



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:54 PM UTC

PDB ID : 5UOB / pdb_00005uob
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 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)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

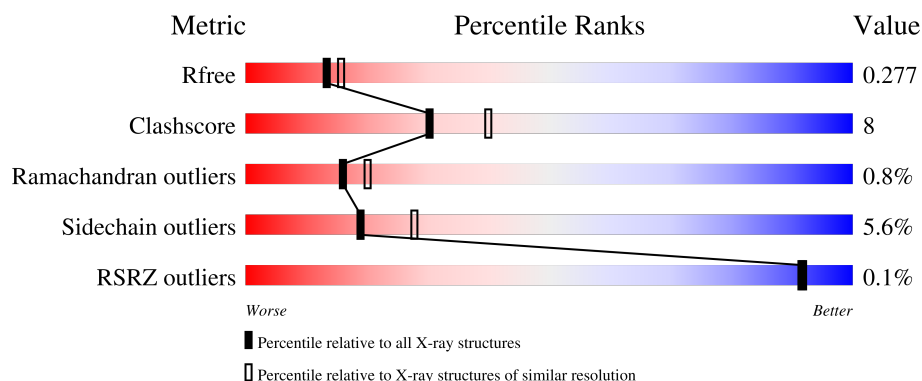
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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	 70% 20% • 8%
1	B	440	 77% 12% • 9%
1	C	440	 70% 20% • 9%
1	D	440	 67% 23% • 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:

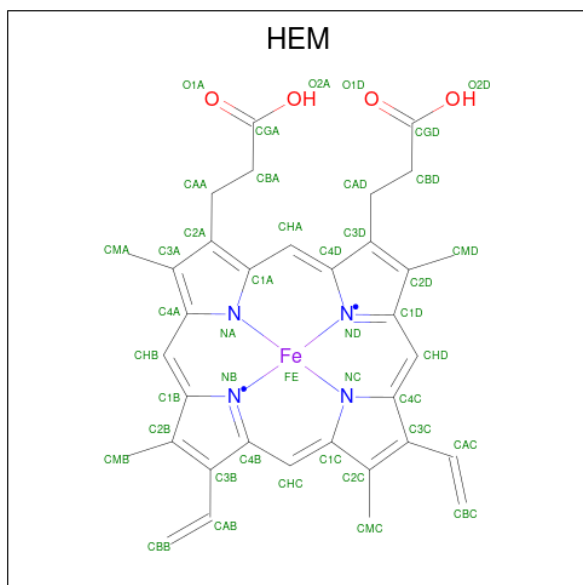
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BTB	D	505	-	-	X	-

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 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 (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



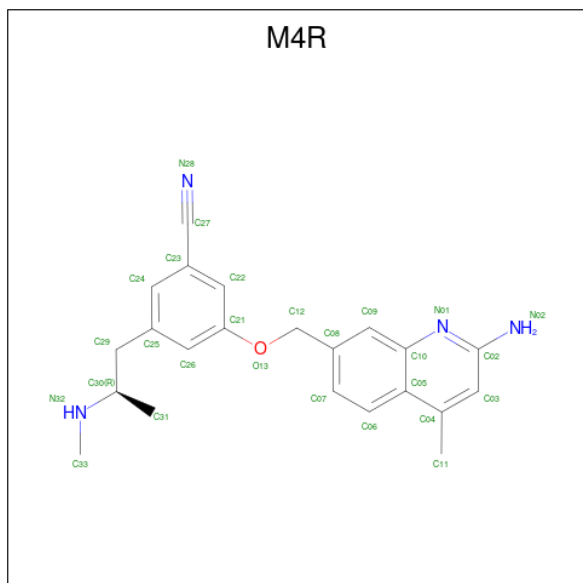
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

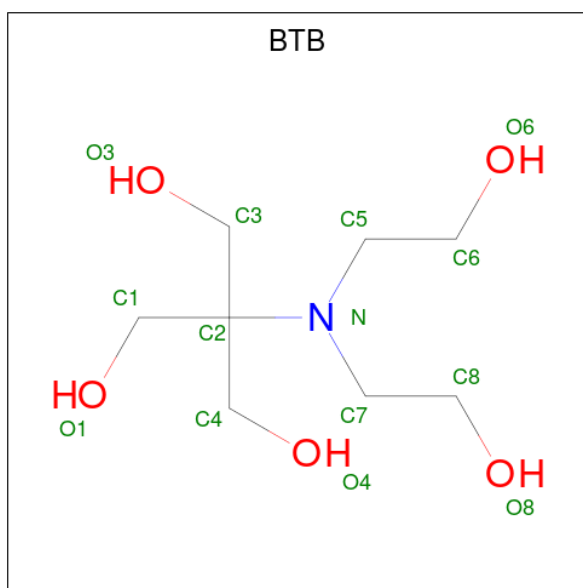
- Molecule 3 is 3-[(2-amino-4-methylquinolin-7-yl)methoxy]-5-[(2R)-2-(methylamino)propyl]benzonitrile (CCD ID: M4R) (formula: C₂₂H₂₄N₄O).



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 (CCD ID: 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 (CCD ID: 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 (CCD ID: 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 (CCD ID: 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 (CCD ID: GD) (formula: Gd).

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

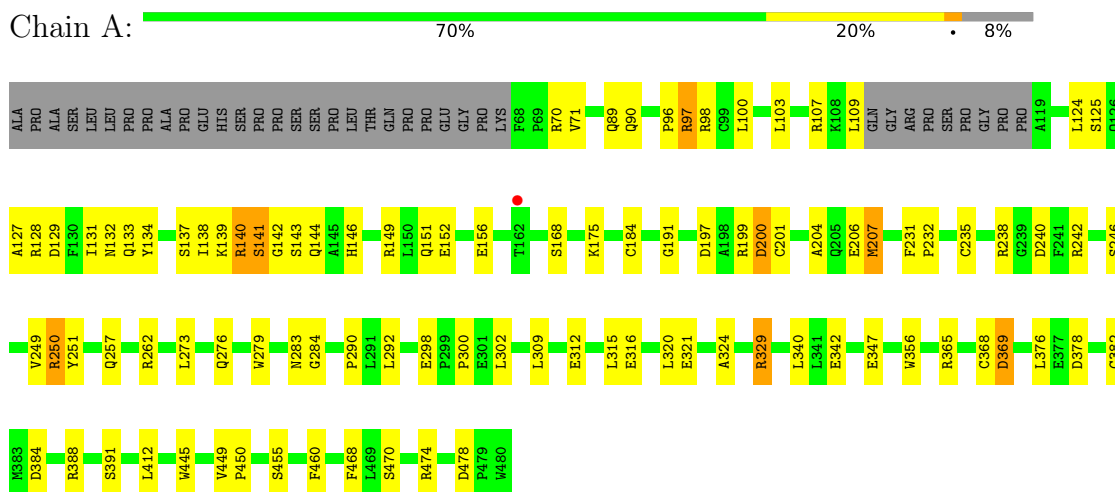
- Molecule 9 is water.

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

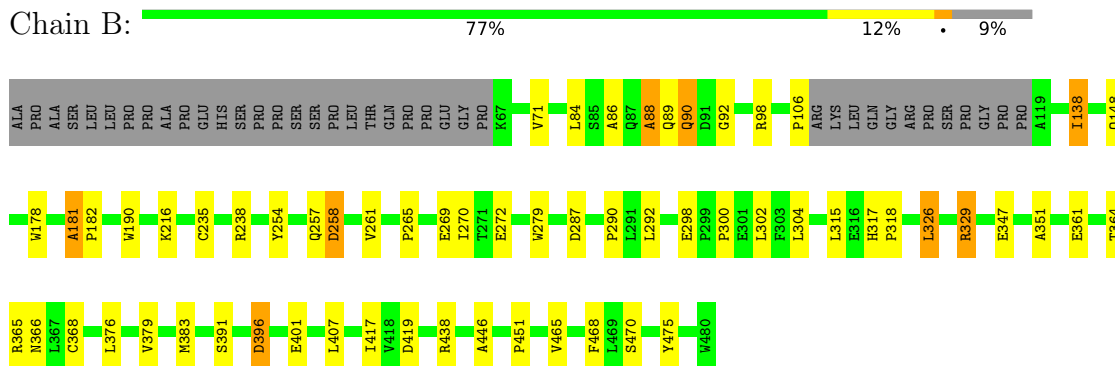
3 Residue-property plots

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

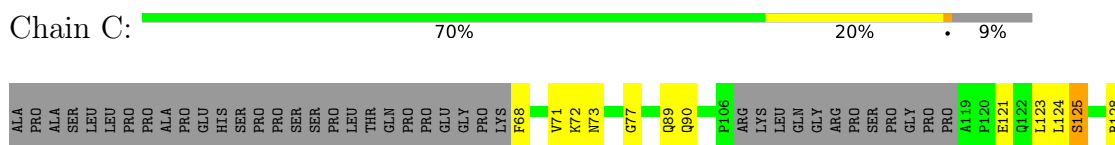
- Molecule 1: Nitric oxide synthase, endothelial

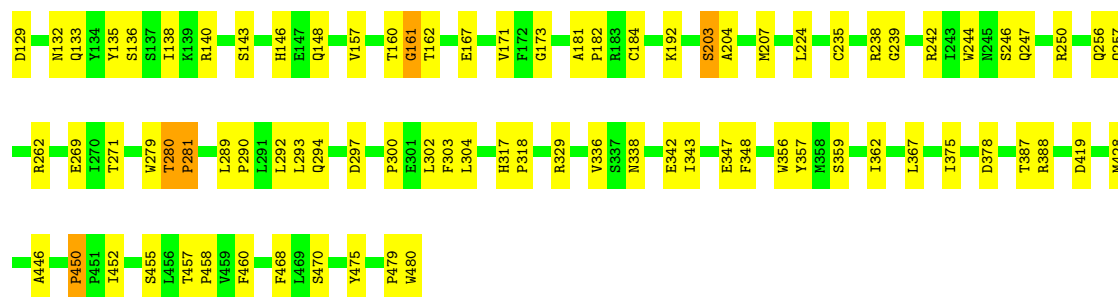


- Molecule 1: Nitric oxide synthase, endothelial



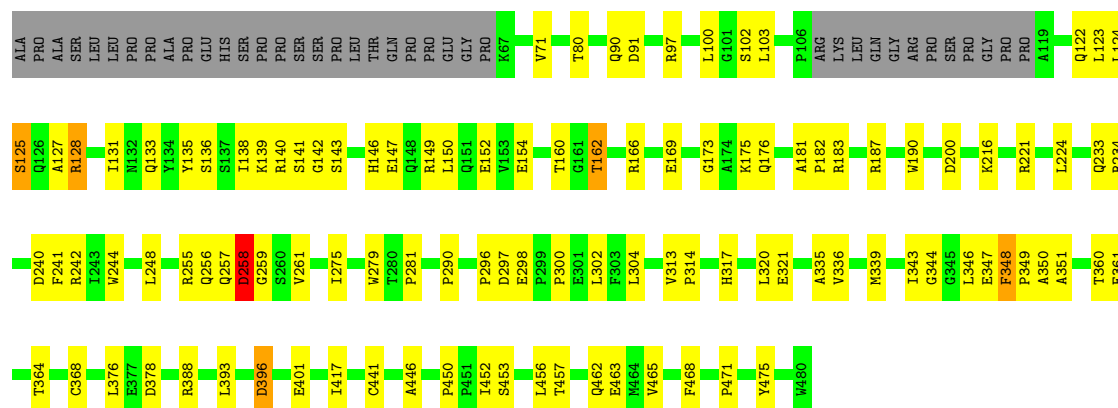
- Molecule 1: Nitric oxide synthase, endothelial





