



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:22 PM UTC

PDB ID : 9CWI / pdb_00009cwi
Title : Structure of human endothelial nitric oxide synthase heme domain bound with 6-(5-((3,3-difluoroazetidin-1-yl)methyl)-2,3-difluorophenyl)-4-methylpyridin-2-amine dihydrochloride
Authors : Li, H.; Poulos, T.L.
Deposited on : 2024-07-29
Resolution : 1.73 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

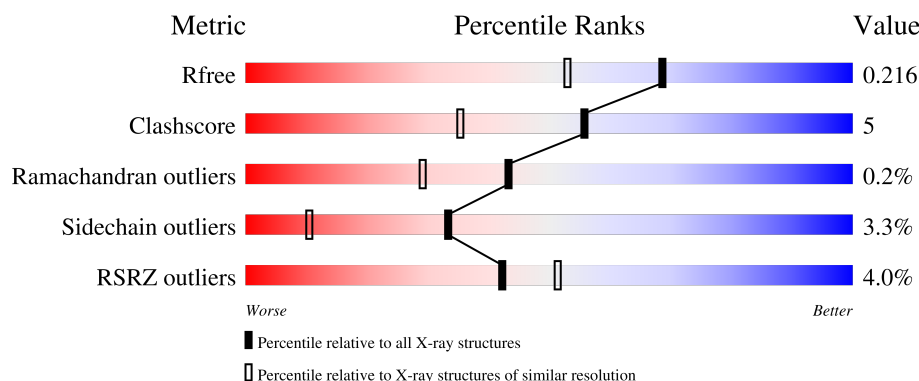
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	
1	B	440	
1	C	440	
1	D	440	

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
6	GOL	C	507	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14367 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	401	Total	C	N	O	S	0	1	0
			3207	2043	564	584	16			
1	B	401	Total	C	N	O	S	0	3	0
			3211	2045	564	586	16			
1	C	401	Total	C	N	O	S	0	1	0
			3203	2040	563	584	16			
1	D	402	Total	C	N	O	S	0	2	0
			3217	2048	567	586	16			

There are 4 discrepancies between the modelled and reference sequences:

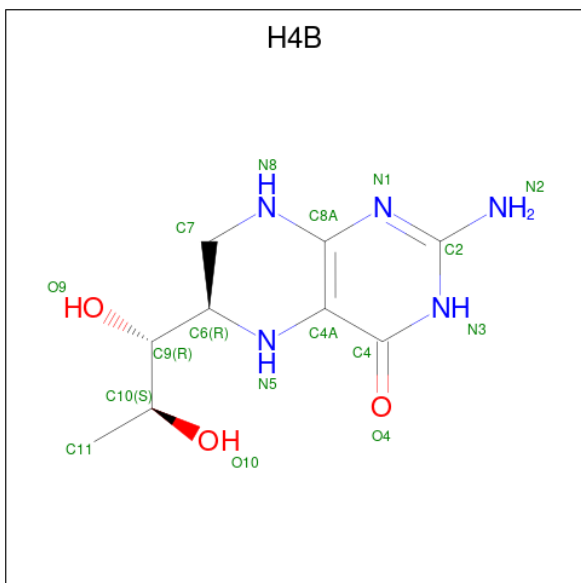
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	variant	UNP P29474
B	298	GLU	ASP	variant	UNP P29474
C	298	GLU	ASP	variant	UNP P29474
D	298	GLU	ASP	variant	UNP P29474

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



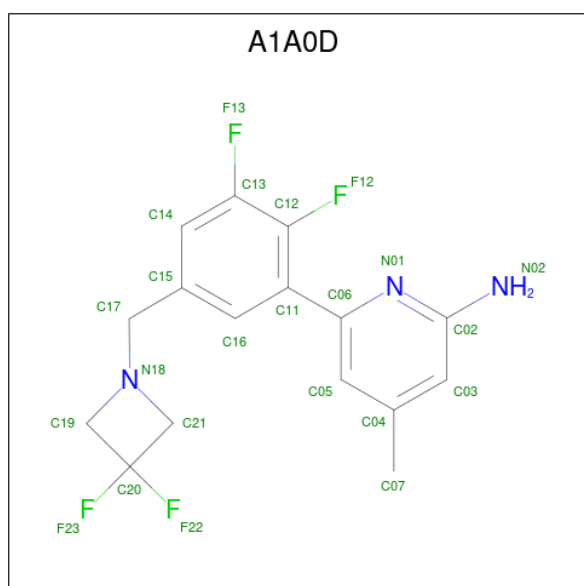
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$).



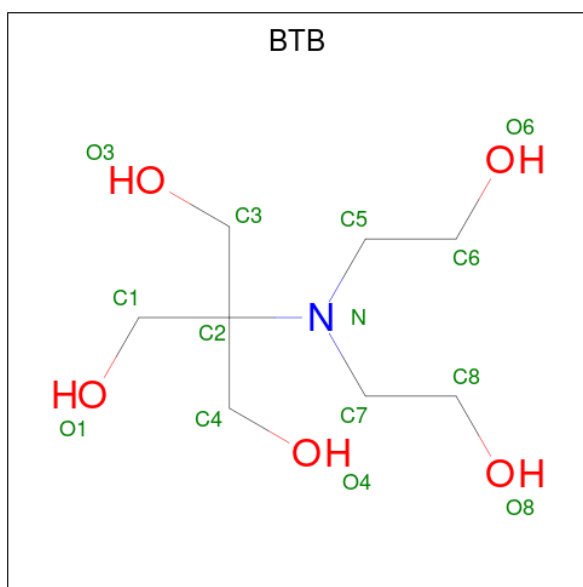
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is (6M)-6-{5-[(3,3-difluoroazetidin-1-yl)methyl]-2,3-difluorophenyl}-4-methylpyridin-2-amine (CCD ID: A1A0D) (formula: C₁₆H₁₅F₄N₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			23	16	4	3		
4	B	1	Total	C	F	N	0	0
			23	16	4	3		
4	C	1	Total	C	F	N	0	0
			23	16	4	3		
4	D	1	Total	C	F	N	0	0
			23	16	4	3		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C₈H₁₉NO₅).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 8 is GADOLINIUM ION (CCD ID: GD3) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	Gd 1	0	0
8	B	2	Total 2	Gd 2	0	0
8	D	1	Total 1	Gd 1	0	0

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total 1	Zn 1	0	0
9	C	1	Total 1	Zn 1	0	0

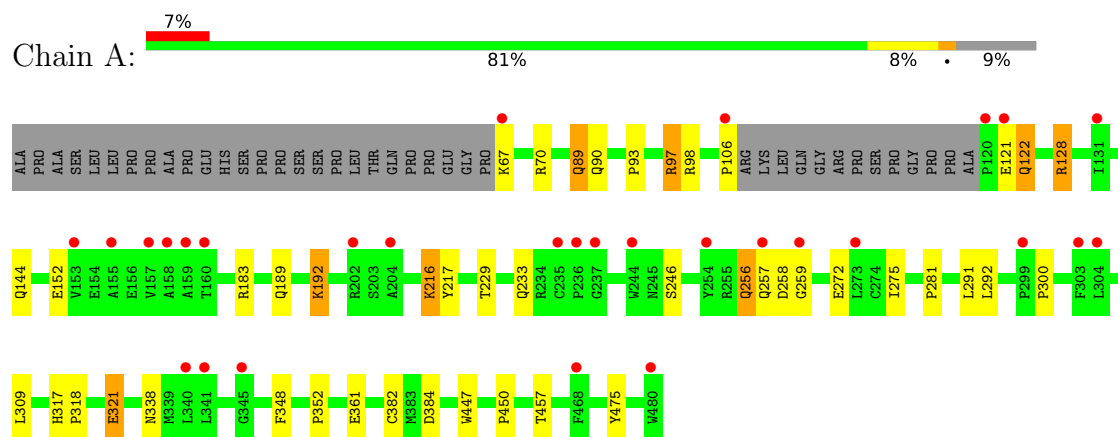
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	196	Total 196	O 196	0	0
10	B	290	Total 290	O 290	0	0
10	C	196	Total 196	O 196	0	0
10	D	305	Total 305	O 305	0	0

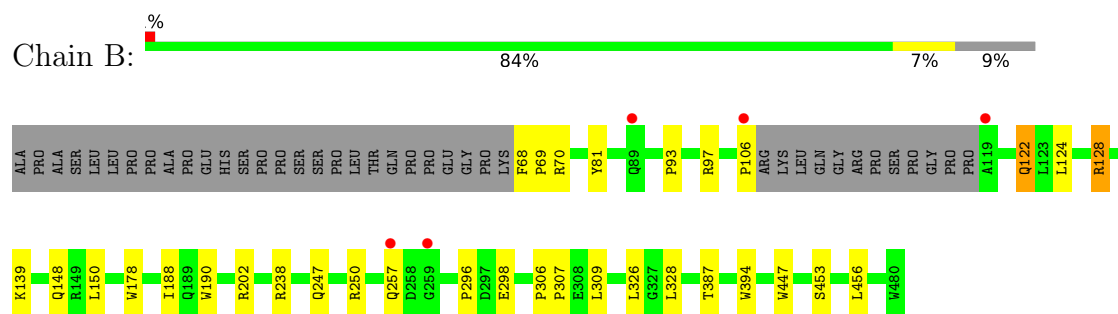
3 Residue-property plots

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.

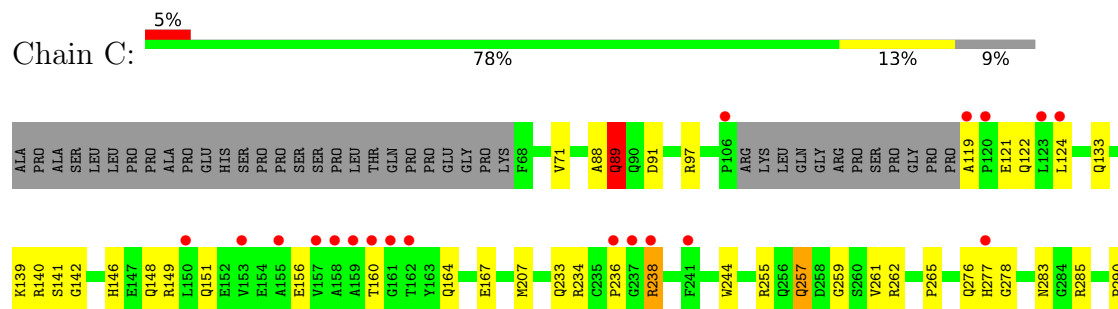
- Molecule 1: Nitric oxide synthase, endothelial

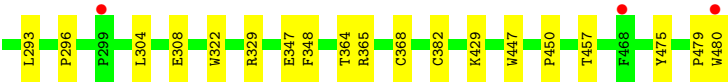


- Molecule 1: Nitric oxide synthase, endothelial

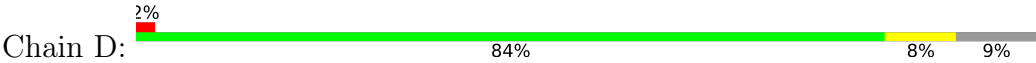


- Molecule 1: Nitric oxide synthase, endothelial





● Molecule 1: Nitric oxide synthase, endothelial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.43Å 152.82Å 108.32Å 90.00° 90.76° 90.00°	Depositor
Resolution (Å)	49.07 – 1.73 49.07 – 1.73	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.07-1.73) 98.5 (49.07-1.73)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.73Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.194 , 0.222 0.188 , 0.216	Depositor DCC
R_{free} test set	9947 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14367	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: BTB, ZN, A1A0D, GOL, CL, H4B, GD3, 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	0.25	0/3302	0.44	0/4498
1	B	0.32	0/3312	0.50	0/4514
1	C	0.26	0/3298	0.44	0/4495
1	D	0.33	0/3315	0.50	0/4517
All	All	0.29	0/13227	0.47	0/18024

There are no bond length outliers.

There are no bond angle outliers.

