



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:26 AM UTC

PDB ID : 9Q51 / pdb_00009q51
Title : Structure of human endothelial nitric oxide synthase heme domain bound with 6-((5-(2-(diethylamino)ethyl)-2,3-difluorophenyl)methyl)-4-methylpyridin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2025-08-20
Resolution : 1.80 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

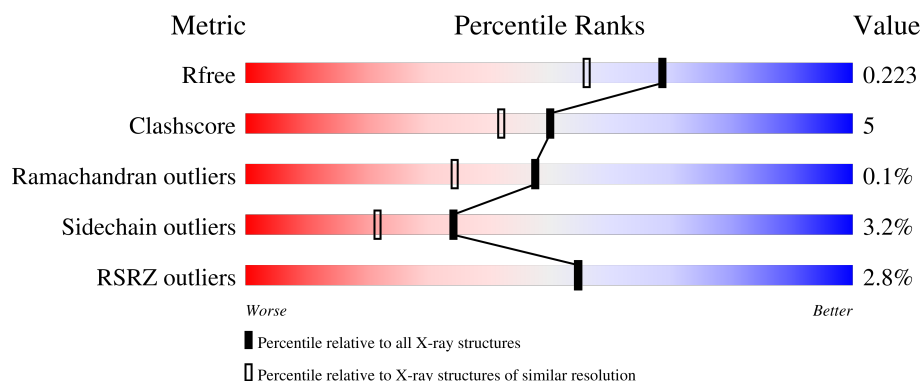
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	4% 80% 11% 9%
1	B	440	2% 81% 10% 9%
1	C	440	4% 79% 11% 9%
1	D	440	0% 83% 8% 9%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14519 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.

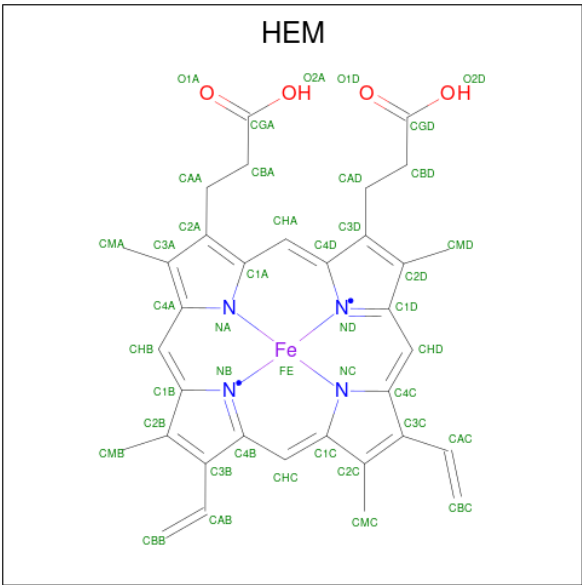
- Molecule 1 is a protein called Nitric oxide synthase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	1	0
			3214	2046	567	585	16			
1	B	402	Total	C	N	O	S	0	1	0
			3212	2046	565	585	16			
1	C	401	Total	C	N	O	S	0	1	0
			3207	2043	564	584	16			
1	D	402	Total	C	N	O	S	0	3	0
			3220	2051	566	587	16			

There are 4 discrepancies between the modelled and reference sequences:

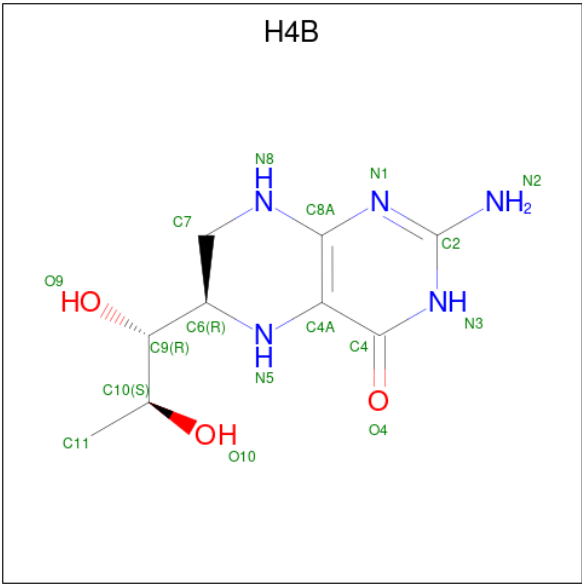
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	GLU	ASP	conflict	UNP P29474
B	298	GLU	ASP	conflict	UNP P29474
C	298	GLU	ASP	conflict	UNP P29474
D	298	GLU	ASP	conflict	UNP P29474