- Molecule 1: Nitric oxide synthase, endothelial

Chain D: 67% 23% 9%



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 38.49 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.1 (38.49-2.29) 95.3 (38.49-2.29)	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 0.221 , 0.277	Depositor DCC
R_{free} test set	4257 reflections (2.24%)	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)	0.34 , 48.6	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	0.96	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, GOL, M4R, GD, BTB, CL, 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	0.49	0/3335	0.85	4/4543 (0.1%)
1	B	0.50	0/3319	0.86	4/4523 (0.1%)
1	C	0.50	0/3301	0.90	9/4499 (0.2%)
1	D	0.55	0/3319	0.93	13/4523 (0.3%)
All	All	0.51	0/13274	0.88	30/18088 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	348	PHE	CA-C-N	6.81	127.09	119.32
1	C	348	PHE	C-N-CA	6.81	127.09	119.32
1	D	259	GLY	N-CA-C	-6.29	106.43	113.79
1	D	91	ASP	N-CA-C	6.17	119.18	110.23
1	B	181	ALA	CA-C-N	6.10	125.99	119.28
1	B	181	ALA	C-N-CA	6.10	125.99	119.28
1	A	369	ASP	CA-C-N	5.86	125.33	119.24
1	A	369	ASP	C-N-CA	5.86	125.33	119.24
1	C	280	THR	CA-C-N	5.62	126.87	119.84
1	C	280	THR	C-N-CA	5.62	126.87	119.84
1	D	457	THR	CA-C-N	5.61	125.32	119.82
1	D	457	THR	C-N-CA	5.61	125.32	119.82
1	D	348	PHE	CA-C-N	5.56	125.40	119.28
1	D	348	PHE	C-N-CA	5.56	125.40	119.28
1	D	450	PRO	O-C-N	5.56	123.87	121.31
1	A	143	SER	CB-CA-C	-5.53	110.18	116.54
1	C	68	PHE	CA-C-N	5.36	126.19	119.98
1	C	68	PHE	C-N-CA	5.36	126.19	119.98
1	D	351	ALA	CA-C-N	5.32	125.57	119.83
1	D	351	ALA	C-N-CA	5.32	125.57	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	338	ASN	N-CA-C	5.30	119.62	113.20
1	C	450	PRO	CA-C-N	5.29	124.95	119.56
1	C	450	PRO	C-N-CA	5.29	124.95	119.56
1	D	224	LEU	N-CA-C	5.24	117.81	109.96
1	A	450	PRO	O-C-N	5.17	123.69	121.31
1	B	351	ALA	CA-C-N	5.11	125.40	119.93
1	B	351	ALA	C-N-CA	5.11	125.40	119.93
1	D	450	PRO	CA-C-N	5.10	125.18	119.87
1	D	450	PRO	C-N-CA	5.10	125.18	119.87
1	D	258	ASP	N-CA-C	-5.09	106.58	112.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3237	0	3146	50	1
1	B	3221	0	3126	36	0
1	C	3206	0	3104	53	0
1	D	3221	0	3126	65	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0
2	C	43	0	30	5	0
2	D	43	0	30	3	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	15	1
5	A	3	0	0	0	0
5	C	3	0	0	0	0
6	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	221	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 (221) 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
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
1:C:342:GLU:OE1	9:C:601:HOH:O	2.09	0.71
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	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:OD1	1:D:258:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HBB2	2:C:501:HEM:HHC	1.81	0.61
1:B:368:CYS:SG	1:B:376:LEU:HD13	2.41	0.61
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	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:HMC2	2:D:501:HEM:HBC2	1.83	0.60
1:A:321:GLU:H	1:A:321:GLU:CD	2.09	0.59
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:HMC2	2:A:501:HEM:HBC2	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:D:138:ILE:C	1:D:140:ARG:H	2.12	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
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:B:254:TYR:OH	1:B:287:ASP:OD2	2.22	0.56
1:D:298:GLU:CD	4:D:506:BTB:H82	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:455:SER:HA	1:A:460:PHE:CG	2.45	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: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:D:139:LYS:C	1:D:141[A]:SER:H	2.19	0.50
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:73:ASN:O	1:C:77:GLY:N	2.36	0.50
1:C:138:ILE:HG13	1:C:140:ARG:HG3	1.93	0.50
4:D:505:BTB:O4	4:D:505:BTB:O1	2.29	0.50
1:A:100:LEU:HD21	1:B:465:VAL:HG22	1.92	0.50
1:D:139:LYS:C	1:D:141[B]:SER:H	2.19	0.50
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:B:257:GLN:H	1:B:257:GLN:CD	2.20	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:475:TYR:OH	2:C:501:HEM:O1D	2.25	0.48
1:C:279:TRP:HB2	1:C:302:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:OD1	1:B:396:ASP:N	2.47	0.47
4:D:506:BTB:H41	4:D:506:BTB:H71	1.41	0.47
4:A:504:BTB:H42	4:A:504:BTB:H71	1.58	0.47
1:A:388:ARG:HH12	1:C:257:GLN:CD	2.20	0.47
1:B:84:LEU:HB2	1:B:438:ARG:O	2.15	0.47
1:A:97:ARG:HH12	1:B:86:ALA:C	2.23	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
4:D:505:BTB:H52	4:D:505:BTB:H11	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:H31	4:C:504:BTB:H52	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:255:ARG:HG3	1:D:261:VAL:HG22	1.98	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
4:D:505:BTB:H42	4:D:505:BTB:H71	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:C:247:GLN:HB2	1:C:250:ARG:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:B:138:ILE:HG12	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:125:SER:OG	4:D:505:BTB:H31	2.17	0.44
1:D:240:ASP:HB3	1:D:349:PRO:HG3	1.99	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:O1	4:D:504:BTB:H52	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:OD1	1:D:396:ASP:N	2.44	0.43
1:A:238:ARG:HH11	1:A:238:ARG:H	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:122:GLN:NE2	4:D:505:BTB:O8	2.48	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: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
4:C:504:BTB:H71	4:C:504:BTB:H42	1.76	0.42
1:A:279:TRP:CE2	1:A:290:PRO:HD3	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:D:123:LEU:HA	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:H42	4:B:504:BTB:H71	1.89	0.41
1:D:128:ARG:HH21	1:D:154:GLU:CD	2.29	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
1:D:143:SER:O	1:D:147:GLU:HG2	2.21	0.40
4:D:504:BTB:H71	4:D:504:BTB:H42	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

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 [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%)	12	15
1	B	401/440 (91%)	379 (94%)	21 (5%)	1 (0%)	43	55
1	C	398/440 (90%)	365 (92%)	29 (7%)	4 (1%)	12	15
1	D	401/440 (91%)	375 (94%)	23 (6%)	3 (1%)	18	23
All	All	1602/1760 (91%)	1486 (93%)	104 (6%)	12 (1%)	16	23

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 [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%)	314 (91%)	31 (9%)	9	12
1	B	344/373 (92%)	328 (95%)	16 (5%)	23	35
1	C	341/373 (91%)	329 (96%)	12 (4%)	32	48
1	D	344/373 (92%)	327 (95%)	17 (5%)	22	34
All	All	1374/1492 (92%)	1298 (94%)	76 (6%)	19	28

All (76) 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	98	ARG
1	A	103	LEU
1	A	107	ARG
1	A	109	LEU
1	A	124	LEU
1	A	129	ASP
1	A	133	GLN
1	A	138	ILE
1	A	140	ARG
1	A	141	SER
1	A	149	ARG
1	A	151	GLN
1	A	168	SER
1	A	200	ASP
1	A	207	MET
1	A	235	CYS
1	A	240	ASP
1	A	242	ARG
1	A	250	ARG
1	A	257	GLN
1	A	302	LEU
1	A	309	LEU
1	A	329	ARG
1	A	391	SER

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Mol	Chain	Res	Type
1	A	412	LEU
1	A	470	SER
1	A	478	ASP
1	B	71	VAL
1	B	89	GLN
1	B	90	GLN
1	B	98	ARG
1	B	138	ILE
1	B	148	GLN
1	B	216	LYS
1	B	258	ASP
1	B	270	ILE
1	B	298	GLU
1	B	326	LEU
1	B	329	ARG
1	B	391	SER
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	387	THR
1	C	452	ILE
1	C	470	SER
1	D	80	THR
1	D	97	ARG
1	D	124	LEU
1	D	125	SER
1	D	128	ARG
1	D	133	GLN
1	D	162	THR
1	D	169	GLU
1	D	216	LYS
1	D	257	GLN
1	D	258	ASP

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Mol	Chain	Res	Type
1	D	297	ASP
1	D	378	ASP
1	D	388	ARG
1	D	393	LEU
1	D	396	ASP
1	D	417	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	151	GLN
1	A	194	GLN
1	A	223	ASN
1	A	277	HIS
1	B	73	ASN
1	C	148	GLN
1	C	205	GLN
1	D	132	ASN
1	D	133	GLN
1	D	176	GLN
1	D	205	GLN
1	D	408	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	HEM	A	501	1	50,50,50	1.99	9 (18%)	67,82,82	1.55	7 (10%)
4	BTB	D	507	-	13,13,13	0.38	0	7,16,16	0.53	0
4	BTB	B	506	-	13,13,13	0.59	0	7,16,16	0.89	0
4	BTB	A	504	8	13,13,13	0.44	0	7,16,16	1.38	1 (14%)
4	BTB	D	505	-	13,13,13	0.42	0	7,16,16	0.69	0
2	HEM	B	501	1	50,50,50	1.95	10 (20%)	67,82,82	1.41	9 (13%)
3	M4R	D	503	-	29,29,29	1.59	1 (3%)	38,40,40	1.16	3 (7%)
4	BTB	B	504	8	13,13,13	0.58	0	7,16,16	0.47	0
4	BTB	D	504	8	13,13,13	0.58	0	7,16,16	0.56	0
6	GOL	C	508	-	5,5,5	0.29	0	5,5,5	0.45	0
3	M4R	C	503	-	29,29,29	1.61	2 (6%)	38,40,40	1.36	6 (15%)
6	GOL	A	508	-	5,5,5	0.45	0	5,5,5	0.49	0
3	M4R	A	502	-	29,29,29	1.61	2 (6%)	38,40,40	1.05	4 (10%)
4	BTB	C	505	-	13,13,13	0.39	0	7,16,16	1.10	0
4	BTB	A	505	-	13,13,13	0.36	0	7,16,16	0.57	0
2	HEM	C	501	1	50,50,50	2.11	10 (20%)	67,82,82	1.33	4 (5%)
3	M4R	B	502	-	29,29,29	1.62	3 (10%)	38,40,40	1.12	4 (10%)
4	BTB	B	505	-	13,13,13	0.42	0	7,16,16	0.61	0
3	M4R	D	502	-	29,29,29	1.65	1 (3%)	38,40,40	1.23	5 (13%)
3	M4R	B	503	-	29,29,29	1.58	2 (6%)	38,40,40	1.10	2 (5%)
2	HEM	D	501	1	50,50,50	2.03	10 (20%)	67,82,82	1.48	10 (14%)
3	M4R	C	502	-	29,29,29	1.65	2 (6%)	38,40,40	1.36	4 (10%)
4	BTB	D	506	-	13,13,13	0.36	0	7,16,16	0.71	0
3	M4R	A	503	-	29,29,29	1.58	2 (6%)	38,40,40	1.30	5 (13%)
4	BTB	C	504	8	13,13,13	0.37	0	7,16,16	0.55	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
2	HEM	A	501	1	-	6/14/54/54	-
4	BTB	D	507	-	-	9/21/21/21	-
4	BTB	B	506	-	-	3/21/21/21	-
4	BTB	A	504	8	-	8/21/21/21	-
4	BTB	D	505	-	-	3/21/21/21	-
2	HEM	B	501	1	-	6/14/54/54	-
3	M4R	D	503	-	-	5/13/13/13	0/3/3/3
4	BTB	B	504	8	-	2/21/21/21	-
4	BTB	D	504	8	-	3/21/21/21	-
6	GOL	C	508	-	-	3/4/4/4	-
3	M4R	C	503	-	-	8/13/13/13	0/3/3/3
6	GOL	A	508	-	-	2/4/4/4	-
3	M4R	A	502	-	-	3/13/13/13	0/3/3/3
4	BTB	C	505	-	-	4/21/21/21	-
4	BTB	A	505	-	-	4/21/21/21	-
2	HEM	C	501	1	-	2/14/54/54	-
3	M4R	B	502	-	-	5/13/13/13	0/3/3/3
4	BTB	B	505	-	-	7/21/21/21	-
3	M4R	D	502	-	-	3/13/13/13	0/3/3/3
3	M4R	B	503	-	-	8/13/13/13	0/3/3/3
2	HEM	D	501	1	-	4/14/54/54	-
3	M4R	C	502	-	-	7/13/13/13	0/3/3/3
4	BTB	D	506	-	-	10/21/21/21	-
3	M4R	A	503	-	-	3/13/13/13	0/3/3/3
4	BTB	C	504	8	-	4/21/21/21	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3D-C2D	8.12	1.54	1.36
2	A	501	HEM	C3D-C2D	7.94	1.53	1.36
2	D	501	HEM	C3D-C2D	7.66	1.53	1.36
3	C	502	M4R	C23-C27	-7.50	1.28	1.44
3	D	502	M4R	C23-C27	-7.38	1.29	1.44
3	B	502	M4R	C23-C27	-7.25	1.29	1.44
3	A	502	M4R	C23-C27	-7.19	1.29	1.44
2	B	501	HEM	C3D-C2D	7.12	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	M4R	C23-C27	-7.12	1.29	1.44
3	C	503	M4R	C23-C27	-7.10	1.29	1.44
3	D	503	M4R	C23-C27	-7.06	1.29	1.44
3	B	503	M4R	C23-C27	-6.79	1.30	1.44
2	C	501	HEM	FE-NB	6.72	2.15	1.94
2	D	501	HEM	FE-NB	6.11	2.13	1.94
2	B	501	HEM	FE-NB	5.80	2.12	1.94
2	A	501	HEM	FE-NB	5.37	2.11	1.94
2	D	501	HEM	FE-NC	4.62	2.10	1.95
2	C	501	HEM	FE-NA	4.49	2.10	1.95
2	D	501	HEM	FE-NA	4.48	2.10	1.95
2	B	501	HEM	FE-ND	4.43	2.08	1.94
2	A	501	HEM	FE-NC	4.21	2.09	1.95
2	A	501	HEM	FE-NA	4.06	2.08	1.95
2	B	501	HEM	FE-NC	3.80	2.07	1.95
2	C	501	HEM	FE-NC	3.72	2.07	1.95
2	A	501	HEM	FE-ND	3.62	2.06	1.94
2	C	501	HEM	FE-ND	3.61	2.06	1.94
2	B	501	HEM	CAC-C3C	3.21	1.55	1.47
2	D	501	HEM	CAC-C3C	3.15	1.55	1.47
2	A	501	HEM	CAC-C3C	3.12	1.55	1.47
2	B	501	HEM	CAB-C3B	3.06	1.55	1.47
2	C	501	HEM	CAB-C3B	2.95	1.55	1.47
2	D	501	HEM	CAB-C3B	2.89	1.55	1.47
2	D	501	HEM	CMA-C3A	2.85	1.56	1.50
2	C	501	HEM	CAC-C3C	2.83	1.54	1.47
2	C	501	HEM	CMC-C2C	2.83	1.56	1.50
2	A	501	HEM	CAB-C3B	2.80	1.54	1.47
2	D	501	HEM	CMC-C2C	2.66	1.56	1.50
2	B	501	HEM	FE-NA	2.51	2.03	1.95
3	C	503	M4R	C02-N01	2.40	1.36	1.33
3	B	503	M4R	C09-C10	-2.38	1.38	1.41
2	D	501	HEM	CMB-C2B	2.37	1.55	1.50
2	A	501	HEM	CMC-C2C	2.37	1.55	1.50
2	C	501	HEM	CMB-C2B	2.29	1.55	1.50
2	B	501	HEM	CMB-C2B	2.28	1.55	1.50
3	A	502	M4R	C05-C10	-2.28	1.38	1.42
2	D	501	HEM	FE-ND	2.26	2.01	1.94
3	A	503	M4R	C02-N01	2.26	1.36	1.33
2	C	501	HEM	CMD-C2D	2.21	1.55	1.50
2	A	501	HEM	CMB-C2B	2.12	1.55	1.50
2	B	501	HEM	CMC-C2C	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	M4R	C09-C10	-2.07	1.38	1.41
2	B	501	HEM	CMA-C3A	2.06	1.55	1.50
3	B	502	M4R	C10-N01	-2.05	1.34	1.37
3	C	502	M4R	C05-C10	-2.01	1.39	1.42