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	3207	0	3112	23	1
1	B	3211	0	3114	18	0
1	C	3203	0	3103	35	0
1	D	3217	0	3121	19	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
2	C	43	0	30	4	0
2	D	43	0	30	2	0
3	A	17	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	1	0
3	C	17	0	15	2	0
3	D	17	0	15	0	0
4	A	23	0	0	1	0
4	B	23	0	0	1	0
4	C	23	0	0	2	0
4	D	23	0	0	1	0
5	A	42	0	56	9	0
5	B	42	0	56	10	0
5	C	28	0	38	4	0
5	D	28	0	36	5	1
6	A	18	0	23	0	0
6	B	12	0	16	0	0
6	C	24	0	31	2	0
6	D	6	0	8	0	0
7	A	1	0	0	0	0
7	B	1	0	0	1	0
7	C	1	0	0	1	0
7	D	1	0	0	1	0
8	A	1	0	0	0	0
8	B	2	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	196	0	0	2	0
10	B	290	0	0	2	0
10	C	196	0	0	3	0
10	D	305	0	0	3	0
All	All	14367	0	12894	123	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 5.

All (123) 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)
5:B:510:BTB:O3	10:B:601:HOH:O	2.03	0.77
4:C:503:A1A0D:F13	7:C:510:CL:CL	2.30	0.76
1:B:70:ARG:NH1	10:B:602:HOH:O	2.19	0.74
1:A:97:ARG:HG2	1:A:98:ARG:HG2	1.71	0.73
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.78	0.64
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.78	0.64
1:B:298:GLU:OE1	5:B:505:BTB:H42	1.98	0.64
1:A:321:GLU:H	1:A:321:GLU:CD	2.05	0.64
1:A:70:ARG:NH2	10:A:602:HOH:O	2.31	0.63
1:C:347:GLU:OE2	10:C:601:HOH:O	2.14	0.63
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.82	0.61
1:C:91:ASP:OD1	1:D:97:ARG:NH1	2.33	0.61
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.86	0.58
1:B:298:GLU:OE1	5:B:505:BTB:H72	2.02	0.58
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.85	0.58
1:C:238:ARG:HH12	1:C:296:PRO:HG2	1.68	0.57
1:B:238:ARG:HG2	1:B:296:PRO:HB3	1.86	0.57
1:A:275:ILE:HD11	1:A:281:PRO:HB3	1.86	0.55
1:C:257:GLN:OE1	6:C:507:GOL:O2	2.24	0.55
4:D:503:A1A0D:F13	7:D:507:CL:CL	2.52	0.54
1:B:453:SER:HB3	1:B:456:LEU:HD12	1.89	0.54
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.89	0.54
1:A:128:ARG:HH11	1:A:128:ARG:HB2	1.71	0.54
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.89	0.54
1:C:207:MET:HE3	1:C:293:LEU:HB3	1.90	0.54
1:C:276:GLN:O	1:C:278:GLY:N	2.38	0.53
1:A:256:GLN:C	1:A:258:ASP:H	2.16	0.53
1:C:234:ARG:NH1	1:C:347:GLU:OE1	2.42	0.53
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.90	0.52
5:A:505:BTB:O4	5:A:505:BTB:O3	2.16	0.52
5:B:504:BTB:H12	10:C:683:HOH:O	2.09	0.52
1:A:183:ARG:HD3	1:A:447:TRP:CD2	2.45	0.52
1:C:475:TYR:OH	2:C:501:HEM:O1D	2.28	0.51
4:B:503:A1A0D:F13	7:B:508:CL:CL	2.56	0.51
1:C:283:ASN:O	1:C:283:ASN:ND2	2.44	0.51
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.31	0.49
1:A:361:GLU:OE2	4:A:503:A1A0D:N02	2.46	0.48
5:C:505:BTB:O4	5:C:505:BTB:O3	2.30	0.48
1:A:384:ASP:OD1	5:A:504:BTB:O3	2.32	0.48
1:D:93:PRO:HB3	1:D:106:PRO:HB3	1.96	0.48
1:C:119:ALA:HB1	1:C:122:GLN:HG3	1.95	0.48
1:A:93:PRO:HB3	1:A:106:PRO:HB3	1.95	0.48
5:C:504:BTB:H42	5:C:504:BTB:H51	1.46	0.47
5:D:505:BTB:H82	5:D:505:BTB:H51	1.63	0.47
1:D:275:ILE:HD12	1:D:281:PRO:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:GLN:NE2	10:D:607:HOH:O	2.35	0.46
1:D:91:ASP:OD1	10:D:601:HOH:O	2.21	0.46
1:C:233:GLN:HB3	1:C:348:PHE:CE2	2.51	0.46
1:A:89:GLN:HG3	1:A:90:GLN:N	2.30	0.46
1:A:122:GLN:H	1:A:122:GLN:HG3	1.45	0.46
1:C:429:LYS:HA	1:C:429:LYS:HD2	1.77	0.46
5:B:510:BTB:O8	5:B:510:BTB:H62	2.15	0.46
1:C:97:ARG:HG3	1:D:88:ALA:HB3	1.99	0.45
1:C:365:ARG:HH12	3:C:502:H4B:C4	2.29	0.45
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.52	0.45
1:A:259:GLY:N	10:A:609:HOH:O	2.41	0.45
5:B:505:BTB:H12	5:B:505:BTB:H51	1.74	0.45
5:B:510:BTB:H12	1:C:382:CYS:HA	1.99	0.45
1:D:271:THR:O	1:D:275:ILE:HG12	2.17	0.45
5:A:506:BTB:H72	5:A:506:BTB:H41	1.44	0.45
1:C:88:ALA:HB3	1:D:97:ARG:CD	2.47	0.45
1:D:453:SER:HB3	1:D:456:LEU:HD12	1.99	0.45
1:B:124:LEU:HB3	1:B:128:ARG:HH12	1.81	0.44
1:B:326:LEU:HB3	1:B:328:LEU:HG	1.99	0.44
1:C:290:PRO:HB3	1:C:304:LEU:HD12	1.99	0.44
1:A:292:LEU:HD22	1:A:300:PRO:HB2	1.98	0.44
1:C:450:PRO:HG2	1:C:457:THR:HG21	2.00	0.44
5:A:504:BTB:H12	5:A:504:BTB:H72	1.35	0.44
1:C:236:PRO:C	1:C:238:ARG:H	2.25	0.44
1:C:364:THR:O	1:C:368:CYS:HB2	2.16	0.44
1:C:447:TRP:HH2	4:C:503:A1A0D:F22	1.90	0.44
1:C:238:ARG:NH1	1:C:296:PRO:HG2	2.33	0.44
1:C:261:VAL:HG11	1:C:265:PRO:HA	2.00	0.43
5:C:505:BTB:O4	5:C:505:BTB:O1	2.33	0.43
1:C:479:PRO:HD2	1:C:480:TRP:CZ3	2.54	0.43
2:C:501:HEM:HBB2	2:C:501:HEM:CHC	2.45	0.43
1:C:89:GLN:H	1:C:89:GLN:HG2	1.56	0.43
1:C:142:GLY:H	1:C:146:HIS:HD1	1.67	0.43
1:A:216:LYS:HG3	1:A:217:TYR:N	2.34	0.43
1:C:167:GLU:OE1	6:C:506:GOL:O2	2.32	0.43
1:B:128:ARG:HG3	1:B:150:LEU:HD22	2.00	0.43
1:D:317:HIS:CG	1:D:318:PRO:HD2	2.54	0.43
5:A:505:BTB:H11	5:A:505:BTB:H51	1.51	0.42
1:B:447:TRP:HA	3:B:502:H4B:N1	2.34	0.42
5:B:505:BTB:O8	5:B:505:BTB:O3	2.34	0.42
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:TRP:CD1	1:C:479:PRO:HG2	2.54	0.42
1:C:262:ARG:NH1	1:C:285:ARG:HG3	2.34	0.42
5:D:505:BTB:H72	5:D:505:BTB:H11	1.77	0.42
5:B:505:BTB:H42	5:B:505:BTB:H72	1.68	0.42
1:C:156:GLU:OE2	1:C:164:GLN:HG2	2.18	0.42
1:B:70:ARG:HD3	1:B:81:TYR:CZ	2.54	0.42
1:B:306:PRO:HA	1:B:307:PRO:HD3	1.96	0.42
1:A:246:SER:HA	1:A:338:ASN:HB3	2.02	0.42
1:A:382:CYS:HA	5:A:504:BTB:H11	2.01	0.42
1:C:257:GLN:C	1:C:259:GLY:H	2.28	0.42
1:D:470:SER:HA	1:D:471:PRO:C	2.44	0.42
1:A:189:GLN:OE1	1:A:192:LYS:HE3	2.20	0.42
1:B:122:GLN:CD	1:B:122:GLN:N	2.77	0.42
1:A:475:TYR:OH	2:A:501:HEM:O2D	2.34	0.41
1:A:229:THR:O	1:A:352:PRO:HD2	2.20	0.41
1:C:149:ARG:NH2	1:C:164:GLN:O	2.39	0.41
5:C:504:BTB:O6	5:C:504:BTB:O1	2.29	0.41
1:D:326:LEU:HB3	1:D:328:LEU:HG	2.03	0.41
1:A:317:HIS:CG	1:A:318:PRO:HD2	2.55	0.41
5:D:504:BTB:H32	5:D:504:BTB:H51	1.91	0.41
1:D:238:ARG:HG2	10:D:883:HOH:O	2.21	0.41
1:B:93:PRO:HG3	1:B:106:PRO:HB3	2.01	0.41
1:C:447:TRP:HA	3:C:502:H4B:N1	2.36	0.41
1:D:298:GLU:CD	5:D:505:BTB:H41	2.45	0.41
1:C:133:GLN:NE2	10:C:613:HOH:O	2.53	0.40
1:D:233:GLN:HB3	1:D:348:PHE:CE2	2.56	0.40
5:A:505:BTB:H41	5:A:505:BTB:H72	1.74	0.40
1:B:68:PHE:HA	1:B:69:PRO:HD3	1.92	0.40
5:B:510:BTB:H61	1:C:322:TRP:CD1	2.56	0.40
1:D:229:THR:O	1:D:351:ALA:HA	2.21	0.40
5:A:504:BTB:H51	5:A:504:BTB:H32	1.63	0.40
1:D:449:VAL:HA	1:D:450:PRO:HD3	1.94	0.40
1:A:450:PRO:HG2	1:A:457:THR:HG21	2.03	0.40
1:B:70:ARG:HD3	1:B:81:TYR:OH	2.21	0.40
1:B:387:THR:HA	1:B:394:TRP:CD1	2.56	0.40
5:A:506:BTB:H11	5:A:506:BTB:H51	1.38	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:152:GLU:OE2	5:D:505:BTB:O4[2_851]	2.12	0.08

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	398/440 (90%)	383 (96%)	14 (4%)	1 (0%)	36	23
1	B	400/440 (91%)	394 (98%)	6 (2%)	0	100	100
1	C	398/440 (90%)	386 (97%)	10 (2%)	2 (0%)	24	12
1	D	400/440 (91%)	393 (98%)	7 (2%)	0	100	100
All	All	1596/1760 (91%)	1556 (98%)	37 (2%)	3 (0%)	43	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	GLN
1	C	277	HIS
1	A	257	GLN

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	342/373 (92%)	328 (96%)	14 (4%)	27	6
1	B	343/373 (92%)	334 (97%)	9 (3%)	40	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	341/373 (91%)	326 (96%)	15 (4%)	25	5
1	D	343/373 (92%)	336 (98%)	7 (2%)	48	26
All	All	1369/1492 (92%)	1324 (97%)	45 (3%)	33	10

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LYS
1	A	89	GLN
1	A	97	ARG
1	A	121	GLU
1	A	122	GLN
1	A	128	ARG
1	A	144	GLN
1	A	192	LYS
1	A	216	LYS
1	A	256	GLN
1	A	272	GLU
1	A	291	LEU
1	A	309	LEU
1	A	321	GLU
1	B	97	ARG
1	B	122	GLN
1	B	128	ARG
1	B	139	LYS
1	B	148	GLN
1	B	188	ILE
1	B	202	ARG
1	B	257	GLN
1	B	309	LEU
1	C	71	VAL
1	C	89	GLN
1	C	121	GLU
1	C	124	LEU
1	C	139	LYS
1	C	140	ARG
1	C	141	SER
1	C	148	GLN
1	C	151	GLN
1	C	160	THR
1	C	238	ARG