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



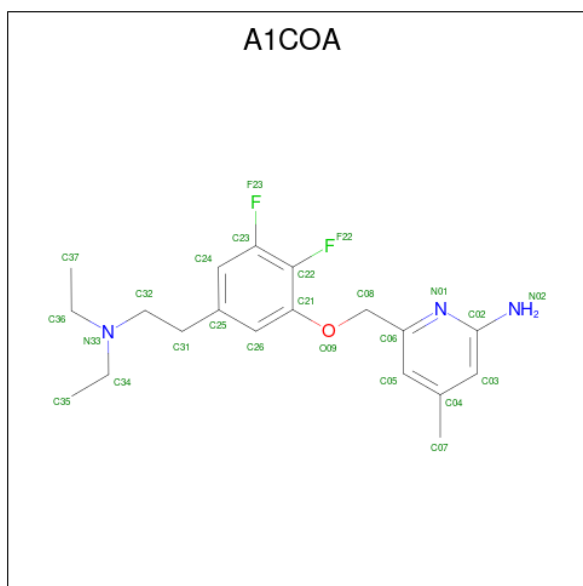
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: C₉H₁₅N₅O₃).



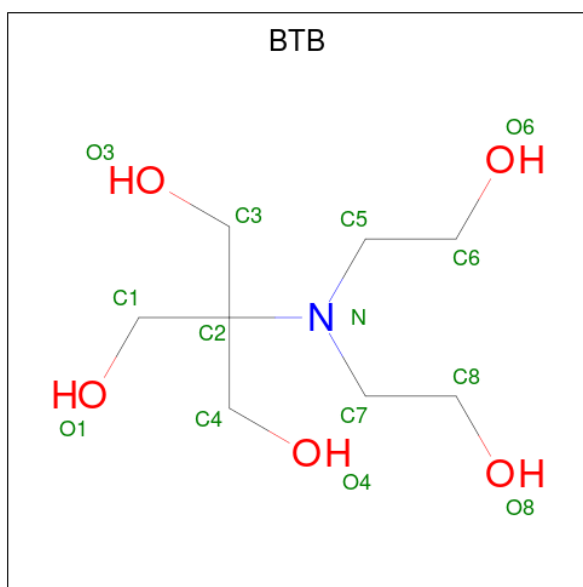
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 6-({5-[2-(diethylamino)ethyl]-2,3-difluorophenoxy}methyl)-4-methylpyridin-2-amine (CCD ID: A1COA) (formula: C₁₉H₂₅F₂N₃O) (labeled as "Ligand of Interest" by depositor).



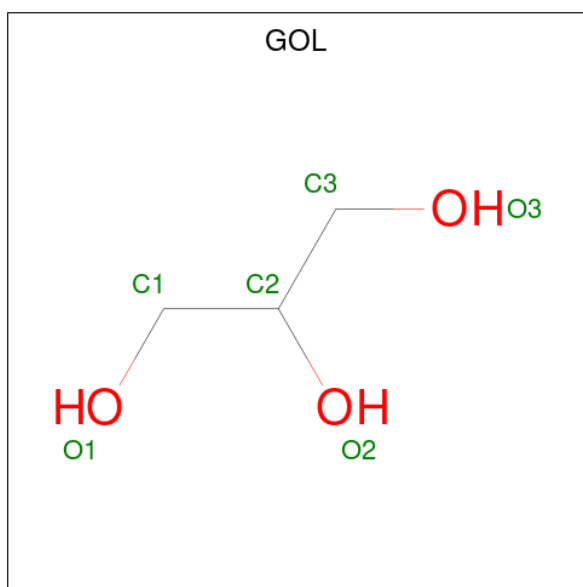
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			25	19	2	3	1		
4	B	1	Total	C	F	N	O	0	0
			25	19	2	3	1		
4	C	1	Total	C	F	N	O	0	0
			25	19	2	3	1		
4	D	1	Total	C	F	N	O	0	0
			25	19	2	3	1		

- 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	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: $C_3H_8O_3$).