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	C4D-ND-C1D	6.53	112.94	105.21
2	C	501	HEM	C4D-ND-C1D	6.06	112.39	105.21
2	A	501	HEM	C4D-ND-C1D	5.79	112.06	105.21
3	C	502	M4R	C33-N32-C30	-5.10	108.29	114.39
2	A	501	HEM	CAD-C3D-C4D	4.99	133.40	124.70
2	B	501	HEM	C4D-ND-C1D	4.70	110.77	105.21
3	B	502	M4R	C33-N32-C30	-3.83	109.81	114.39
2	B	501	HEM	CAD-C3D-C4D	3.65	131.06	124.70
2	B	501	HEM	CAD-CBD-CGD	-3.42	104.58	113.67
3	D	502	M4R	C33-N32-C30	-3.37	110.36	114.39
3	B	503	M4R	C33-N32-C30	-3.37	110.36	114.39
2	A	501	HEM	CAD-C3D-C2D	-3.34	121.61	127.87
2	D	501	HEM	CAD-CBD-CGD	-3.34	104.81	113.67
3	A	503	M4R	C04-C05-C10	3.31	120.02	118.00
4	A	504	BTB	O3-C3-C2	-3.23	103.81	111.40
3	C	503	M4R	C33-N32-C30	-3.20	110.56	114.39
3	D	503	M4R	C05-C10-N01	-3.14	119.47	122.80
2	D	501	HEM	CHB-C1B-NB	3.09	128.19	124.37
3	C	503	M4R	C04-C05-C10	3.08	119.88	118.00
3	C	502	M4R	C04-C05-C10	2.85	119.74	118.00
3	C	502	M4R	C05-C10-N01	-2.85	119.79	122.80
3	A	503	M4R	C33-N32-C30	-2.81	111.04	114.39
3	D	503	M4R	C33-N32-C30	-2.80	111.04	114.39
3	C	503	M4R	N02-C02-N01	2.80	120.55	118.24
3	D	502	M4R	C05-C10-N01	-2.77	119.87	122.80
3	A	503	M4R	C05-C10-N01	-2.77	119.87	122.80
3	D	502	M4R	C12-O13-C21	2.73	124.12	117.62
2	D	501	HEM	C3D-C4D-ND	-2.67	107.24	110.17
2	A	501	HEM	C3B-C4B-NB	-2.64	107.57	109.47
2	A	501	HEM	CHD-C1D-ND	2.64	127.27	124.42
2	B	501	HEM	CMD-C2D-C1D	2.59	129.08	125.03
3	C	503	M4R	C05-C10-N01	-2.58	120.06	122.80
3	B	503	M4R	C12-C08-C09	-2.58	115.49	121.23
2	D	501	HEM	C2A-C1A-NA	-2.56	107.31	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	M4R	C04-C05-C10	2.53	119.54	118.00
2	B	501	HEM	CAD-C3D-C2D	-2.48	123.21	127.87
2	D	501	HEM	CBA-CAA-C2A	-2.48	105.67	112.53
2	D	501	HEM	CHD-C1D-ND	2.45	127.06	124.42
3	A	502	M4R	C05-C10-N01	-2.45	120.21	122.80
3	A	502	M4R	N02-C02-N01	2.43	120.25	118.24
2	D	501	HEM	C3B-C4B-NB	-2.41	107.73	109.47
2	C	501	HEM	C3B-C2B-C1B	2.40	108.22	106.41
3	A	502	M4R	C33-N32-C30	-2.39	111.53	114.39
2	C	501	HEM	CBD-CAD-C3D	-2.36	106.01	112.53
3	B	502	M4R	C08-C09-C10	-2.36	119.23	121.11
2	C	501	HEM	C2A-C1A-NA	-2.33	107.57	110.15
2	D	501	HEM	C1B-NB-C4B	2.31	107.94	105.21
3	D	503	M4R	C04-C05-C10	2.26	119.38	118.00
2	A	501	HEM	C3B-C2B-C1B	2.24	108.09	106.41
3	B	502	M4R	C04-C05-C10	2.23	119.36	118.00
2	B	501	HEM	C1B-NB-C4B	2.17	107.78	105.21
3	C	502	M4R	C29-C25-C26	2.16	124.14	120.43
2	B	501	HEM	CAA-CBA-CGA	-2.15	107.97	113.67
2	B	501	HEM	CHA-C1A-NA	2.12	127.71	123.86
2	B	501	HEM	C3B-C4B-NB	-2.11	107.95	109.47
3	A	503	M4R	C06-C05-C04	-2.10	119.53	123.61
3	C	503	M4R	C12-O13-C21	2.10	122.61	117.62
3	C	503	M4R	C06-C05-C04	-2.09	119.55	123.61
2	D	501	HEM	C3B-C2B-C1B	2.07	107.96	106.41
3	D	502	M4R	C29-C25-C26	2.06	123.97	120.43
3	A	503	M4R	C08-C09-C10	-2.05	119.48	121.11
3	B	502	M4R	C05-C10-N01	-2.04	120.63	122.80
2	A	501	HEM	C1B-NB-C4B	2.02	107.59	105.21
3	A	502	M4R	C03-C04-C05	2.01	119.87	117.84

There are no chirality outliers.

All (122) 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
3	C	503	M4R	C25-C29-C30-C31
3	C	503	M4R	C25-C29-C30-N32

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Mol	Chain	Res	Type	Atoms
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	A	505	BTB	C3-C2-C4-O4
4	A	505	BTB	N-C2-C4-O4
4	B	504	BTB	O1-C1-C2-C4
4	B	504	BTB	O1-C1-C2-N
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	B	506	BTB	C1-C2-C3-O3
4	B	506	BTB	C4-C2-C3-O3
4	B	506	BTB	N-C2-C3-O3
4	C	504	BTB	O1-C1-C2-C3
4	C	504	BTB	O1-C1-C2-C4
4	C	504	BTB	O1-C1-C2-N
4	C	505	BTB	O1-C1-C2-C3
4	C	505	BTB	O1-C1-C2-C4
4	C	505	BTB	O1-C1-C2-N
4	D	504	BTB	O1-C1-C2-C4
4	D	505	BTB	O1-C1-C2-C3
4	D	505	BTB	O1-C1-C2-N
4	D	506	BTB	C1-C2-C4-O4
4	D	506	BTB	C3-C2-C4-O4
4	D	506	BTB	N-C2-C4-O4
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
4	D	507	BTB	N-C2-C4-O4
6	C	508	GOL	O1-C1-C2-C3
4	D	504	BTB	N-C7-C8-O8
3	B	503	M4R	C22-C21-O13-C12
3	B	503	M4R	C26-C21-O13-C12
3	A	502	M4R	C26-C21-O13-C12

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Mol	Chain	Res	Type	Atoms
3	A	502	M4R	C22-C21-O13-C12
4	C	504	BTB	N-C5-C6-O6
2	B	501	HEM	C3D-CAD-CBD-CGD
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
2	A	501	HEM	C3D-CAD-CBD-CGD
3	B	503	M4R	C25-C29-C30-N32
4	A	504	BTB	N-C7-C8-O8
3	D	503	M4R	C31-C30-N32-C33
6	A	508	GOL	O1-C1-C2-O2
3	B	502	M4R	C29-C30-N32-C33
3	B	503	M4R	C29-C30-N32-C33
3	D	502	M4R	C29-C30-N32-C33
3	D	503	M4R	C29-C30-N32-C33
3	D	502	M4R	C26-C25-C29-C30
3	D	502	M4R	C24-C25-C29-C30
3	C	502	M4R	C26-C25-C29-C30
3	C	503	M4R	C22-C21-O13-C12
4	A	504	BTB	C1-C2-C3-O3
3	C	502	M4R	C24-C25-C29-C30
4	A	505	BTB	N-C7-C8-O8
3	C	503	M4R	C26-C21-O13-C12
3	D	503	M4R	C22-C21-O13-C12
4	D	506	BTB	N-C5-C6-O6
3	B	502	M4R	C24-C25-C29-C30
3	B	502	M4R	C26-C25-C29-C30
4	D	507	BTB	N-C7-C8-O8
3	A	502	M4R	C31-C30-N32-C33
6	C	508	GOL	O2-C2-C3-O3
2	D	501	HEM	C3D-CAD-CBD-CGD
3	C	502	M4R	C08-C12-O13-C21
3	D	503	M4R	C26-C21-O13-C12
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
3	C	503	M4R	C29-C30-N32-C33

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Mol	Chain	Res	Type	Atoms
4	B	505	BTB	N-C5-C6-O6
4	C	505	BTB	N-C2-C3-O3
4	D	504	BTB	O1-C1-C2-N
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
3	C	503	M4R	C24-C25-C29-C30
4	D	505	BTB	N-C5-C6-O6
3	C	503	M4R	C26-C25-C29-C30
2	C	501	HEM	C3D-CAD-CBD-CGD
2	D	501	HEM	CAD-CBD-CGD-O1D
3	D	503	M4R	C25-C29-C30-N32
3	A	503	M4R	C29-C30-N32-C33
2	B	501	HEM	CAD-CBD-CGD-O2D
3	B	503	M4R	C31-C30-N32-C33
3	C	502	M4R	C31-C30-N32-C33
2	D	501	HEM	CAD-CBD-CGD-O2D
3	B	503	M4R	C24-C25-C29-C30
2	B	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O2A
3	B	503	M4R	C26-C25-C29-C30
4	D	507	BTB	C3-C2-C4-O4
3	C	503	M4R	C31-C30-N32-C33
3	C	502	M4R	C29-C30-N32-C33
4	A	505	BTB	O1-C1-C2-N
4	D	506	BTB	C3-C2-N-C7
4	D	506	BTB	C4-C2-N-C5

There are no ring outliers.

21 monomers are involved in 55 short contacts:

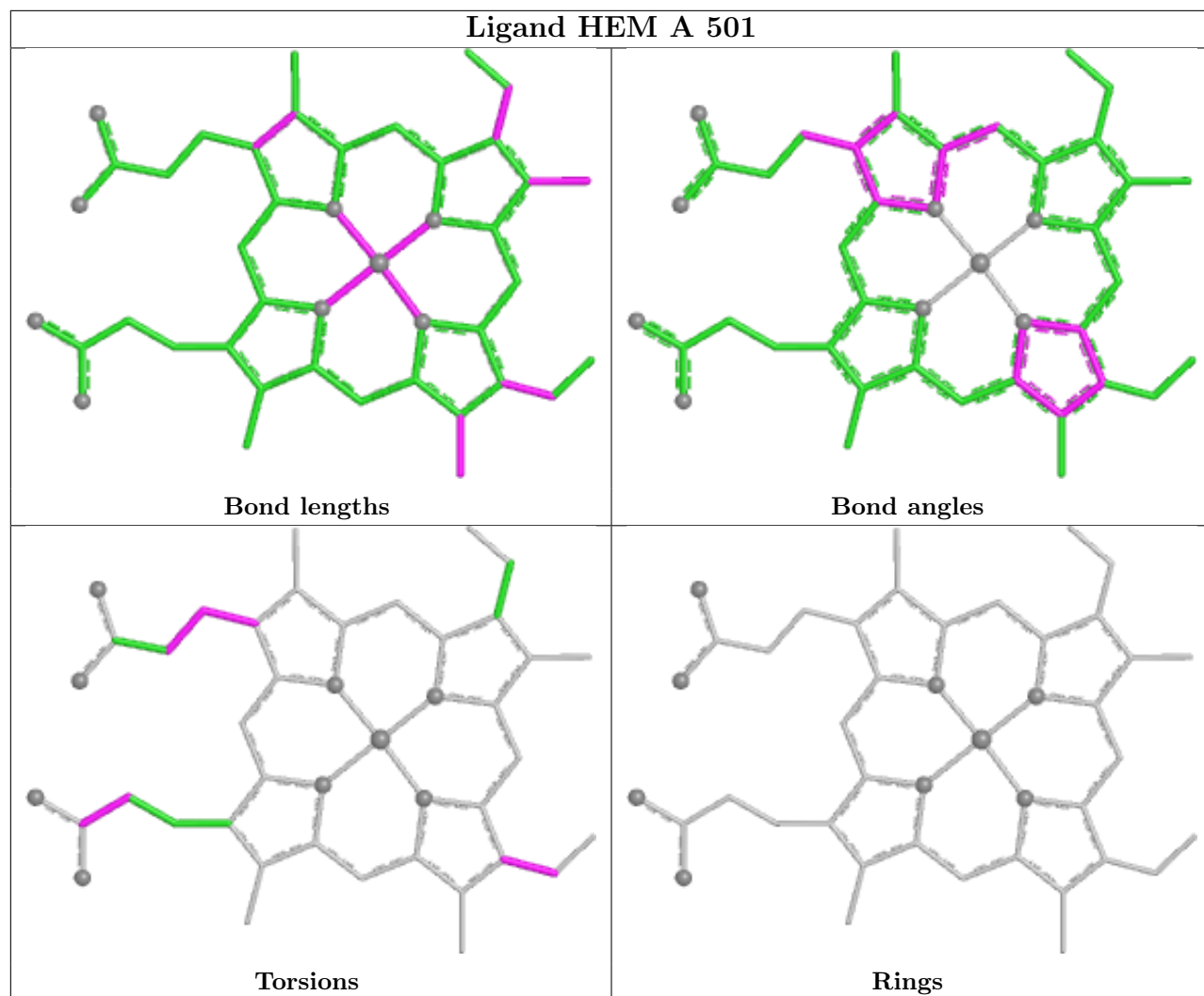
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	4	0
4	D	507	BTB	2	0
4	B	506	BTB	1	0
4	A	504	BTB	3	0
4	D	505	BTB	6	1
2	B	501	HEM	4	0