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Mol	Chain	Res	Type
1	C	255	ARG
1	C	257	GLN
1	C	308	GLU
1	C	329	ARG
1	D	98	ARG
1	D	200	ASP
1	D	257	GLN
1	D	309	LEU
1	D	326	LEU
1	D	342	GLU
1	D	414	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	B	122	GLN
1	C	133	GLN
1	C	403	ASN
1	D	90	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 10 are monoatomic - leaving 32 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
5	BTB	B	504	8	13,13,13	0.48	0	7,16,16	0.53	0
6	GOL	B	507	-	5,5,5	0.85	0	5,5,5	1.02	0
2	HEM	D	501	1	50,50,50	1.49	10 (20%)	67,82,82	1.24	7 (10%)
6	GOL	C	506	-	5,5,5	1.08	0	5,5,5	1.08	0
4	A1A0D	D	503	-	25,25,25	1.06	2 (8%)	33,38,38	2.78	12 (36%)
6	GOL	A	507	-	5,5,5	0.84	0	5,5,5	1.12	1 (20%)
3	H4B	C	502	-	17,18,18	0.94	0	14,26,26	1.82	4 (28%)
6	GOL	B	506	-	5,5,5	0.94	0	5,5,5	0.98	0
6	GOL	A	508	-	5,5,5	1.13	1 (20%)	5,5,5	0.93	0
4	A1A0D	B	503	-	25,25,25	1.03	2 (8%)	33,38,38	2.35	9 (27%)
2	HEM	C	501	1	50,50,50	1.57	8 (16%)	67,82,82	1.38	10 (14%)
5	BTB	A	504	8	13,13,13	0.50	0	7,16,16	1.29	1 (14%)
6	GOL	C	508	-	5,5,5	0.86	0	5,5,5	1.08	0
6	GOL	D	506	-	5,5,5	0.93	0	5,5,5	1.04	0
5	BTB	D	505	-	13,13,13	0.57	0	7,16,16	1.16	0
5	BTB	A	506	-	13,13,13	0.36	0	7,16,16	0.65	0
2	HEM	A	501	1	50,50,50	1.60	8 (16%)	67,82,82	1.41	9 (13%)
3	H4B	B	502	-	17,18,18	1.04	2 (11%)	14,26,26	1.99	5 (35%)
3	H4B	A	502	-	17,18,18	0.89	0	14,26,26	1.91	4 (28%)
5	BTB	D	504	8	13,13,13	0.40	0	7,16,16	0.84	0
6	GOL	A	509	-	5,5,5	0.90	0	5,5,5	1.05	0
4	A1A0D	A	503	-	25,25,25	1.04	1 (4%)	33,38,38	2.57	11 (33%)
2	HEM	B	501	1	50,50,50	1.51	8 (16%)	67,82,82	1.23	5 (7%)
5	BTB	C	505	-	13,13,13	0.36	0	7,16,16	0.47	0
5	BTB	A	505	-	13,13,13	0.52	0	7,16,16	0.72	0
6	GOL	C	509	-	5,5,5	0.88	0	5,5,5	0.94	0
4	A1A0D	C	503	-	25,25,25	0.90	1 (4%)	33,38,38	2.49	5 (15%)
6	GOL	C	507	-	5,5,5	2.26	1 (20%)	5,5,5	1.81	1 (20%)
5	BTB	B	505	-	13,13,13	0.67	0	7,16,16	1.69	1 (14%)
5	BTB	C	504	-	13,13,13	0.72	1 (7%)	7,16,16	1.09	0
3	H4B	D	502	-	17,18,18	0.91	0	14,26,26	1.77	4 (28%)
5	BTB	B	510	8	13,13,13	0.41	0	7,16,16	0.74	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
5	BTB	B	504	8	-	3/21/21/21	-
6	GOL	B	507	-	-	4/4/4/4	-
2	HEM	D	501	1	-	0/14/54/54	-
6	GOL	C	506	-	-	4/4/4/4	-
4	A1A0D	D	503	-	-	0/8/18/18	0/3/3/3
6	GOL	A	507	-	-	4/4/4/4	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
6	GOL	B	506	-	-	2/4/4/4	-
6	GOL	A	508	-	-	0/4/4/4	-
4	A1A0D	B	503	-	-	2/8/18/18	0/3/3/3
2	HEM	C	501	1	-	2/14/54/54	-
5	BTB	A	504	8	-	8/21/21/21	-
6	GOL	C	508	-	-	2/4/4/4	-
6	GOL	D	506	-	-	0/4/4/4	-
5	BTB	D	505	-	-	5/21/21/21	-
5	BTB	A	506	-	-	11/21/21/21	-
2	HEM	A	501	1	-	2/14/54/54	-
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
5	BTB	D	504	8	-	5/21/21/21	-
6	GOL	A	509	-	-	2/4/4/4	-
4	A1A0D	A	503	-	-	1/8/18/18	0/3/3/3
2	HEM	B	501	1	-	0/14/54/54	-
5	BTB	C	505	-	-	12/21/21/21	-
5	BTB	A	505	-	-	10/21/21/21	-
6	GOL	C	509	-	-	4/4/4/4	-
4	A1A0D	C	503	-	-	1/8/18/18	0/3/3/3
6	GOL	C	507	-	-	4/4/4/4	-
5	BTB	B	505	-	-	11/21/21/21	-
5	BTB	C	504	-	-	15/21/21/21	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
5	BTB	B	510	8	-	3/21/21/21	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	FE-NB	4.89	2.10	1.94
2	C	501	HEM	FE-NA	4.62	2.10	1.95
6	C	507	GOL	O2-C2	-4.43	1.30	1.43
2	A	501	HEM	FE-NC	4.22	2.09	1.95
2	A	501	HEM	FE-ND	4.22	2.07	1.94
2	B	501	HEM	FE-NB	4.01	2.07	1.94
2	A	501	HEM	FE-NB	4.00	2.07	1.94
2	D	501	HEM	FE-NB	3.89	2.06	1.94
2	A	501	HEM	FE-NA	3.47	2.06	1.95
2	B	501	HEM	FE-ND	3.40	2.05	1.94
2	B	501	HEM	FE-NA	3.36	2.06	1.95
2	D	501	HEM	FE-NA	3.35	2.06	1.95
4	D	503	A1A0D	C21-C20	-3.19	1.50	1.54
2	A	501	HEM	CAB-C3B	3.13	1.55	1.47
2	D	501	HEM	FE-NC	3.11	2.05	1.95
2	A	501	HEM	CAC-C3C	3.08	1.55	1.47
2	C	501	HEM	FE-NC	3.07	2.05	1.95
2	C	501	HEM	CAC-C3C	2.99	1.55	1.47
2	B	501	HEM	CAC-C3C	2.97	1.55	1.47
2	D	501	HEM	CAC-C3C	2.93	1.55	1.47
2	C	501	HEM	CAB-C3B	2.92	1.55	1.47
2	B	501	HEM	CAB-C3B	2.83	1.54	1.47
2	D	501	HEM	FE-ND	2.77	2.03	1.94
2	B	501	HEM	FE-NC	2.70	2.04	1.95
3	B	502	H4B	C7-C6	2.58	1.54	1.52
2	B	501	HEM	CMB-C2B	2.57	1.56	1.50
4	B	503	A1A0D	C19-C20	-2.47	1.51	1.54
4	A	503	A1A0D	C21-C20	-2.47	1.51	1.54
2	D	501	HEM	CAB-C3B	2.45	1.53	1.47
4	C	503	A1A0D	C21-C20	-2.45	1.51	1.54
2	C	501	HEM	FE-ND	2.43	2.02	1.94
6	A	508	GOL	O2-C2	-2.37	1.36	1.43
2	D	501	HEM	CMA-C3A	2.34	1.55	1.50
2	C	501	HEM	CMC-C2C	2.31	1.55	1.50
2	B	501	HEM	CMA-C3A	2.30	1.55	1.50
2	D	501	HEM	C2A-C3A	-2.29	1.32	1.38
4	B	503	A1A0D	C21-C20	-2.25	1.51	1.54
2	A	501	HEM	CMC-C2C	2.25	1.55	1.50
2	C	501	HEM	CMB-C2B	2.20	1.55	1.50
2	D	501	HEM	CMB-C2B	2.13	1.55	1.50
4	D	503	A1A0D	C19-C20	-2.04	1.52	1.54
3	B	502	H4B	C4-N3	-2.04	1.35	1.38
2	D	501	HEM	CMD-C2D	2.03	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	504	BTB	C3-C2	-2.02	1.50	1.53
2	A	501	HEM	CMB-C2B	2.01	1.54	1.50

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	A1A0D	C06-C11-C12	-11.06	111.04	124.24
4	D	503	A1A0D	C06-C11-C12	-10.25	112.00	124.24
4	B	503	A1A0D	C06-C11-C12	-9.17	113.29	124.24
4	A	503	A1A0D	C06-C11-C12	-9.02	113.48	124.24
4	D	503	A1A0D	C15-C14-C13	6.54	123.65	119.37
4	A	503	A1A0D	C06-N01-C02	6.50	122.56	118.52
4	B	503	A1A0D	C06-N01-C02	5.15	121.72	118.52
4	D	503	A1A0D	C06-N01-C02	5.06	121.66	118.52
4	C	503	A1A0D	C06-N01-C02	4.64	121.40	118.52
4	C	503	A1A0D	C15-C14-C13	4.12	122.07	119.37
3	B	502	H4B	C2-N1-C8A	4.01	120.44	113.36
2	A	501	HEM	CAD-CBD-CGD	-3.94	103.22	113.67
3	A	502	H4B	C2-N1-C8A	3.92	120.28	113.36
3	D	502	H4B	C2-N1-C8A	3.84	120.14	113.36
4	A	503	A1A0D	C15-C14-C13	3.83	121.88	119.37
4	A	503	A1A0D	C05-C06-N01	-3.66	118.09	122.34
4	A	503	A1A0D	N02-C02-N01	3.61	122.39	116.59
3	C	502	H4B	C2-N1-C8A	3.59	119.70	113.36
5	B	505	BTB	O1-C1-C2	-3.56	103.02	111.40
4	C	503	A1A0D	C16-C11-C06	3.45	129.33	119.85
2	C	501	HEM	C3D-C4D-ND	-3.41	106.43	110.17
2	B	501	HEM	CHC-C1C-NC	3.30	128.04	124.45
6	C	507	GOL	O1-C1-C2	-3.26	95.71	110.38
4	A	503	A1A0D	C17-C15-C16	3.22	126.34	120.27
2	A	501	HEM	C3B-C2B-C1B	3.21	108.82	106.41
4	B	503	A1A0D	C05-C06-N01	-3.09	118.76	122.34
4	D	503	A1A0D	C16-C11-C12	3.03	120.66	117.44
4	A	503	A1A0D	C16-C11-C06	3.02	128.16	119.85
4	D	503	A1A0D	C17-C15-C16	3.00	125.93	120.27
2	B	501	HEM	CBA-CAA-C2A	-2.96	104.34	112.53
4	B	503	A1A0D	C17-C15-C14	-2.96	114.70	120.27
2	A	501	HEM	C3D-C4D-ND	-2.87	107.02	110.17
4	A	503	A1A0D	C17-C15-C14	-2.86	114.89	120.27
2	C	501	HEM	C4D-ND-C1D	2.86	108.59	105.21
2	D	501	HEM	CHC-C1C-NC	2.83	127.53	124.45
5	A	504	BTB	O3-C3-C2	2.83	118.05	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CBA-CAA-C2A	-2.81	104.75	112.53
2	A	501	HEM	C1B-NB-C4B	2.80	108.52	105.21
4	B	503	A1A0D	C17-C15-C16	2.79	125.53	120.27
2	C	501	HEM	CAD-CBD-CGD	-2.73	106.42	113.67
4	D	503	A1A0D	C16-C11-C06	2.72	127.32	119.85
3	B	502	H4B	C4A-C4-N3	2.72	119.59	112.13
4	D	503	A1A0D	N02-C02-N01	2.70	120.93	116.59
2	C	501	HEM	CBD-CAD-C3D	-2.69	105.11	112.53
4	B	503	A1A0D	C16-C11-C06	2.67	127.19	119.85
2	B	501	HEM	C2A-C1A-NA	-2.64	107.22	110.15
4	D	503	A1A0D	C05-C04-C03	2.64	121.05	118.11
3	D	502	H4B	C4A-C4-N3	2.63	119.36	112.13
3	B	502	H4B	O4-C4-C4A	-2.62	120.93	127.26
3	C	502	H4B	O4-C4-C4A	-2.60	120.98	127.26
2	A	501	HEM	C3B-C4B-NB	-2.59	107.61	109.47
2	C	501	HEM	CBA-CAA-C2A	-2.56	105.46	112.53
2	B	501	HEM	CAD-CBD-CGD	-2.55	106.91	113.67
4	B	503	A1A0D	N02-C02-N01	2.52	120.63	116.59
3	A	502	H4B	O4-C4-C4A	-2.50	121.23	127.26
3	A	502	H4B	O10-C10-C9	-2.46	105.70	109.77
2	C	501	HEM	C2A-C1A-NA	-2.46	107.42	110.15
2	D	501	HEM	CBD-CAD-C3D	-2.46	105.73	112.53
2	C	501	HEM	C3B-C4B-NB	-2.46	107.70	109.47
3	A	502	H4B	C4A-C4-N3	2.45	118.86	112.13
2	D	501	HEM	C2A-C1A-NA	-2.41	107.48	110.15
3	D	502	H4B	O4-C4-C4A	-2.40	121.48	127.26
4	D	503	A1A0D	C05-C06-N01	-2.39	119.57	122.34
2	A	501	HEM	C4D-ND-C1D	2.37	108.01	105.21
3	C	502	H4B	C4A-C4-N3	2.35	118.59	112.13
3	C	502	H4B	O10-C10-C9	-2.33	105.92	109.77
2	D	501	HEM	C3B-C2B-C1B	2.31	108.15	106.41
4	A	503	A1A0D	C05-C04-C03	2.29	120.66	118.11
4	B	503	A1A0D	C15-C14-C13	2.27	120.86	119.37
3	D	502	H4B	C2-N3-C4	-2.27	121.00	125.11
2	A	501	HEM	C2A-C1A-NA	-2.26	107.65	110.15
6	A	507	GOL	C3-C2-C1	-2.23	103.60	111.80
2	A	501	HEM	C2B-C1B-NB	-2.19	107.32	109.84
4	D	503	A1A0D	F13-C13-C12	2.18	121.28	118.32
2	A	501	HEM	CBA-CAA-C2A	-2.17	106.53	112.53
2	C	501	HEM	CHA-C4D-ND	2.13	127.01	124.37
4	D	503	A1A0D	C17-C15-C14	-2.13	116.26	120.27
2	D	501	HEM	C3D-C4D-ND	-2.12	107.84	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C3B-C2B-C1B	2.12	108.00	106.41
3	B	502	H4B	O9-C9-C6	2.09	114.28	109.28
4	A	503	A1A0D	F13-C13-C12	2.07	121.13	118.32
4	D	503	A1A0D	C11-C16-C15	-2.07	118.35	121.81
4	C	503	A1A0D	C16-C11-C12	2.06	119.63	117.44
2	D	501	HEM	CAD-CBD-CGD	-2.06	108.21	113.67
2	C	501	HEM	C3B-C2B-C1B	2.04	107.94	106.41
4	B	503	A1A0D	C05-C04-C03	2.03	120.37	118.11
2	C	501	HEM	O1D-CGD-CBD	-2.02	116.68	123.09
4	A	503	A1A0D	C03-C02-N02	-2.01	117.47	121.81
3	B	502	H4B	N3-C2-N1	-2.01	119.64	123.32

