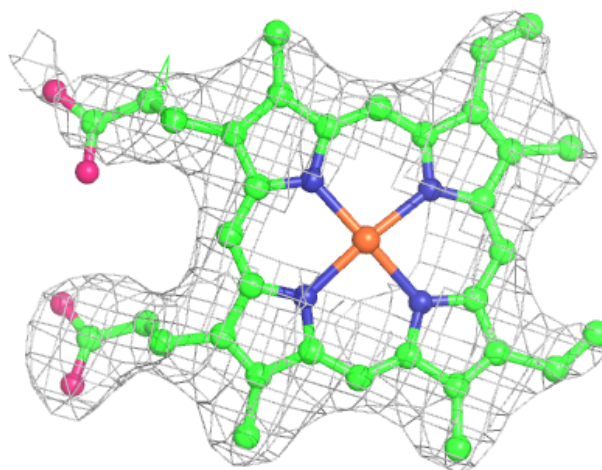
Electron density around HEM B 501:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.