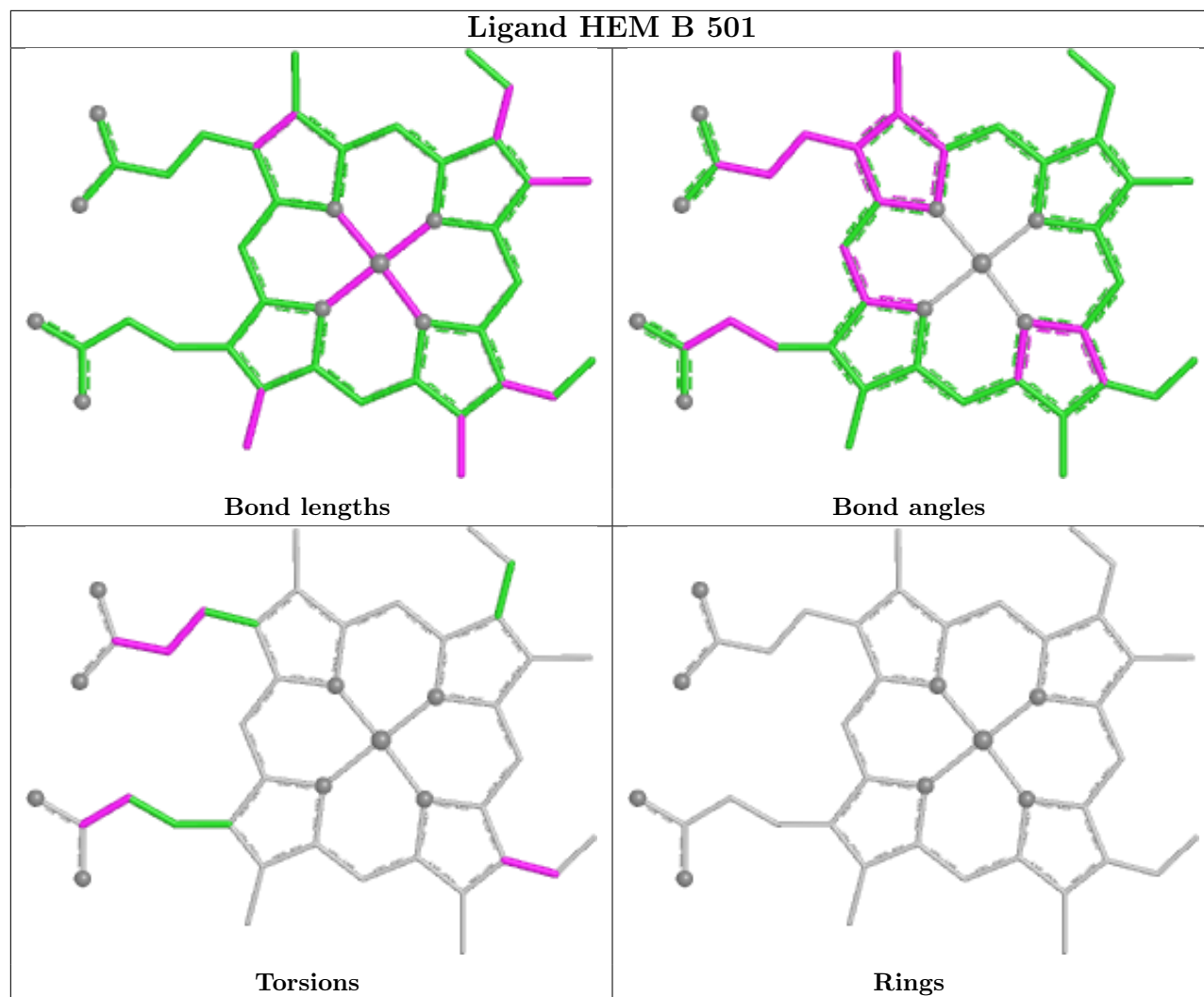
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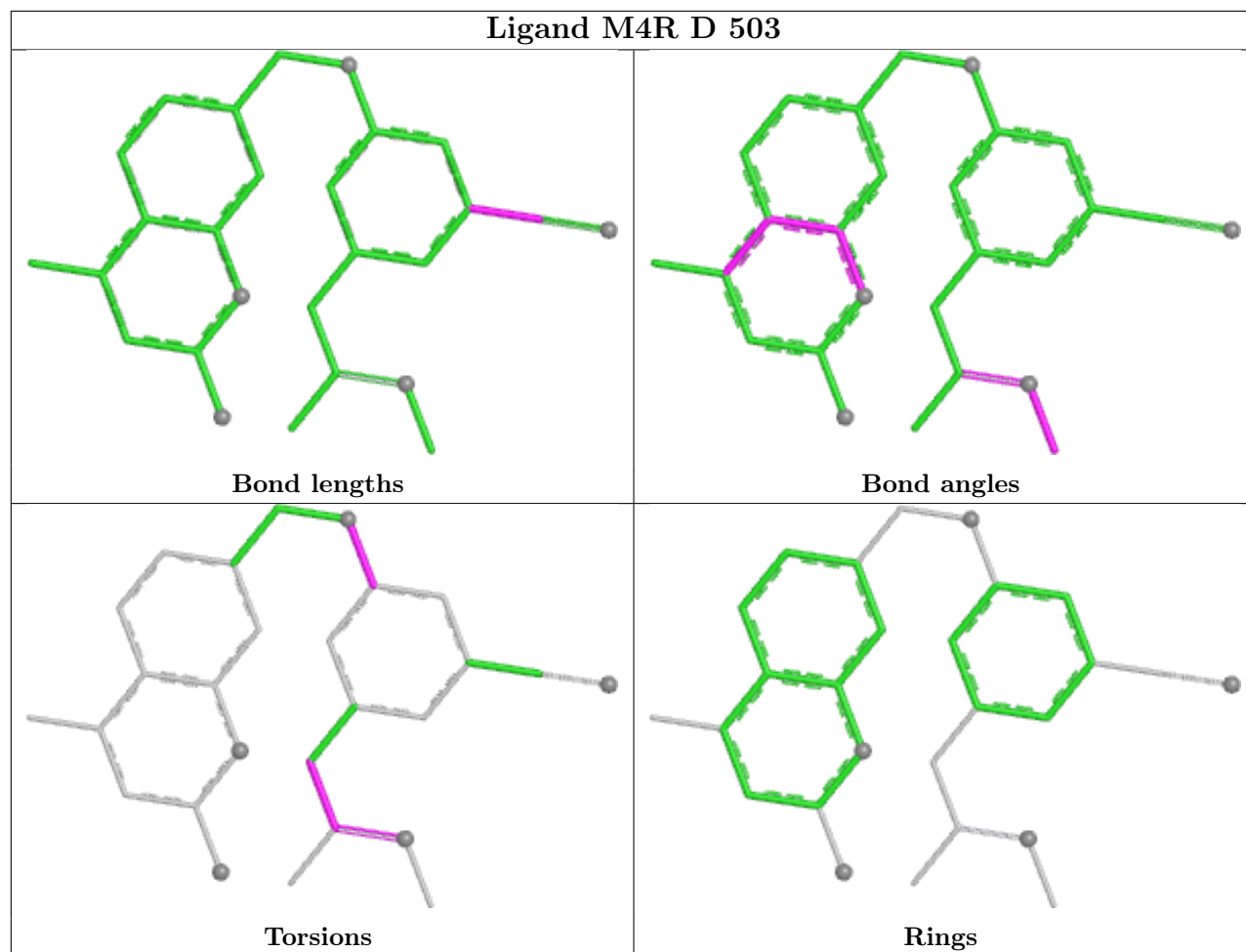
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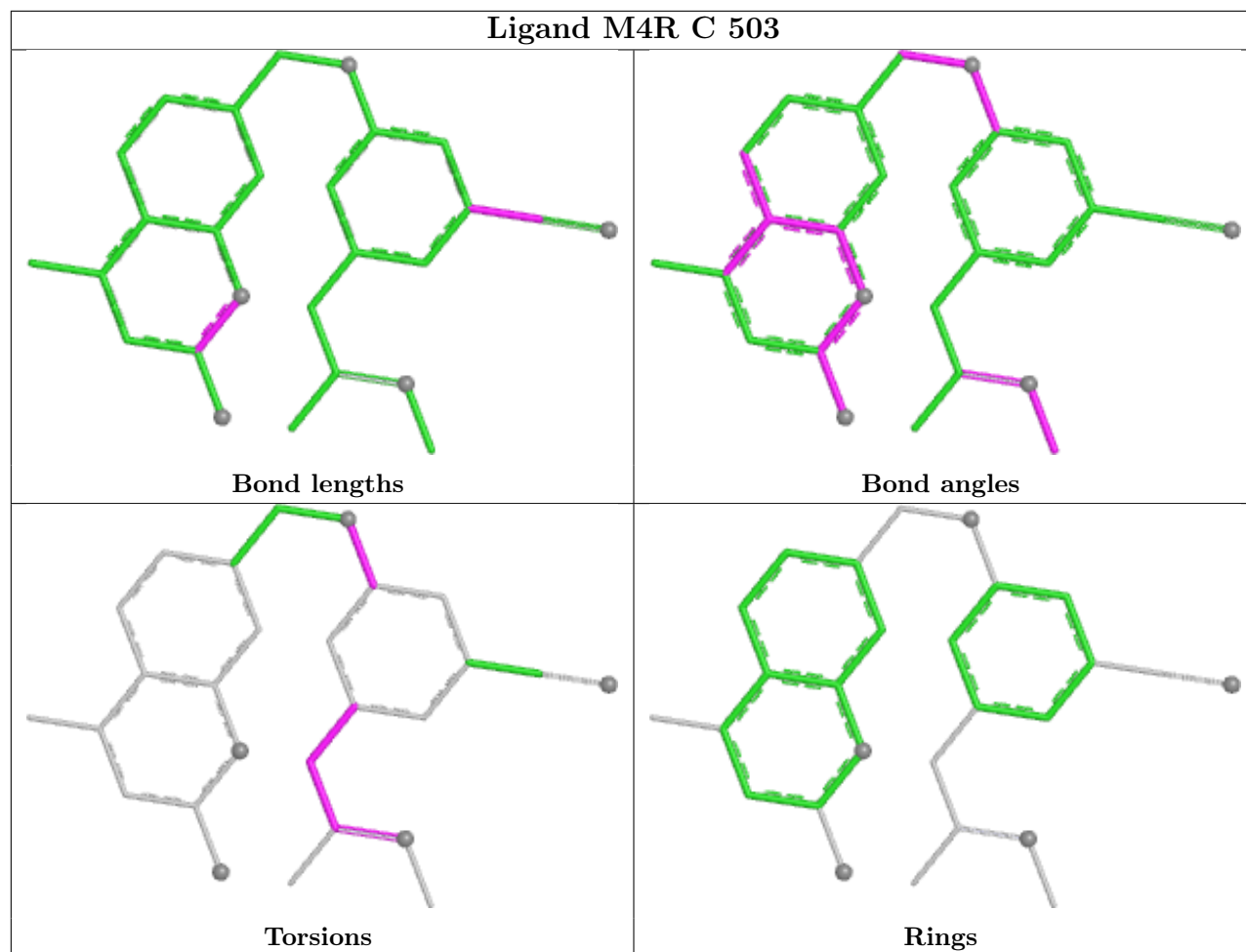
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	503	M4R	1	0
4	B	504	BTB	2	0
4	D	504	BTB	3	0
3	C	503	M4R	1	0
3	A	502	M4R	1	0
4	C	505	BTB	1	0
4	A	505	BTB	2	0
2	C	501	HEM	5	0
3	B	502	M4R	2	0
3	D	502	M4R	3	0
3	B	503	M4R	1	0
2	D	501	HEM	3	0
3	C	502	M4R	3	0
4	D	506	BTB	4	0
4	C	504	BTB	3	0