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	A1A0D	C05-C06-C11-C12
4	B	503	A1A0D	C15-C17-N18-C19
5	A	504	BTB	O1-C1-C2-N
5	A	504	BTB	C1-C2-C4-O4
5	A	504	BTB	C3-C2-C4-O4
5	A	504	BTB	N-C2-C4-O4
5	A	505	BTB	C1-C2-C4-O4
5	A	505	BTB	C3-C2-C4-O4
5	A	505	BTB	N-C2-C4-O4
5	A	506	BTB	O1-C1-C2-N
5	A	506	BTB	C1-C2-C3-O3
5	A	506	BTB	N-C2-C3-O3
5	A	506	BTB	C1-C2-N-C5
5	A	506	BTB	C1-C2-N-C7
5	A	506	BTB	C3-C2-N-C5
5	A	506	BTB	C3-C2-N-C7
5	A	506	BTB	C4-C2-N-C5
5	A	506	BTB	C4-C2-N-C7
5	B	504	BTB	O1-C1-C2-C3
5	B	504	BTB	O1-C1-C2-C4
5	B	504	BTB	O1-C1-C2-N
5	B	505	BTB	C1-C2-C3-O3
5	B	505	BTB	C4-C2-C3-O3
5	B	505	BTB	N-C2-C3-O3
5	B	505	BTB	C1-C2-N-C5
5	B	505	BTB	C1-C2-N-C7

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Mol	Chain	Res	Type	Atoms
5	B	505	BTB	C3-C2-N-C5
5	B	505	BTB	C3-C2-N-C7
5	B	505	BTB	C4-C2-N-C5
5	B	505	BTB	C4-C2-N-C7
5	B	510	BTB	C4-C2-C3-O3
5	C	504	BTB	O1-C1-C2-C3
5	C	504	BTB	O1-C1-C2-C4
5	C	504	BTB	O1-C1-C2-N
5	C	504	BTB	C1-C2-C4-O4
5	C	504	BTB	C3-C2-C4-O4
5	C	504	BTB	N-C2-C4-O4
5	C	504	BTB	C1-C2-N-C5
5	C	504	BTB	C1-C2-N-C7
5	C	504	BTB	C3-C2-N-C5
5	C	504	BTB	C3-C2-N-C7
5	C	504	BTB	C4-C2-N-C5
5	C	504	BTB	C4-C2-N-C7
5	C	505	BTB	O1-C1-C2-N
5	C	505	BTB	C1-C2-C3-O3
5	C	505	BTB	C4-C2-C3-O3
5	C	505	BTB	N-C2-C3-O3
5	D	504	BTB	O1-C1-C2-C3
5	D	504	BTB	O1-C1-C2-C4
5	D	504	BTB	O1-C1-C2-N
5	D	504	BTB	C3-C2-C4-O4
5	D	505	BTB	C1-C2-C3-O3
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	N-C2-C3-O3
6	A	507	GOL	O1-C1-C2-O2
6	A	507	GOL	O1-C1-C2-C3
6	A	507	GOL	C1-C2-C3-O3
6	A	509	GOL	C1-C2-C3-O3
6	B	506	GOL	O1-C1-C2-C3
6	B	507	GOL	O1-C1-C2-C3
6	C	506	GOL	O1-C1-C2-C3
6	C	506	GOL	C1-C2-C3-O3
6	C	507	GOL	O1-C1-C2-C3
6	C	507	GOL	C1-C2-C3-O3
6	C	507	GOL	O2-C2-C3-O3
6	C	508	GOL	O1-C1-C2-C3
6	C	509	GOL	O1-C1-C2-O2
6	C	509	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	504	BTB	N-C7-C8-O8
5	A	505	BTB	N-C7-C8-O8
5	C	504	BTB	N-C5-C6-O6
6	B	507	GOL	C1-C2-C3-O3
6	C	509	GOL	C1-C2-C3-O3
5	B	505	BTB	N-C5-C6-O6
5	C	504	BTB	N-C7-C8-O8
6	A	507	GOL	O2-C2-C3-O3
6	B	506	GOL	O1-C1-C2-O2
6	B	507	GOL	O1-C1-C2-O2
6	B	507	GOL	O2-C2-C3-O3
5	D	505	BTB	N-C7-C8-O8
2	A	501	HEM	C4B-C3B-CAB-CBB
6	A	509	GOL	O2-C2-C3-O3
6	C	506	GOL	O1-C1-C2-O2
6	C	506	GOL	O2-C2-C3-O3
6	C	507	GOL	O1-C1-C2-O2
5	B	505	BTB	N-C7-C8-O8
5	C	505	BTB	O1-C1-C2-C3
6	C	509	GOL	O2-C2-C3-O3
5	D	505	BTB	C6-C5-N-C2
5	A	506	BTB	N-C5-C6-O6
5	A	504	BTB	C3-C2-N-C5
5	A	505	BTB	C1-C2-N-C5
5	A	505	BTB	C3-C2-N-C5
5	A	505	BTB	C3-C2-N-C7
5	A	505	BTB	C4-C2-N-C5
5	A	505	BTB	C4-C2-N-C7
5	B	510	BTB	N-C2-C3-O3
5	C	505	BTB	C1-C2-N-C7
5	C	505	BTB	C3-C2-N-C5
5	C	505	BTB	C3-C2-N-C7
5	C	505	BTB	C4-C2-N-C5
6	C	508	GOL	O1-C1-C2-O2
5	C	505	BTB	N-C5-C6-O6
2	A	501	HEM	C2A-CAA-CBA-CGA
5	B	510	BTB	C1-C2-C3-O3
5	C	505	BTB	N-C7-C8-O8
4	B	503	A1A0D	C05-C06-C11-C12
4	C	503	A1A0D	C05-C06-C11-C12
2	C	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
5	A	504	BTB	N-C5-C6-O6
5	A	506	BTB	O1-C1-C2-C4
5	C	504	BTB	C6-C5-N-C7
5	A	504	BTB	C1-C2-N-C5
5	A	505	BTB	C1-C2-N-C7
5	C	505	BTB	C1-C2-N-C5
5	D	504	BTB	N-C2-C4-O4

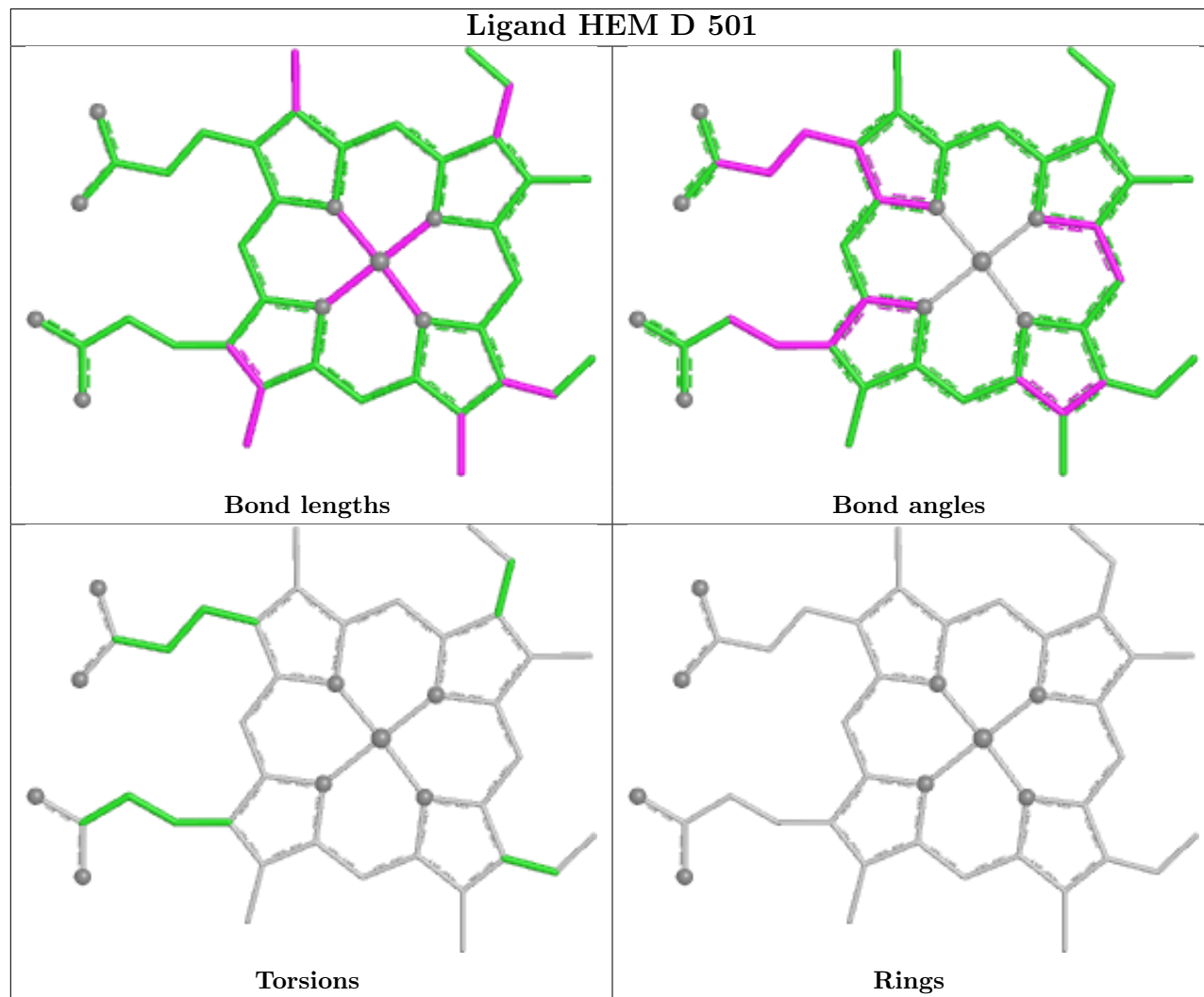
There are no ring outliers.

22 monomers are involved in 49 short contacts:

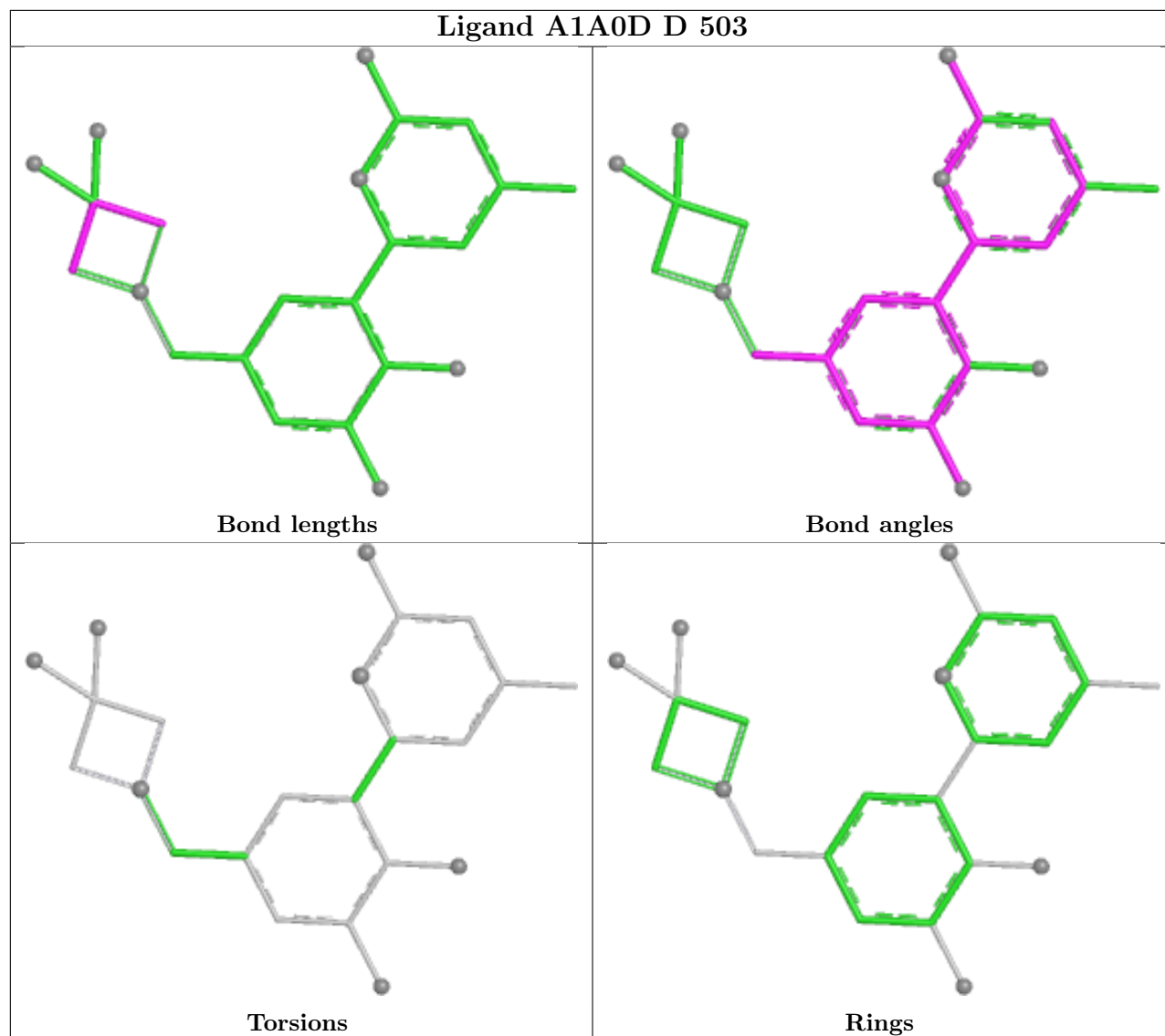
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504	BTB	1	0
2	D	501	HEM	2	0
6	C	506	GOL	1	0
4	D	503	A1A0D	1	0
3	C	502	H4B	2	0
4	B	503	A1A0D	1	0
2	C	501	HEM	4	0
5	A	504	BTB	4	0
5	D	505	BTB	3	1
5	A	506	BTB	2	0
2	A	501	HEM	3	0
3	B	502	H4B	1	0
5	D	504	BTB	2	0
4	A	503	A1A0D	1	0
2	B	501	HEM	1	0
5	C	505	BTB	2	0
5	A	505	BTB	3	0
4	C	503	A1A0D	2	0
6	C	507	GOL	1	0
5	B	505	BTB	5	0
5	C	504	BTB	2	0
5	B	510	BTB	4	0

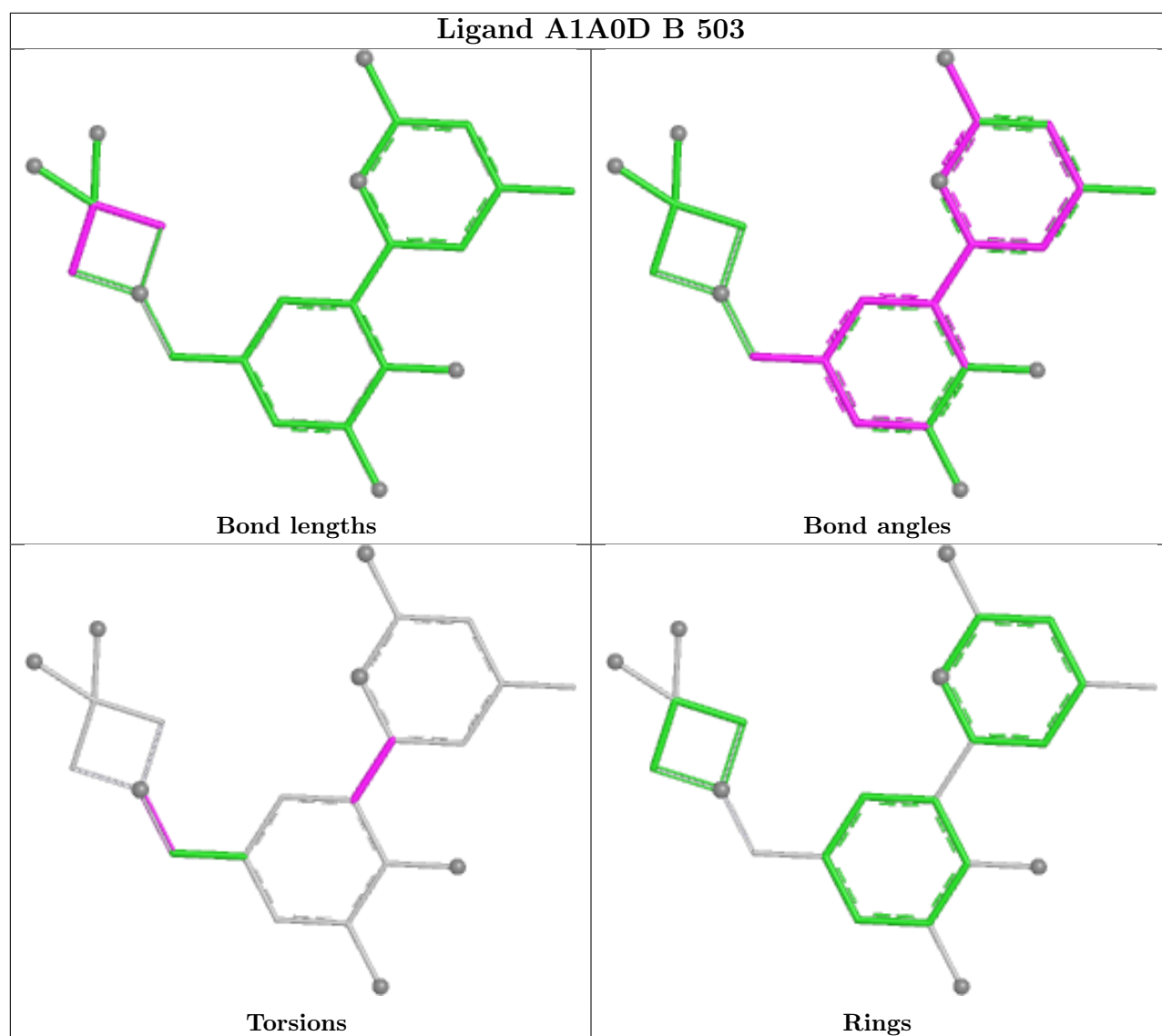
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

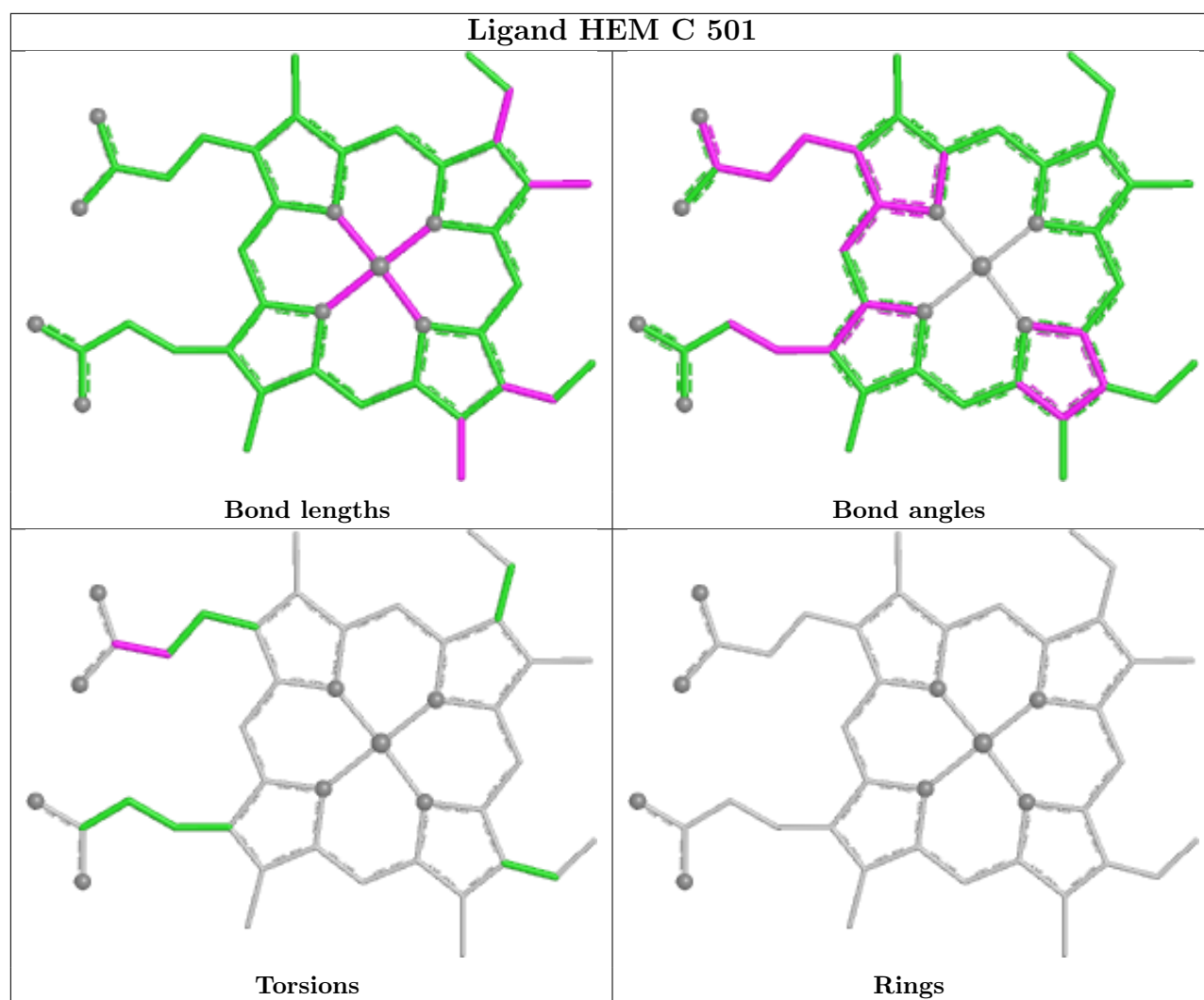
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