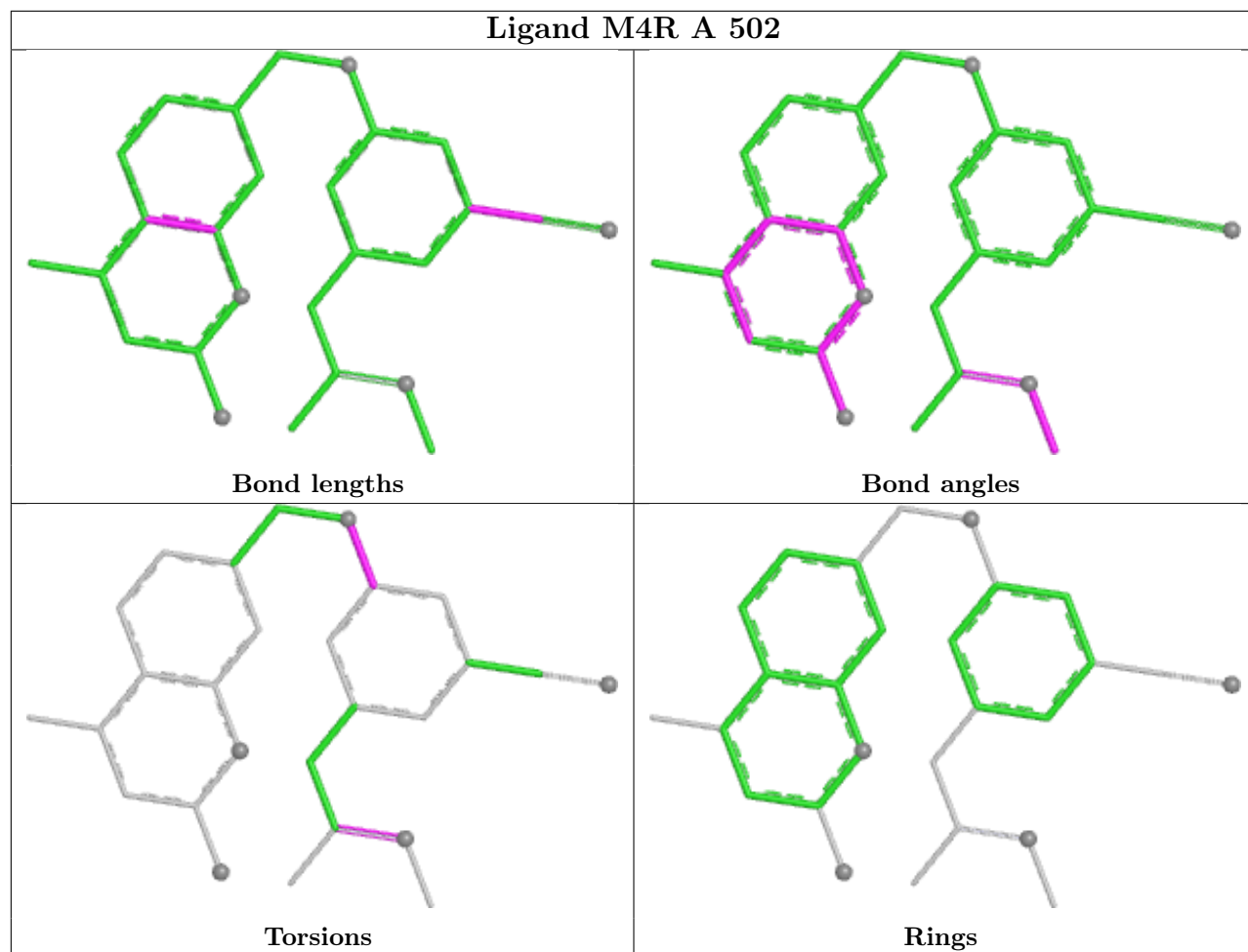
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