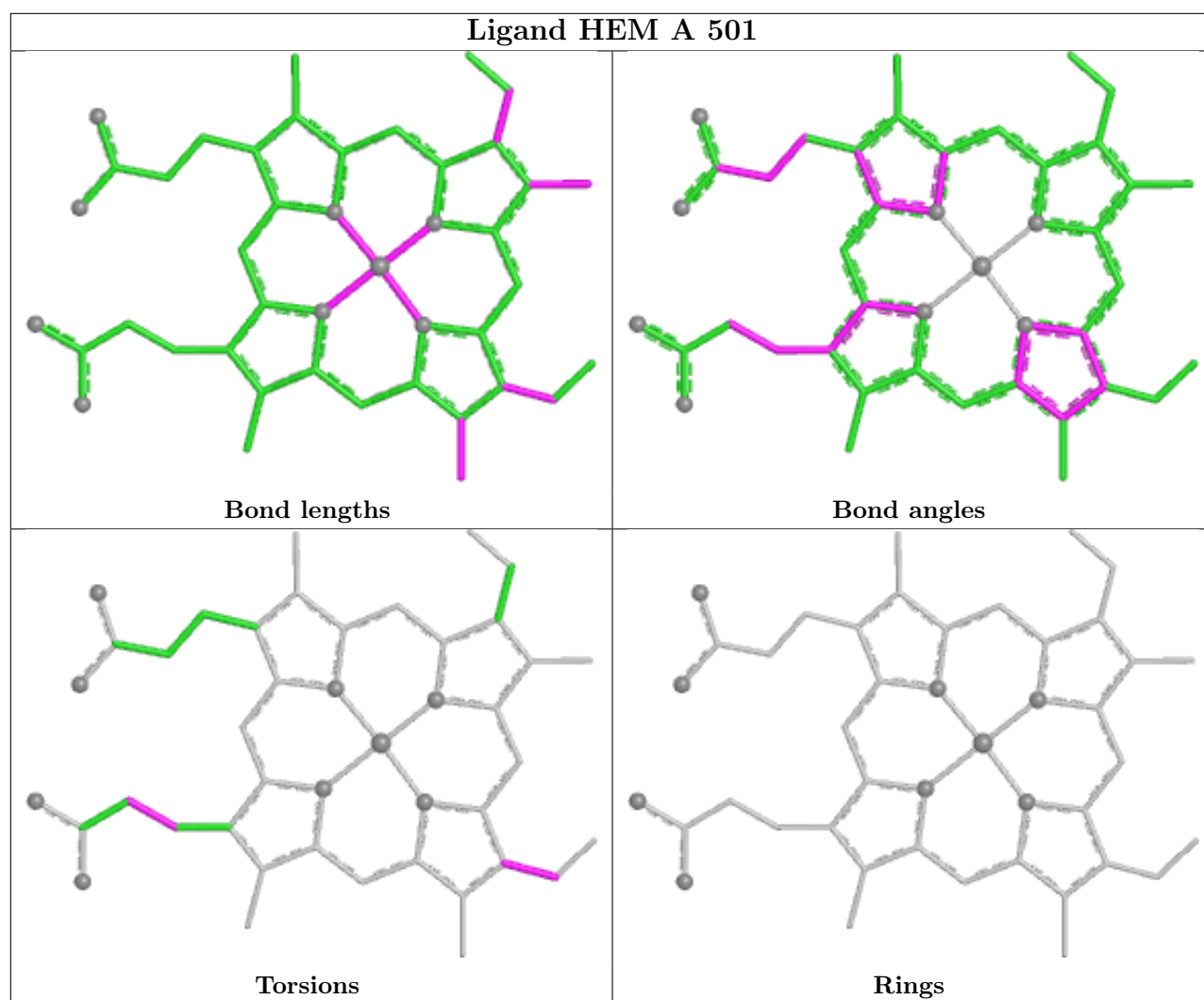


Ligand A1A0D D 503

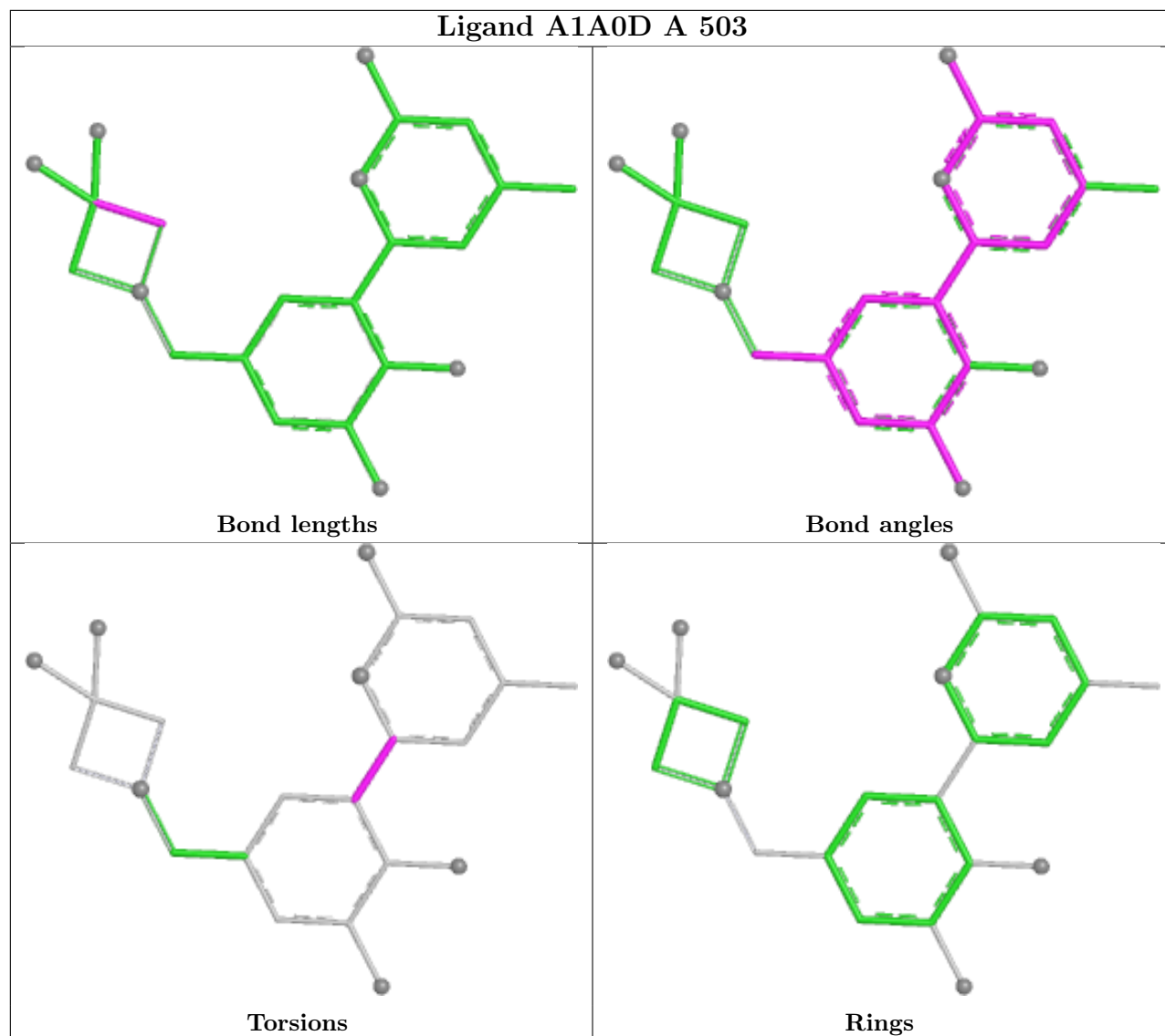


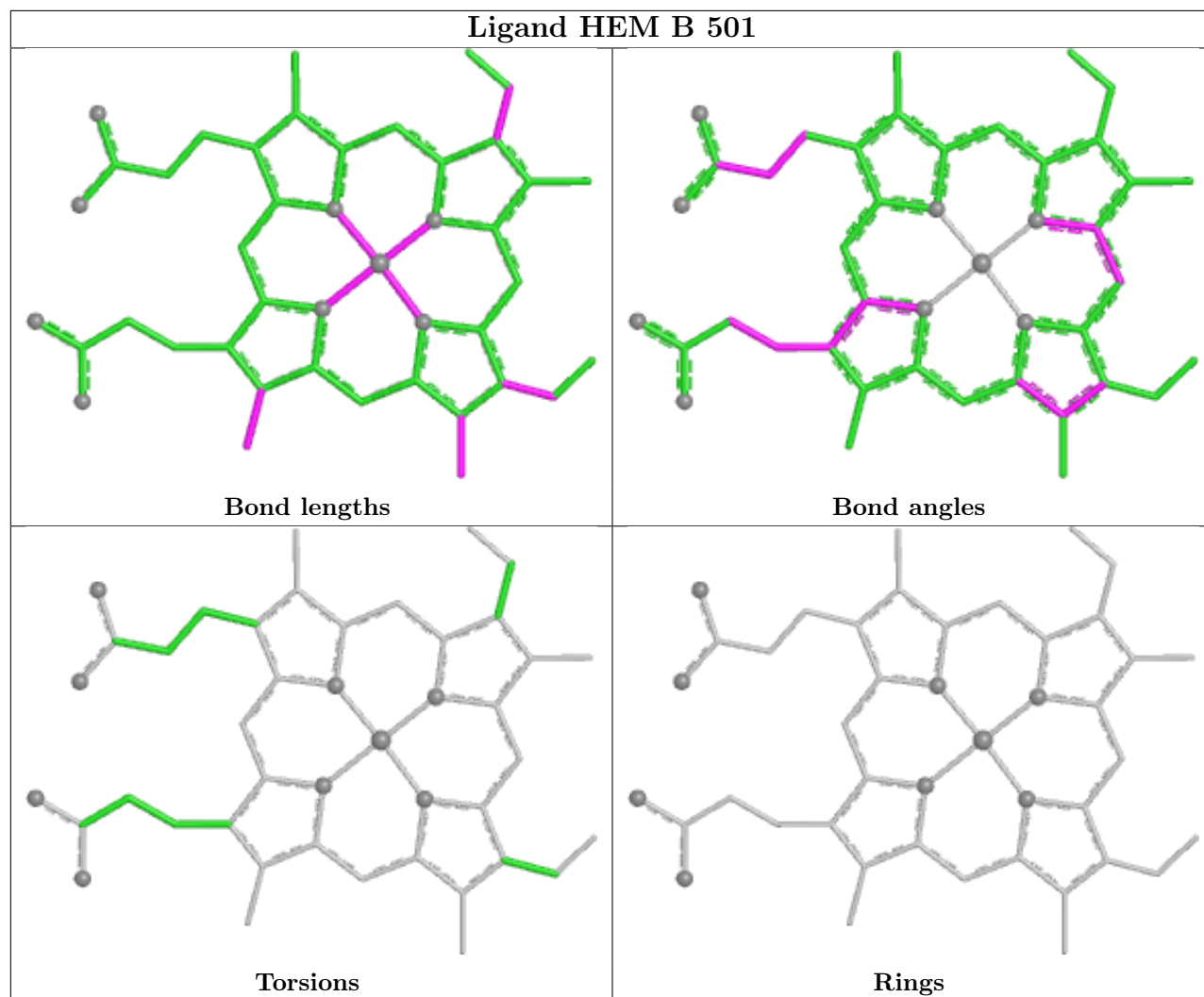


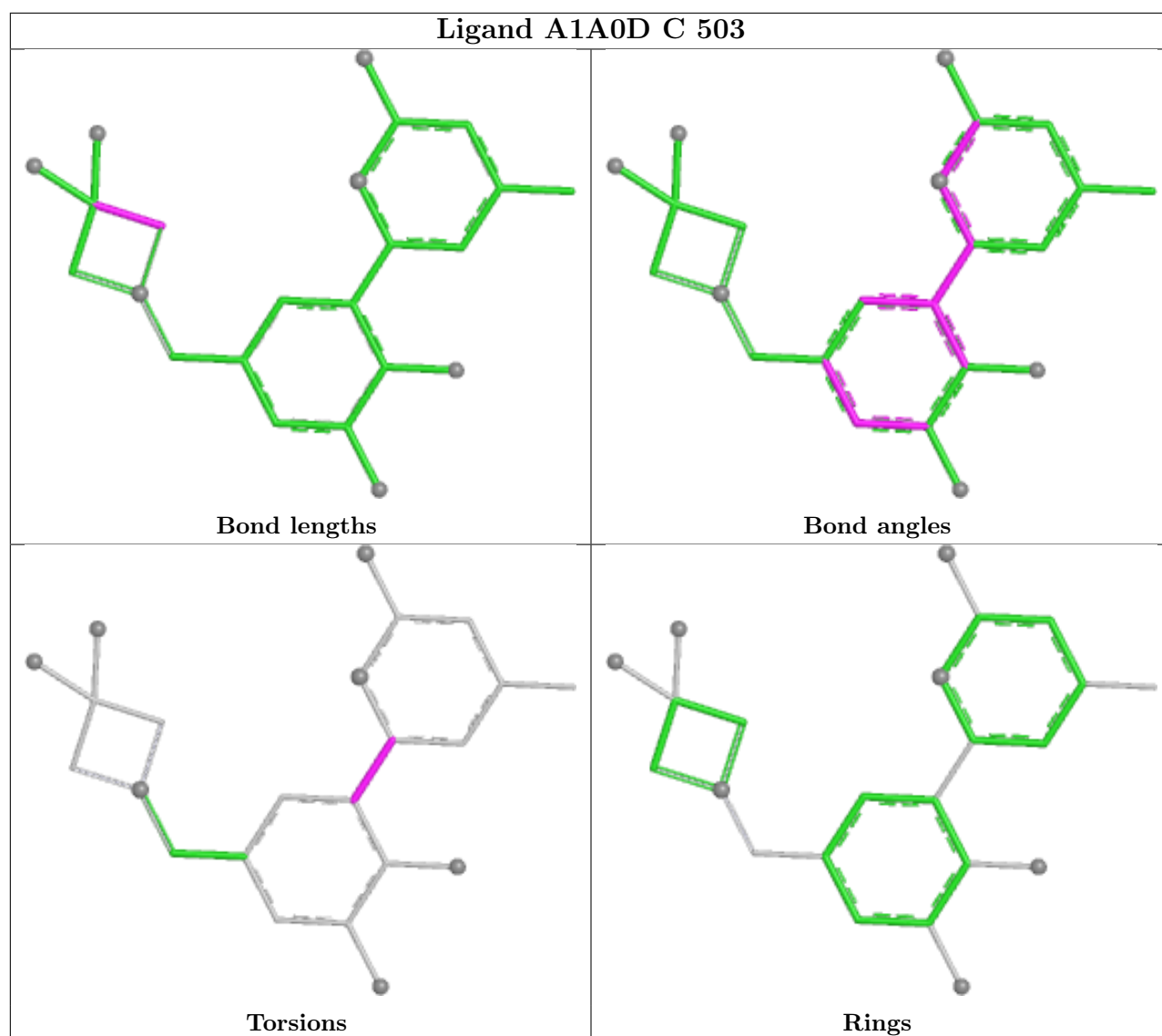




Ligand A1A0D A 503







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	401/440 (91%)	0.69	29 (7%)	21 27	22, 52, 96, 121	1 (0%)
1	B	401/440 (91%)	0.10	5 (1%)	76 83	20, 35, 64, 111	3 (0%)
1	C	401/440 (91%)	0.53	22 (5%)	30 37	24, 48, 89, 115	1 (0%)
1	D	402/440 (91%)	0.04	9 (2%)	62 70	21, 35, 55, 109	2 (0%)
All	All	1605/1760 (91%)	0.34	65 (4%)	42 51	20, 42, 87, 121	7 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	106	PRO	4.9
1	C	155	ALA	4.6
1	A	106	PRO	4.3
1	A	204	ALA	4.2
1	B	106	PRO	4.0
1	C	480	TRP	3.9
1	D	119	ALA	3.6
1	A	120	PRO	3.6
1	A	480	TRP	3.5
1	C	157	VAL	3.4
1	C	158	ALA	3.4
1	A	237	GLY	3.2
1	C	159	ALA	3.2
1	D	89	GLN	3.1
1	D	106	PRO	3.1
1	A	158	ALA	3.1
1	B	119	ALA	3.0
1	C	468	PHE	3.0
1	B	89	GLN	3.0
1	A	155	ALA	2.9
1	A	341	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	258	ASP	2.8
1	A	304	LEU	2.8
1	C	277	HIS	2.8
1	A	345	GLY	2.7
1	B	257	GLN	2.7
1	A	257	GLN	2.7
1	A	153	VAL	2.7
1	C	150	LEU	2.7
1	A	157	VAL	2.6
1	A	202	ARG	2.6
1	A	244	TRP	2.5
1	C	160	THR	2.5
1	A	236	PRO	2.5
1	C	124	LEU	2.4
1	C	161	GLY	2.4
1	D	257	GLN	2.4
1	D	255	ARG	2.4
1	C	120	PRO	2.3
1	C	119	ALA	2.3
1	C	123	LEU	2.3
1	A	259	GLY	2.3
1	A	67	LYS	2.3
1	C	236	PRO	2.3
1	A	160	THR	2.3
1	A	159	ALA	2.3
1	D	468	PHE	2.3
1	A	254	TYR	2.3
1	C	237	GLY	2.3
1	D	259	GLY	2.3
1	C	153	VAL	2.2
1	B	259	GLY	2.2
1	A	121	GLU	2.2
1	C	238	ARG	2.2
1	C	299	PRO	2.2
1	A	273	LEU	2.2
1	A	303	PHE	2.2
1	A	131	ILE	2.2
1	C	162	THR	2.1
1	A	299	PRO	2.1
1	D	107	ARG	2.1
1	C	241	PHE	2.1
1	A	340	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	468	PHE	2.0
1	A	235	CYS	2.0

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
6	GOL	A	509	6/6	0.59	0.14	71,76,77,80	0
6	GOL	C	509	6/6	0.68	0.14	72,76,80,83	0
6	GOL	B	507	6/6	0.69	0.14	67,69,71,71	0
5	BTB	A	506	14/14	0.70	0.16	86,93,97,97	0
5	BTB	C	505	14/14	0.74	0.15	85,88,91,91	0
4	A1A0D	C	503	23/23	0.74	0.19	39,73,93,96	0
6	GOL	A	507	6/6	0.76	0.16	50,63,67,68	0
4	A1A0D	A	503	23/23	0.77	0.19	41,69,93,96	0
5	BTB	A	505	14/14	0.78	0.16	63,71,77,78	0
5	BTB	D	505	14/14	0.78	0.18	59,65,71,75	0
5	BTB	B	505	14/14	0.78	0.15	53,64,68,70	0
6	GOL	C	508	6/6	0.79	0.13	59,67,73,76	0
4	A1A0D	B	503	23/23	0.79	0.17	29,52,87,93	0
5	BTB	C	504	14/14	0.80	0.18	50,63,67,71	0
5	BTB	D	504	14/14	0.82	0.16	48,55,66,75	0
6	GOL	A	508	6/6	0.82	0.17	53,64,65,65	0
4	A1A0D	D	503	23/23	0.83	0.15	25,56,84,88	0
5	BTB	A	504	14/14	0.84	0.16	54,60,67,74	0
6	GOL	D	506	6/6	0.87	0.13	47,56,59,59	0
6	GOL	C	507	6/6	0.88	0.17	36,44,56,60	0
5	BTB	B	504	14/14	0.88	0.13	41,45,56,62	0

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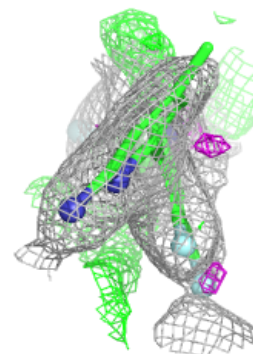
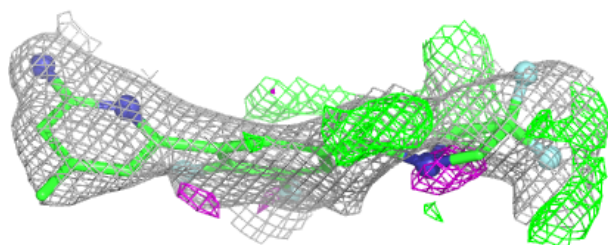
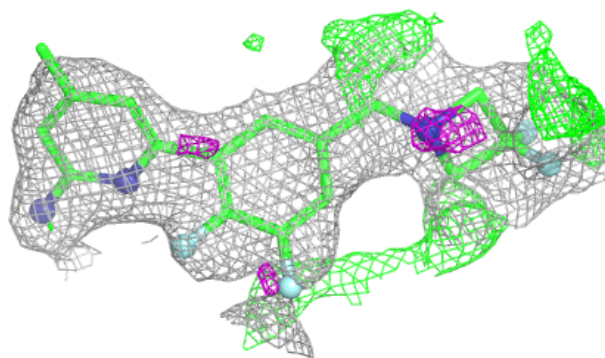
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BTB	B	510	14/14	0.89	0.14	31,53,63,64	0
6	GOL	C	506	6/6	0.89	0.10	54,61,63,66	0
6	GOL	B	506	6/6	0.90	0.12	41,47,55,56	0
3	H4B	C	502	17/17	0.91	0.09	33,37,40,41	0
3	H4B	A	502	17/17	0.93	0.08	37,43,45,46	0
7	CL	B	508	1/1	0.94	0.11	43,43,43,43	0
3	H4B	D	502	17/17	0.95	0.07	29,33,38,38	0
3	H4B	B	502	17/17	0.96	0.07	30,32,35,39	0
7	CL	A	510	1/1	0.96	0.07	54,54,54,54	0
2	HEM	A	501	43/43	0.96	0.11	36,43,59,89	0
2	HEM	C	501	43/43	0.97	0.08	32,39,57,77	0
7	CL	C	510	1/1	0.97	0.07	48,48,48,48	0
7	CL	D	507	1/1	0.97	0.07	44,44,44,44	0
8	GD3	D	508	1/1	0.97	0.05	41,41,41,41	0
2	HEM	D	501	43/43	0.98	0.07	19,25,48,72	0
8	GD3	A	511	1/1	0.98	0.04	49,49,49,49	1
2	HEM	B	501	43/43	0.98	0.07	22,27,44,71	0
9	ZN	A	512	1/1	0.98	0.04	38,38,38,38	0
8	GD3	B	509	1/1	0.99	0.04	37,37,37,37	0
8	GD3	B	511	1/1	0.99	0.03	42,42,42,42	1
9	ZN	C	511	1/1	0.99	0.03	30,30,30,30	0

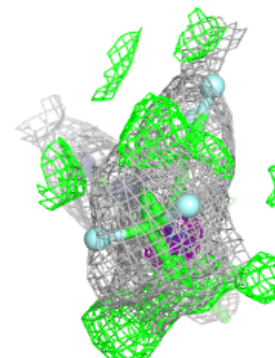
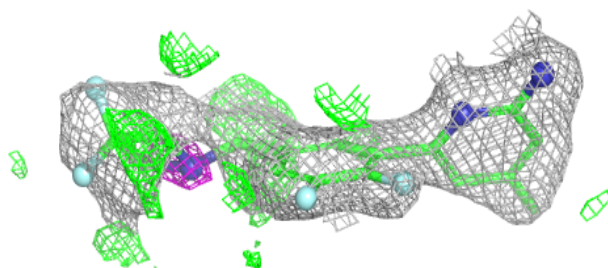
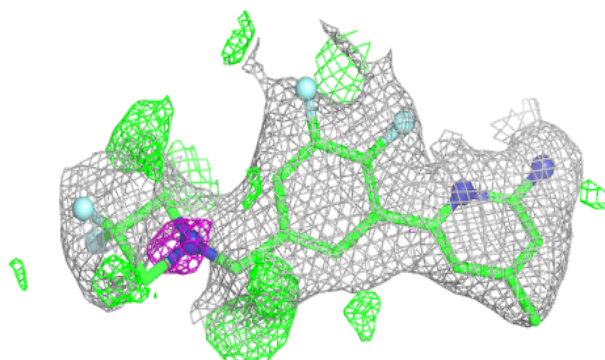
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1A0D 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)