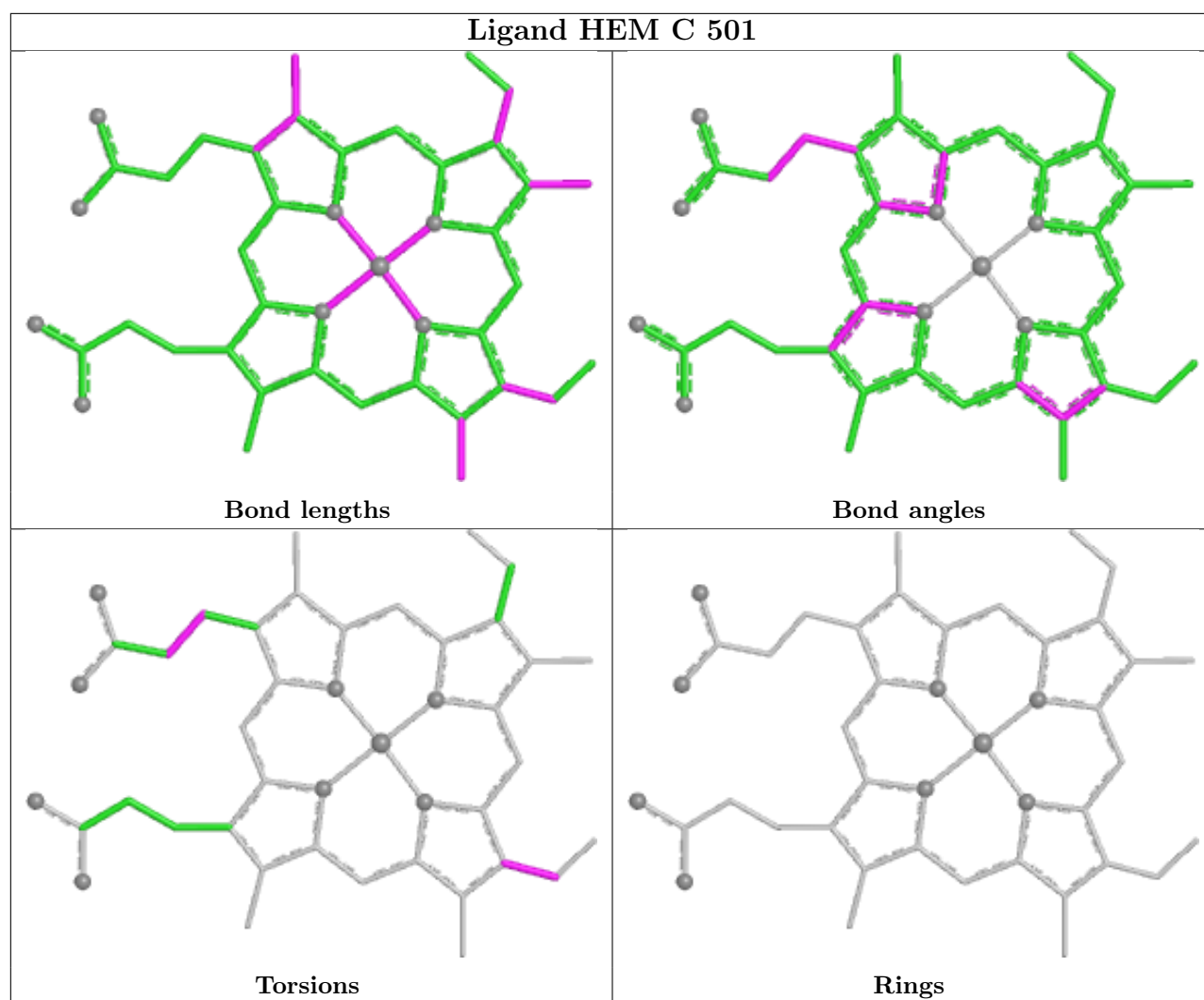


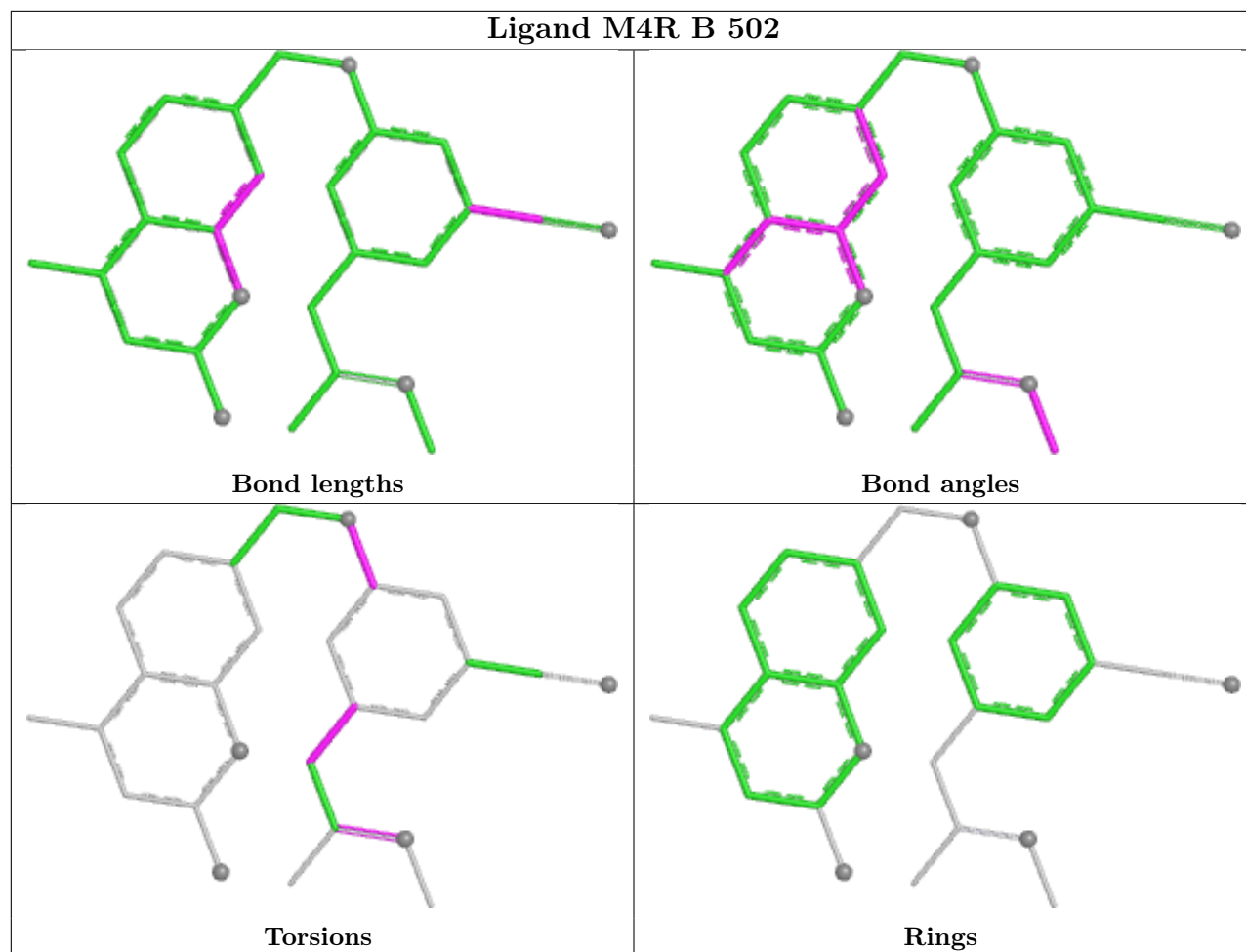


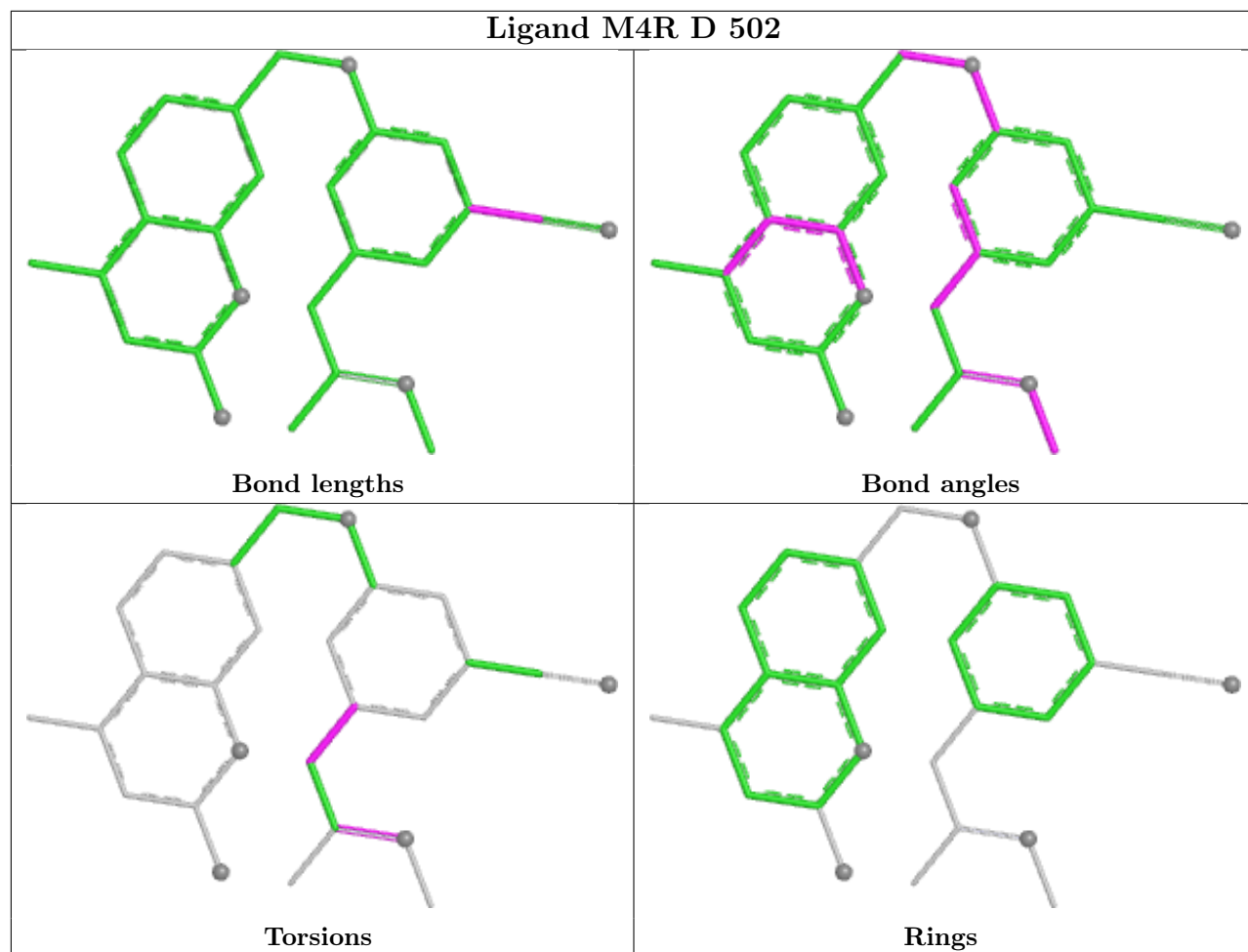


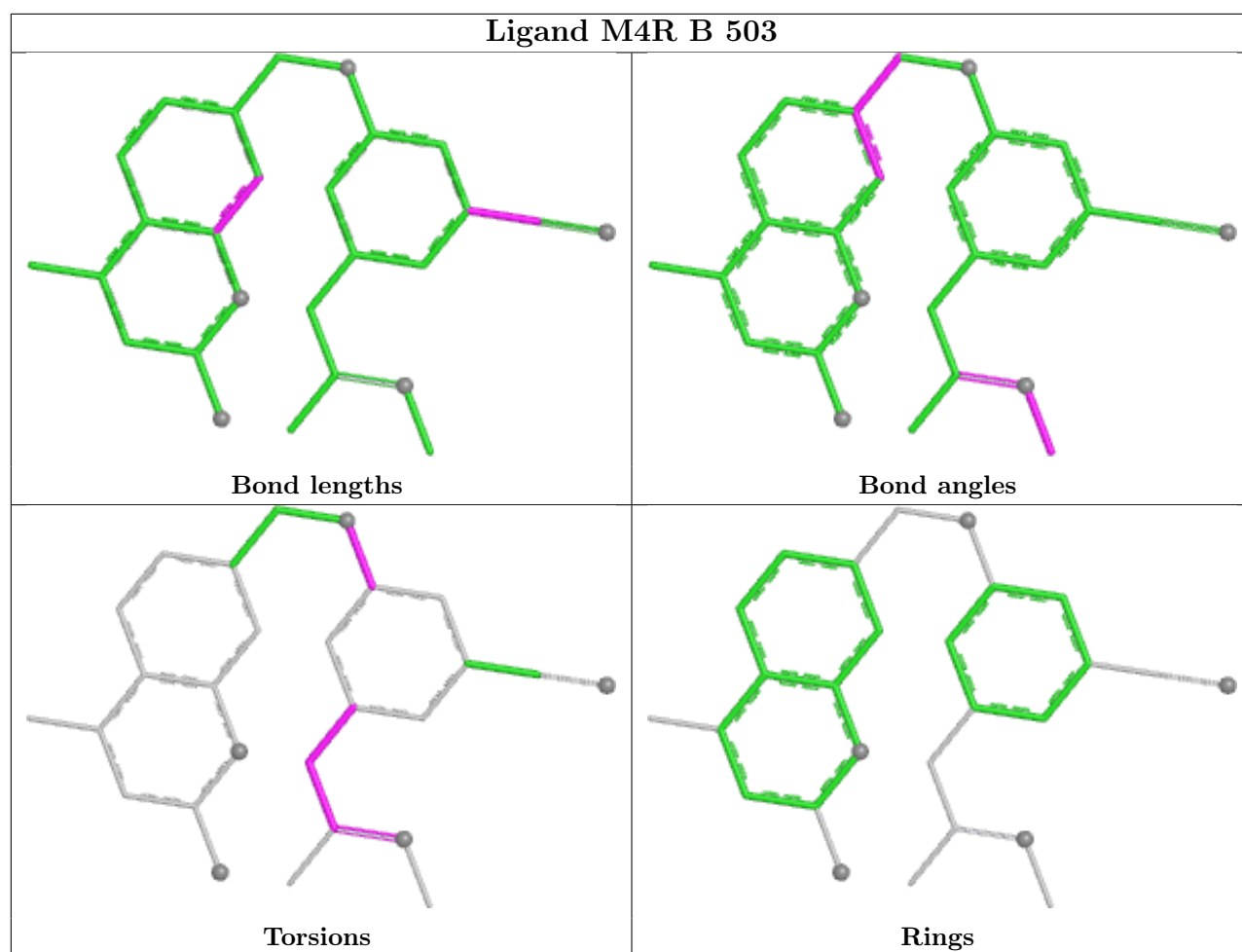


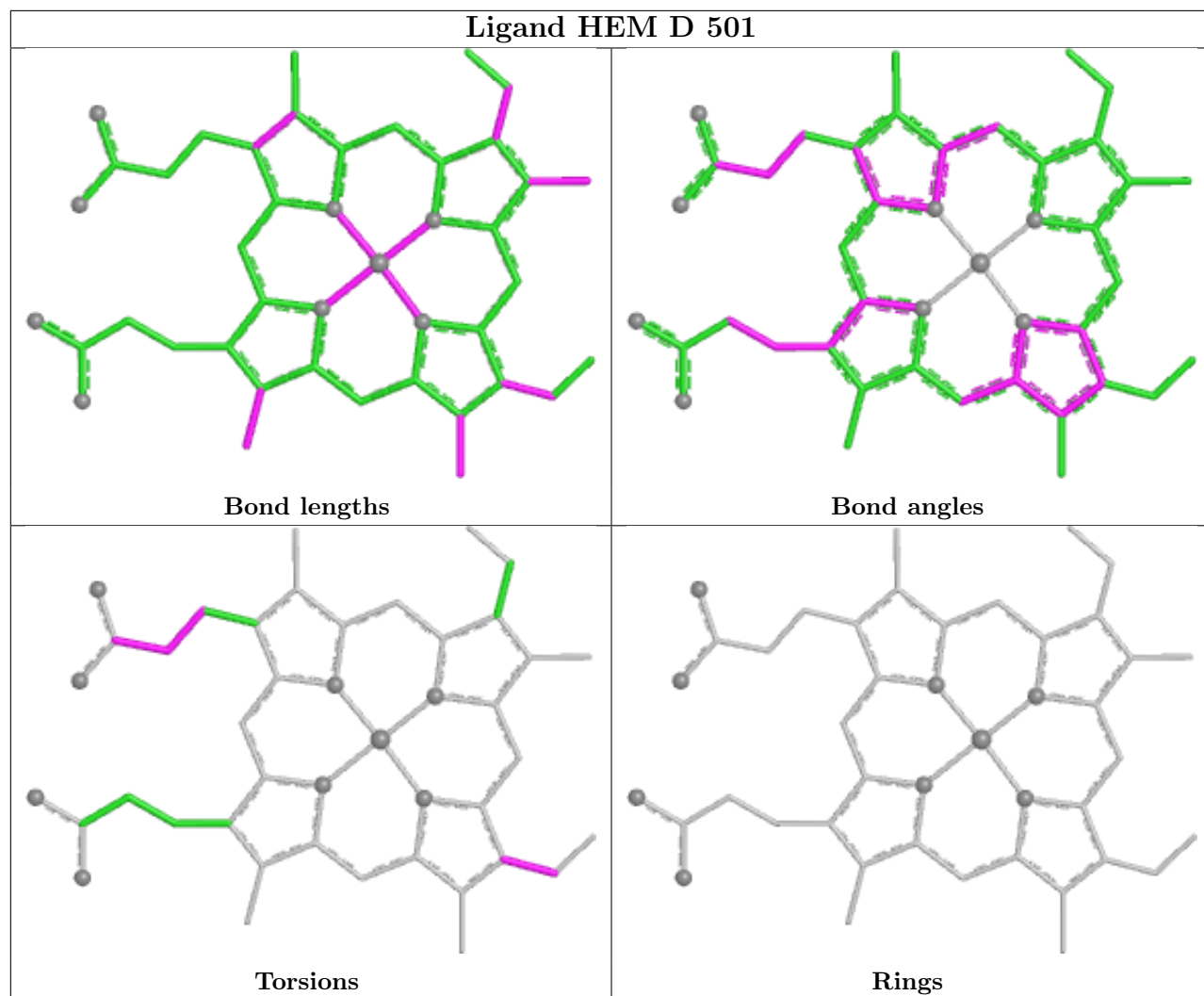


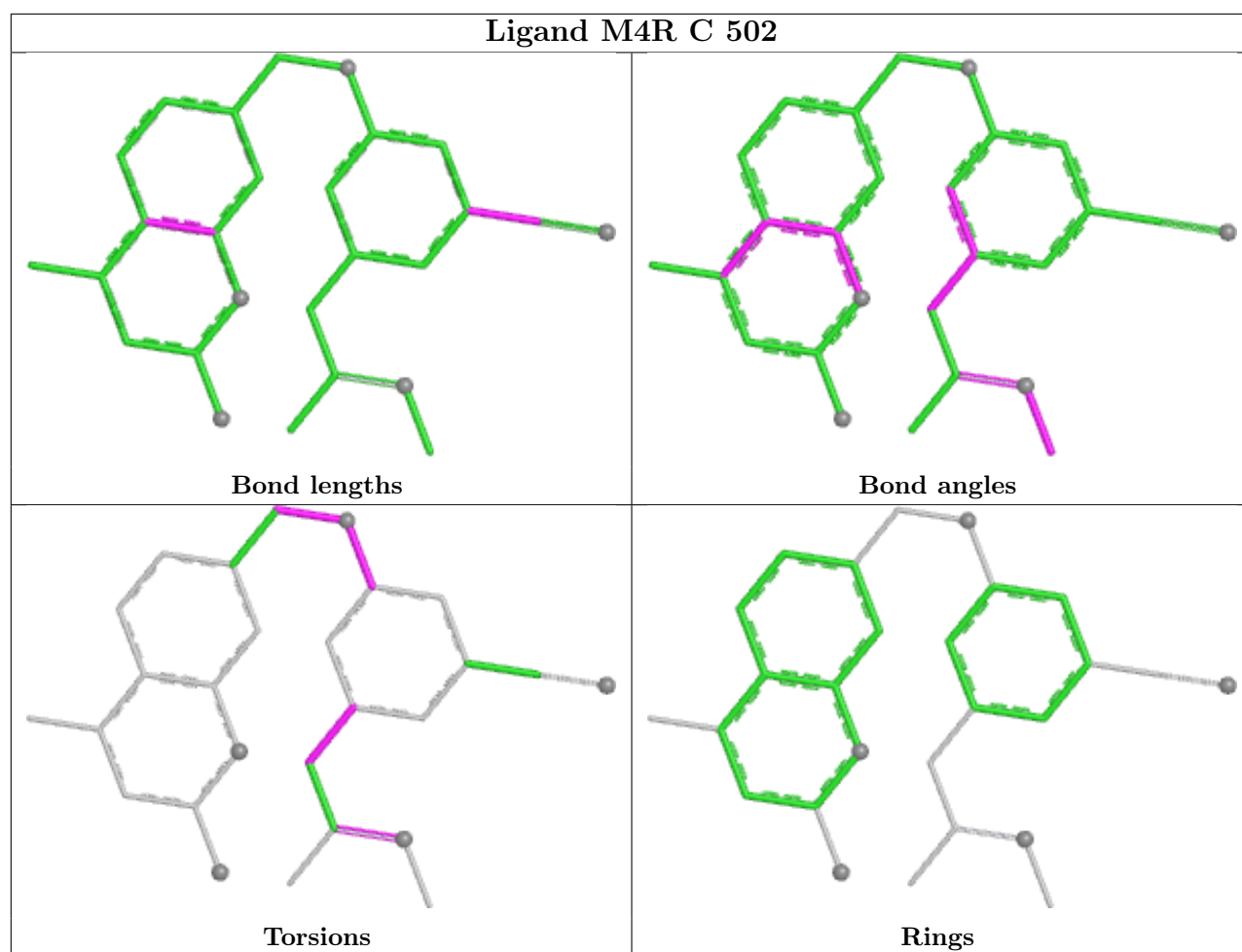


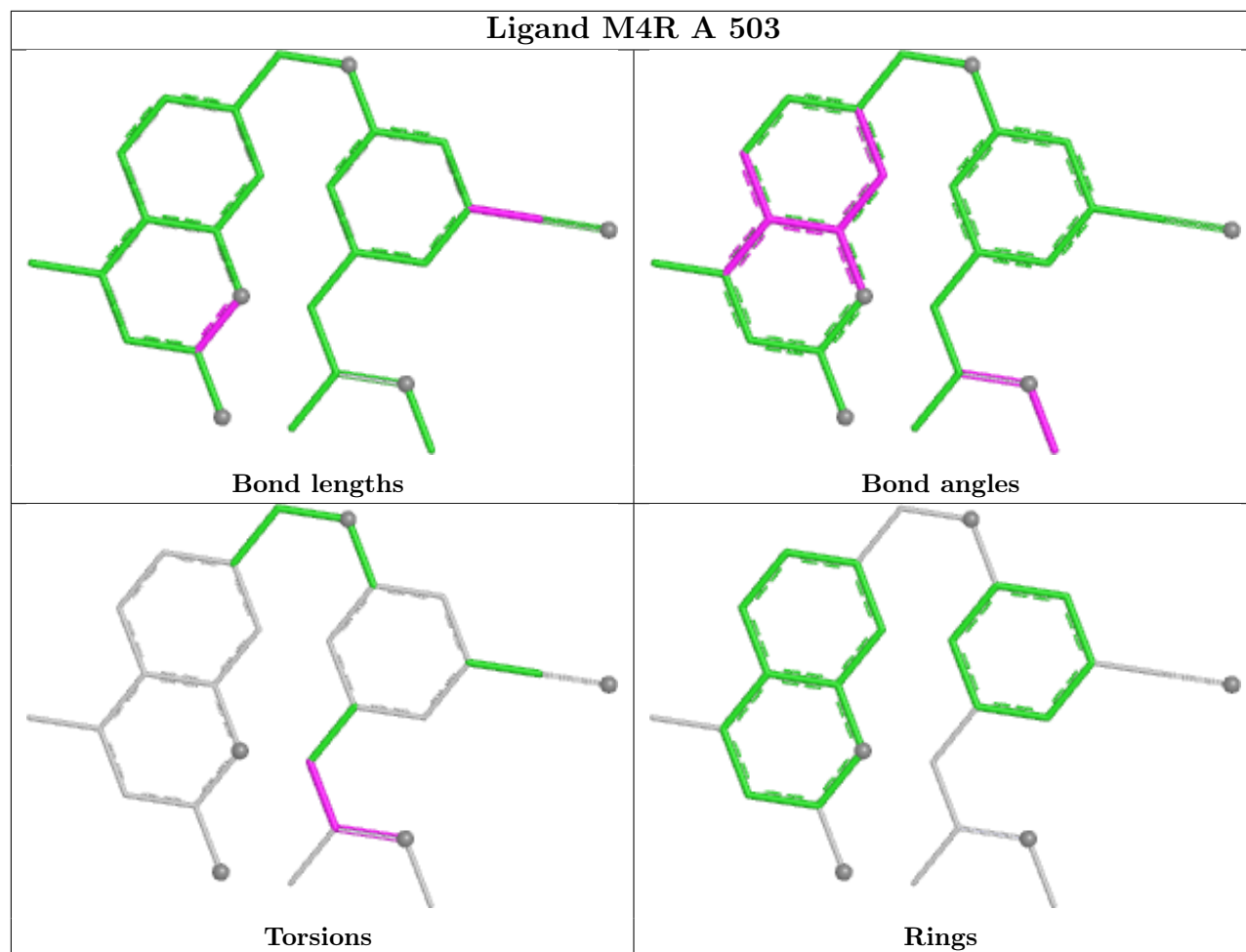












5.7 Other polymers [i](#)

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 [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%)	-0.71	1 (0%) 91 91	32, 70, 121, 159	2 (0%)
1	B	402/440 (91%)	-1.03	0 100 100	35, 58, 97, 141	3 (0%)
1	C	401/440 (91%)	-0.98	0 100 100	29, 60, 111, 147	1 (0%)
1	D	402/440 (91%)	-0.94	0 100 100	36, 56, 112, 140	3 (0%)
All	All	1609/1760 (91%)	-0.91	1 (0%) 92 91	29, 61, 113, 159	9 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	THR	2.2

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 oligosaccharides 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(Å ²)	Q<0.9
4	BTB	D	505	14/14	0.95	0.06	107,111,113,114	0

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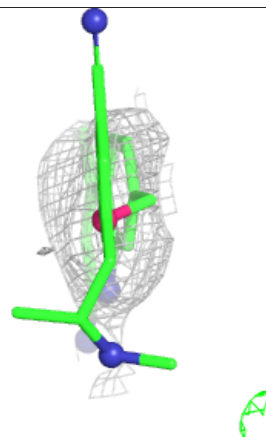
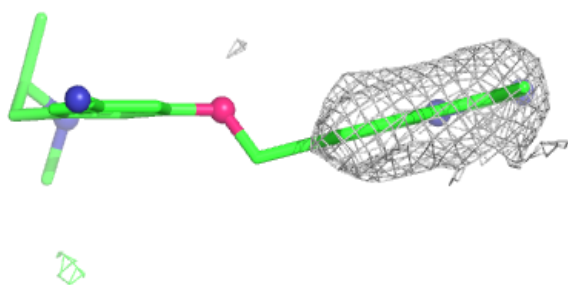
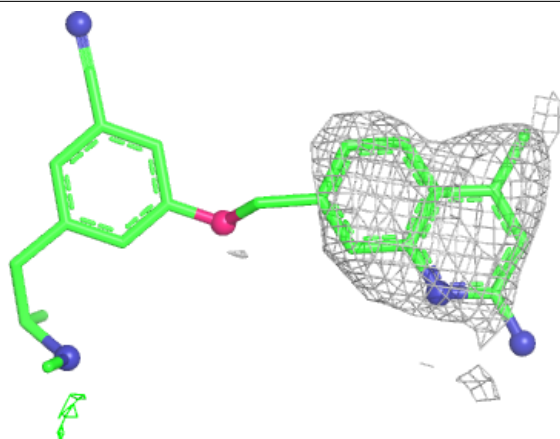
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BTB	A	505	14/14	0.96	0.05	98,103,107,107	0
4	BTB	B	505	14/14	0.96	0.06	83,95,103,105	0
3	M4R	B	502	27/27	0.96	0.10	59,94,116,119	0
4	BTB	D	507	14/14	0.96	0.05	86,96,100,102	0
6	GOL	C	508	6/6	0.96	0.05	71,80,87,89	0
3	M4R	D	502	27/27	0.97	0.10	69,89,109,111	0
4	BTB	D	506	14/14	0.97	0.04	100,103,107,107	0
3	M4R	A	503	27/27	0.97	0.07	43,61,88,90	0
6	GOL	A	508	6/6	0.97	0.05	77,87,89,91	0
3	M4R	A	502	27/27	0.97	0.10	92,106,121,121	0
4	BTB	D	504	14/14	0.98	0.07	53,88,93,95	0
3	M4R	C	502	27/27	0.98	0.12	116,126,135,136	0
3	M4R	B	503	27/27	0.98	0.06	41,56,85,94	0