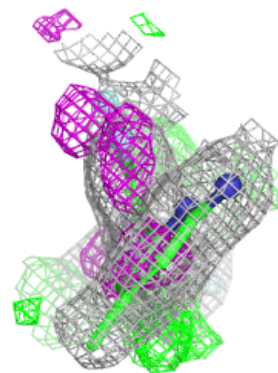
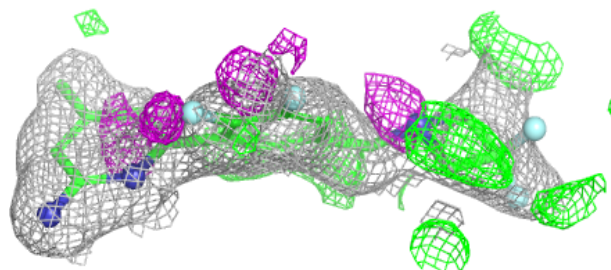
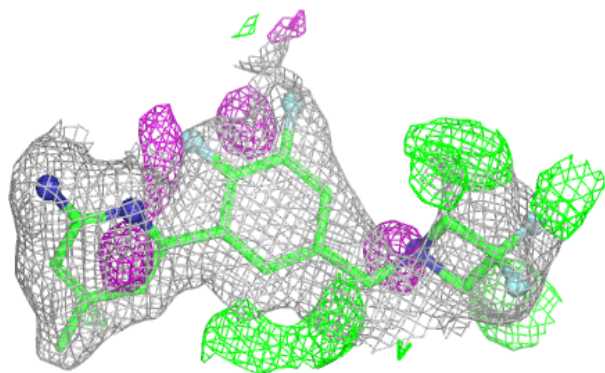
**Electron density around A1A0D A 503:**

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

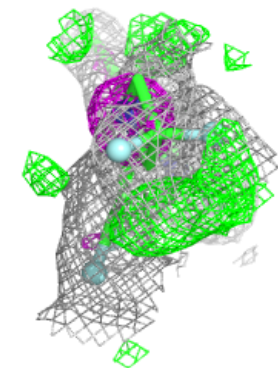
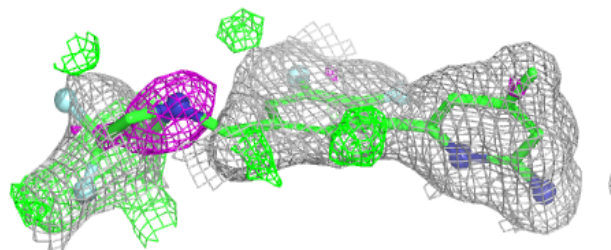
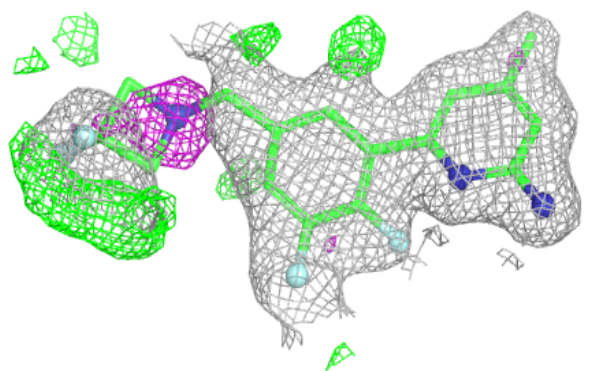


Electron density around A1A0D B 503:

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

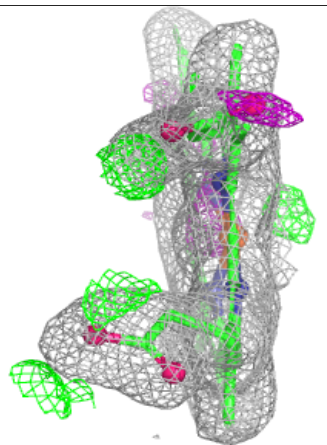
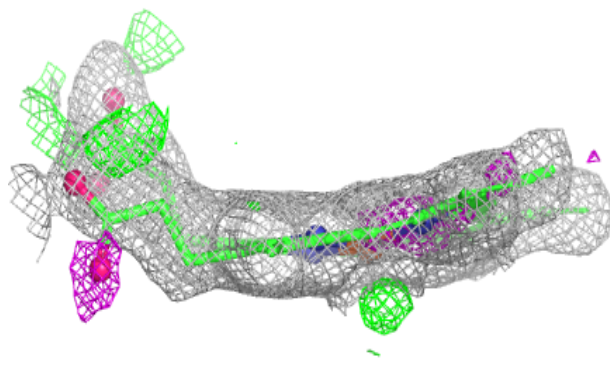
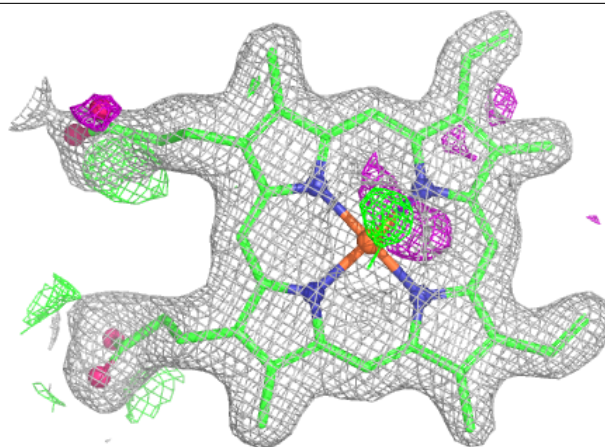
**Electron density around A1A0D D 503:**

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



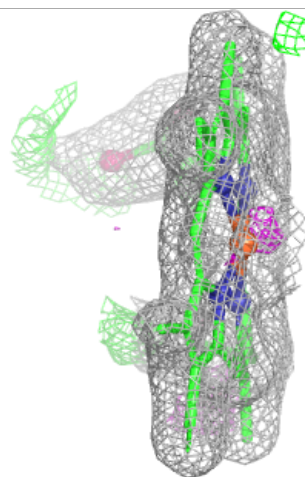
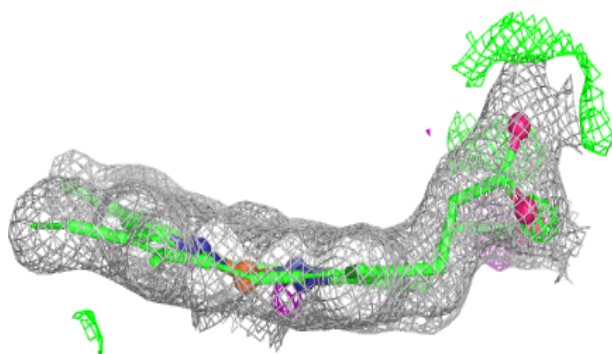
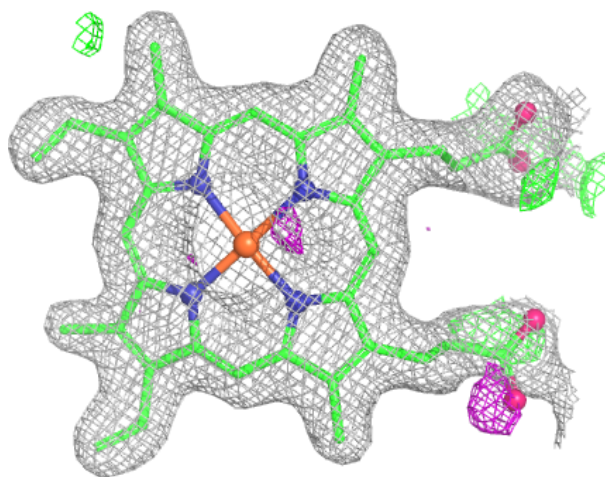
Electron density around HEM A 501:

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



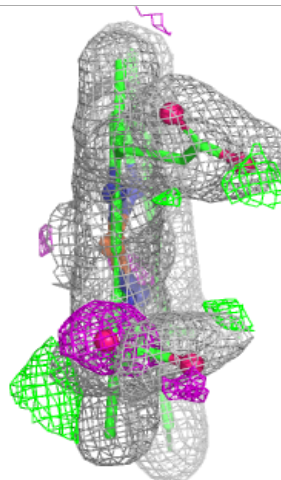
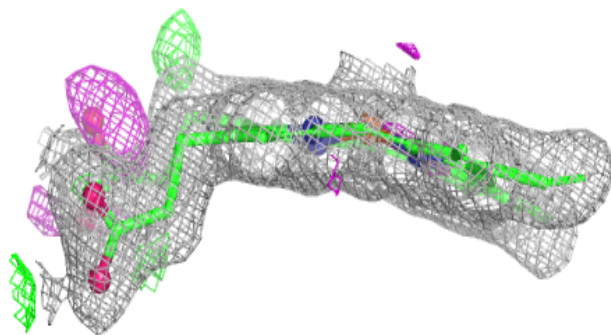
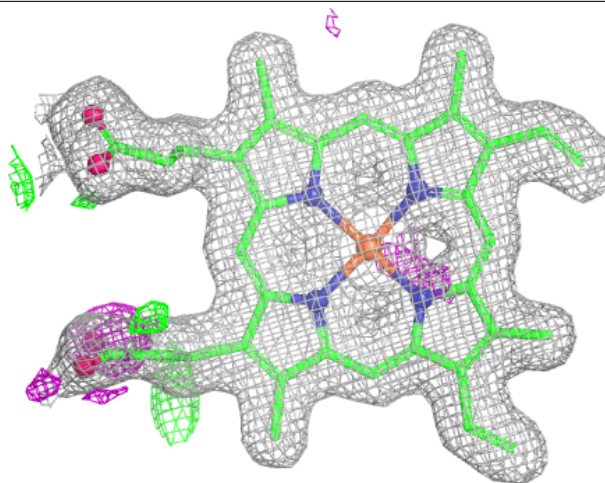
Electron density around HEM C 501:

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



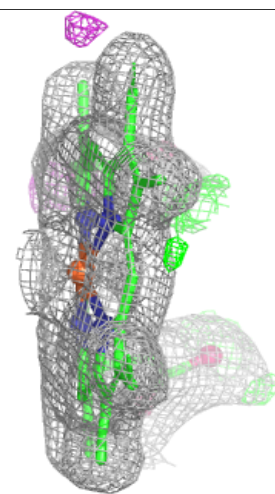
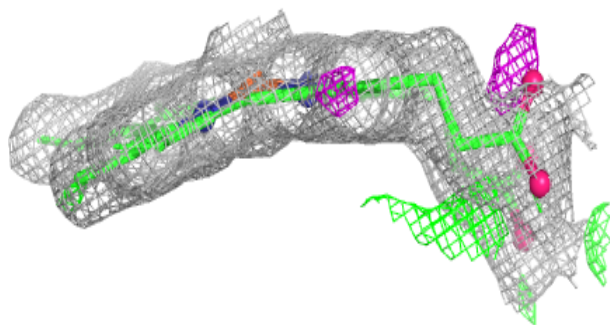
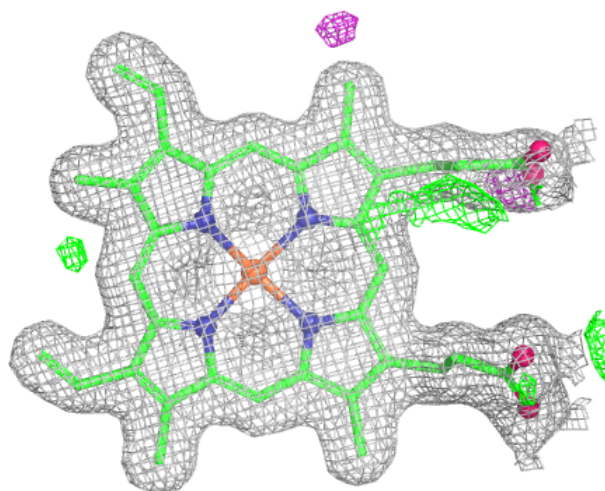
Electron density around HEM D 501:

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



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.