4	BTB	B	506	14/14	0.98	0.06	98,104,107,110	0
4	BTB	C	504	14/14	0.98	0.07	95,107,111,112	0
4	BTB	C	505	14/14	0.98	0.04	76,88,91,91	0
7	CL	B	507	1/1	0.98	0.10	47,47,47,47	0
4	BTB	B	504	14/14	0.99	0.04	55,67,78,81	0
3	M4R	C	503	27/27	0.99	0.06	49,69,92,93	0
2	HEM	C	501	43/43	0.99	0.04	41,54,75,88	0
5	ZN	C	511	1/1	0.99	0.02	55,55,55,55	1
3	M4R	D	503	27/27	0.99	0.05	35,55,70,72	0
4	BTB	A	504	14/14	0.99	0.04	37,83,86,87	0
7	CL	A	509	1/1	0.99	0.04	71,71,71,71	0
2	HEM	A	501	43/43	0.99	0.04	46,56,79,91	0
7	CL	C	509	1/1	0.99	0.03	64,64,64,64	0
7	CL	D	509	1/1	0.99	0.05	48,48,48,48	0
2	HEM	D	501	43/43	1.00	0.04	32,54,77,86	0
2	HEM	B	501	43/43	1.00	0.04	36,46,68,84	0
5	ZN	A	506	1/1	1.00	0.02	54,54,54,54	0
5	ZN	A	507	1/1	1.00	0.02	53,53,53,53	0
5	ZN	A	511	1/1	1.00	0.01	64,64,64,64	0
5	ZN	C	506	1/1	1.00	0.01	50,50,50,50	0
5	ZN	C	507	1/1	1.00	0.02	57,57,57,57	0
8	GD	A	510	1/1	1.00	0.02	171,171,171,171	0
8	GD	B	508	1/1	1.00	0.01	62,62,62,62	0
8	GD	C	510	1/1	1.00	0.01	117,117,117,117	0
8	GD	D	508	1/1	1.00	0.01	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.

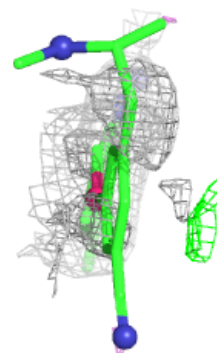
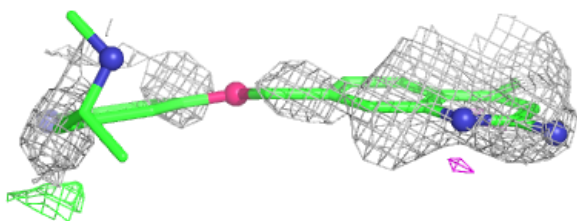
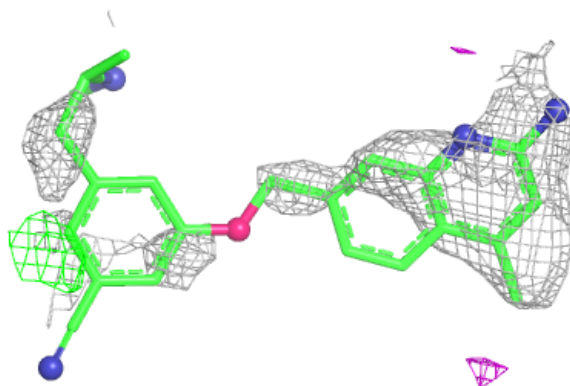
Electron density around M4R B 502:

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

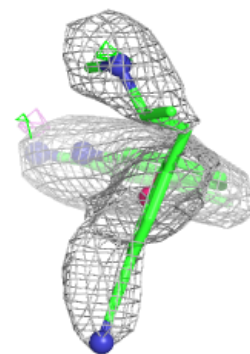
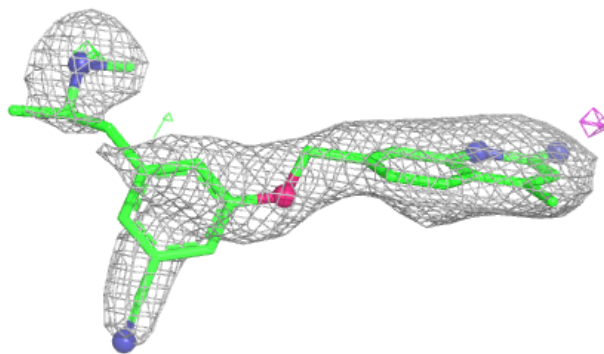


Electron density around M4R D 502:

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

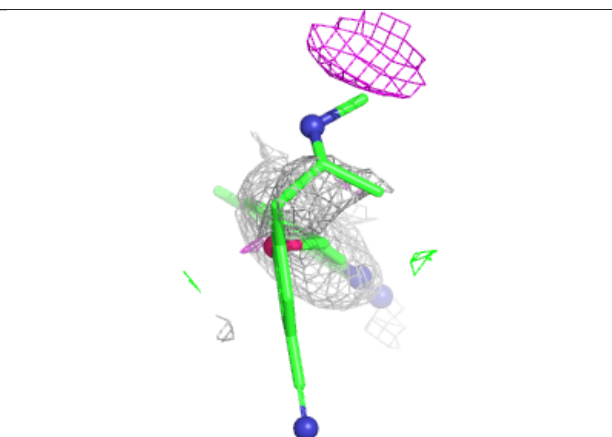
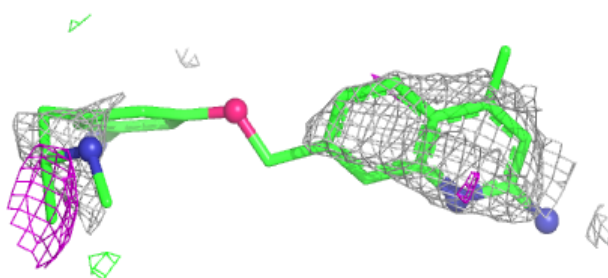
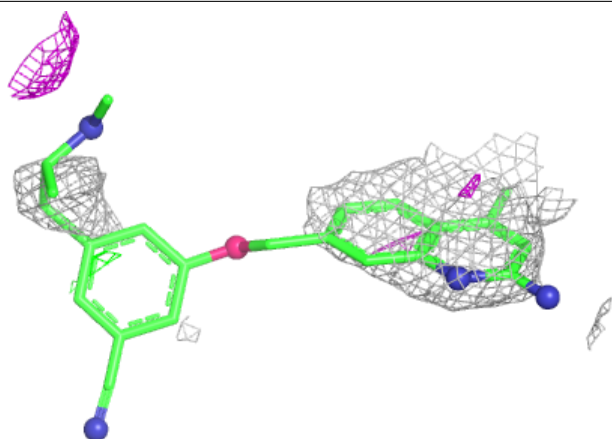
**Electron density around M4R A 503:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

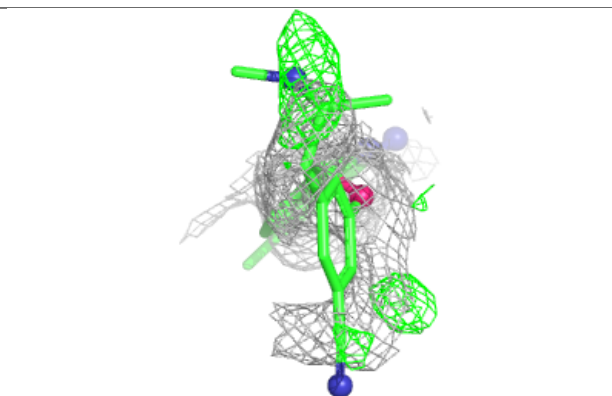
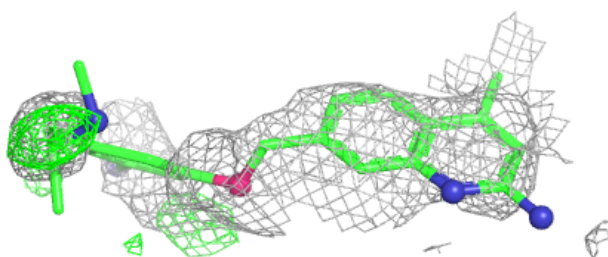
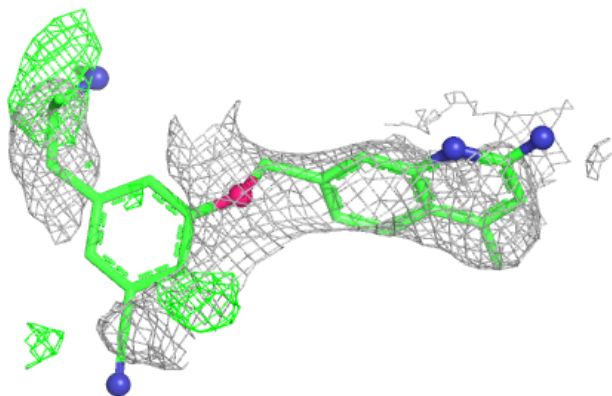


Electron density around M4R A 502:

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

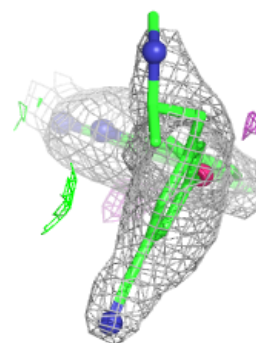
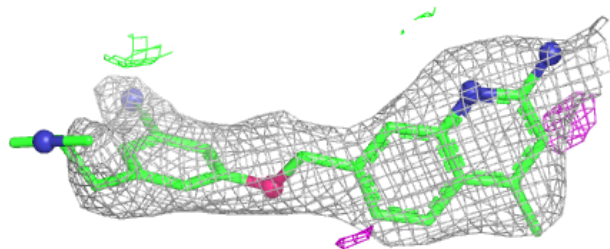
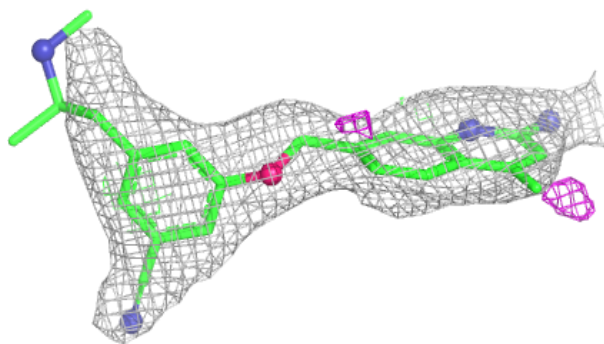
**Electron density around M4R C 502:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

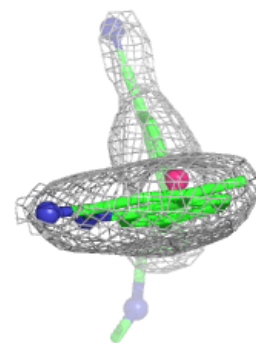
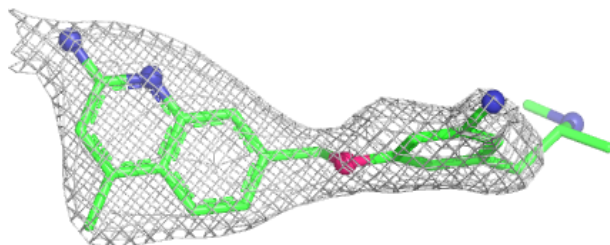
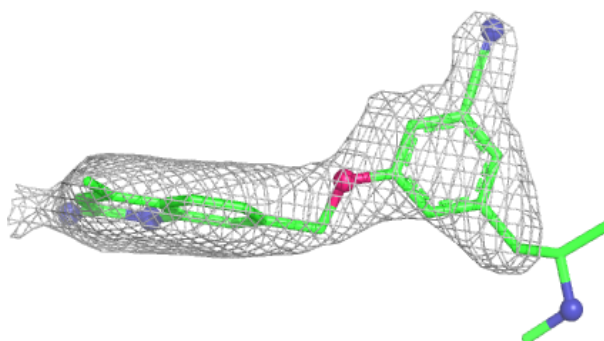


Electron density around M4R B 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

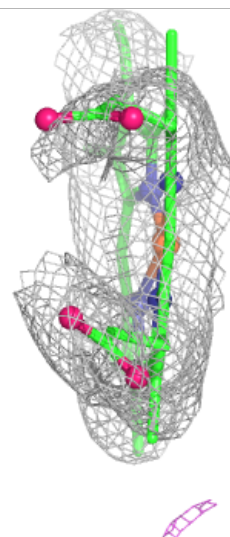
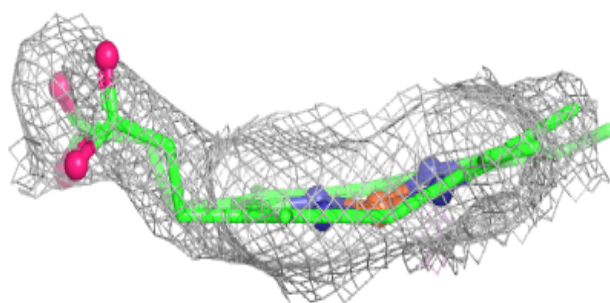
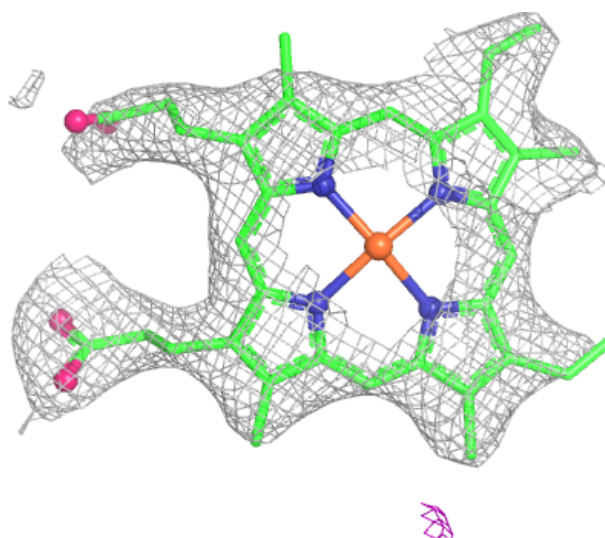
**Electron density around M4R C 503:**

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



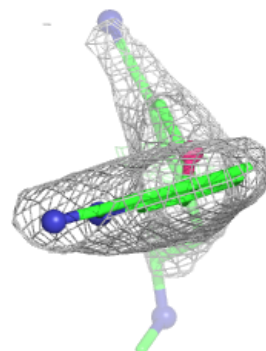
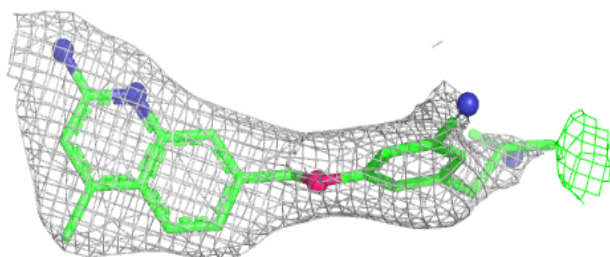
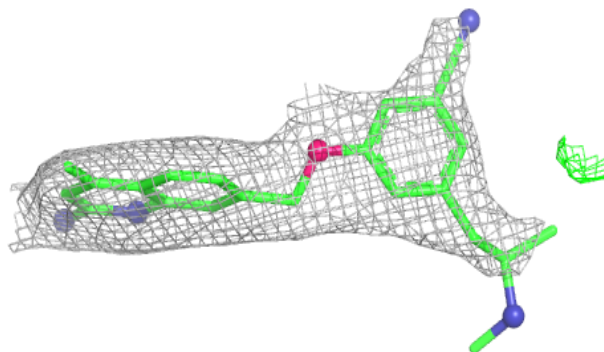
Electron density around HEM C 501:

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

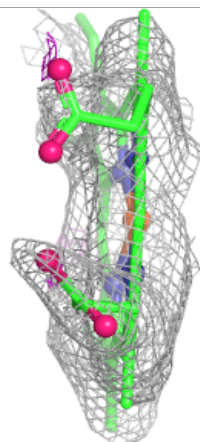
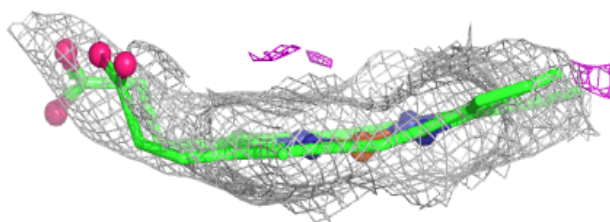
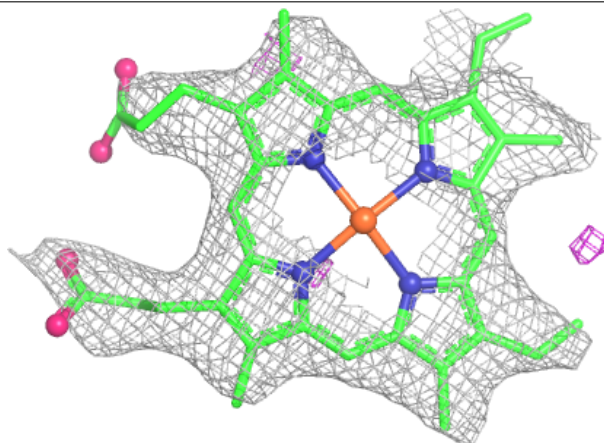


Electron density around M4R D 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

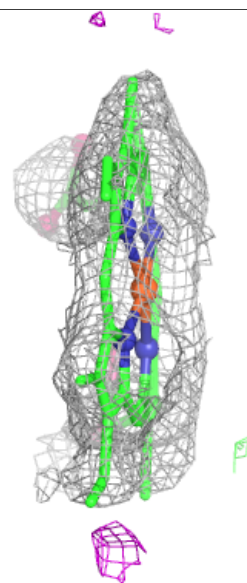
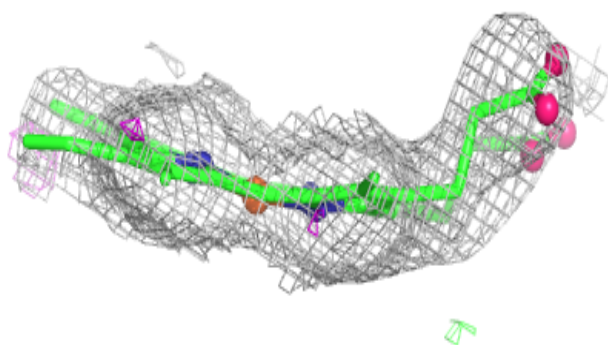
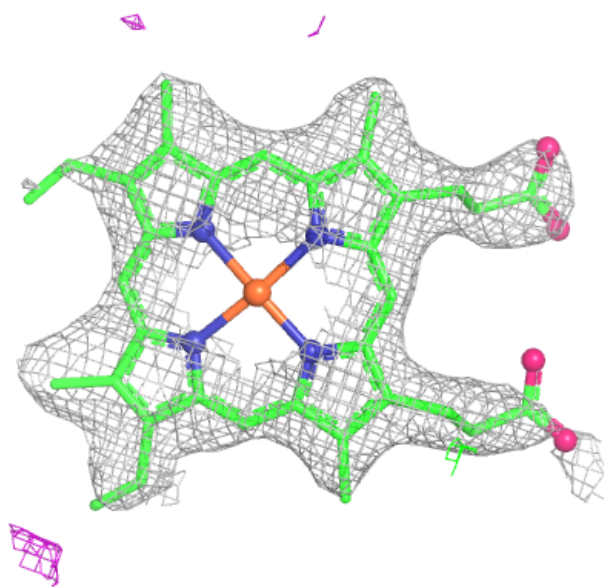
**Electron density around HEM A 501:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



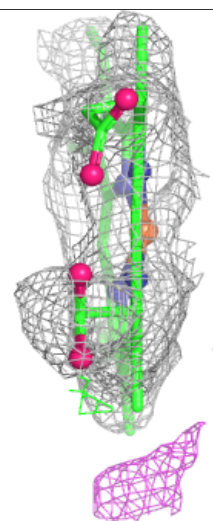
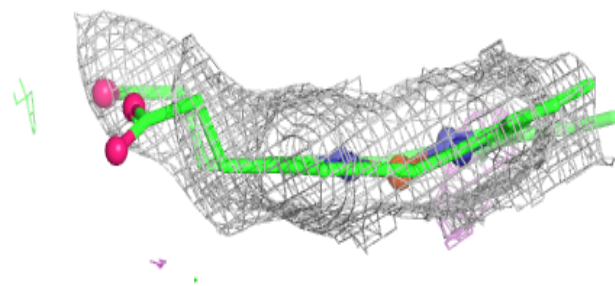
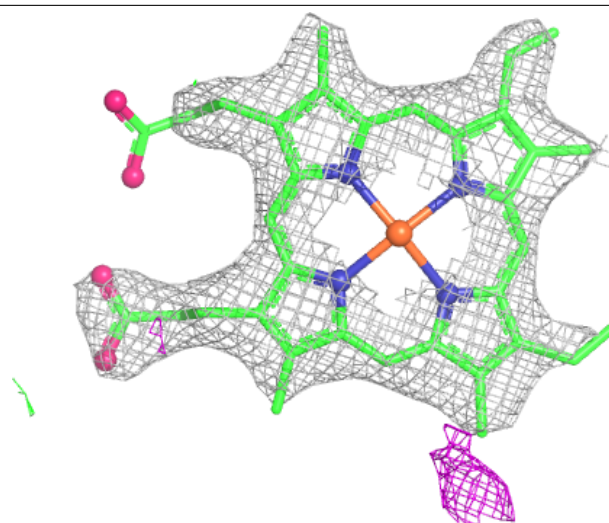
Electron density around HEM D 501:

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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.