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	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		
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		
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 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 CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total 1	Ca 1	0	0

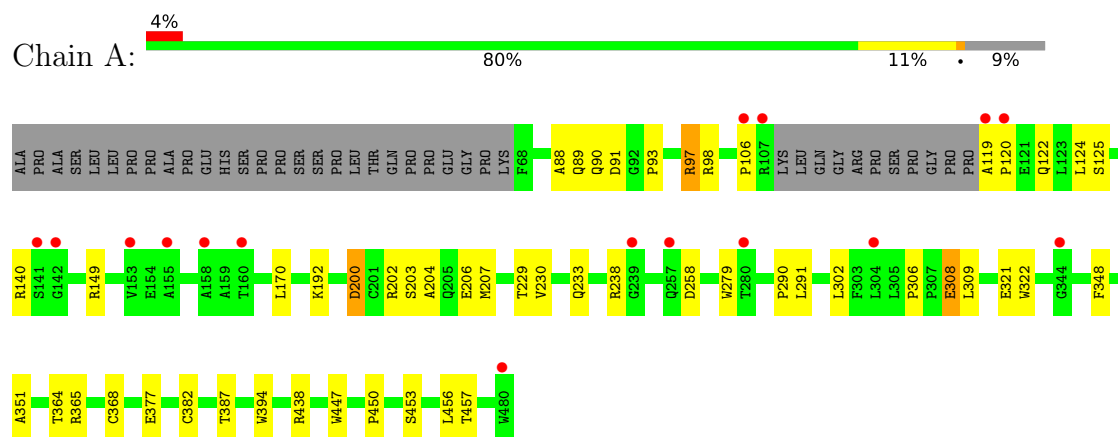
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	259	Total 259	O 259	0	0
11	B	345	Total 345	O 345	0	0
11	C	218	Total 218	O 218	0	0
11	D	333	Total 333	O 333	0	0

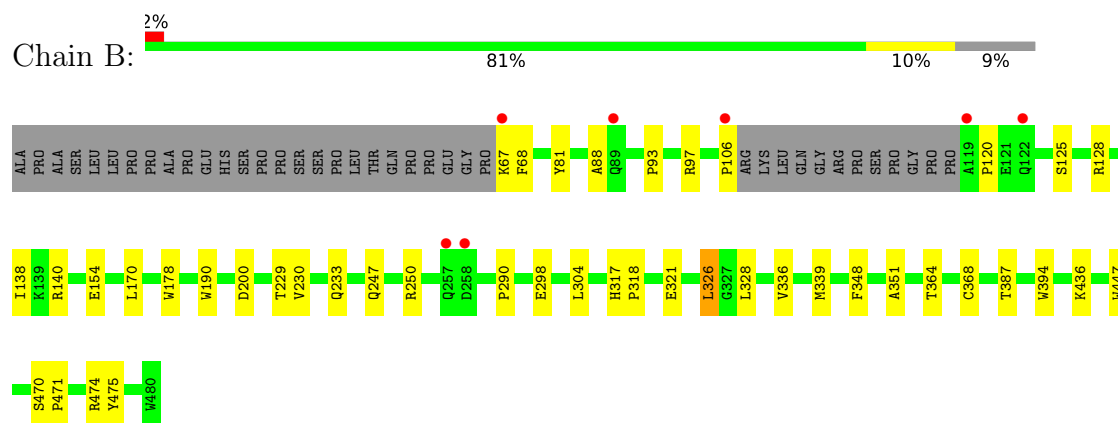
3 Residue-property plots [i](#)

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.

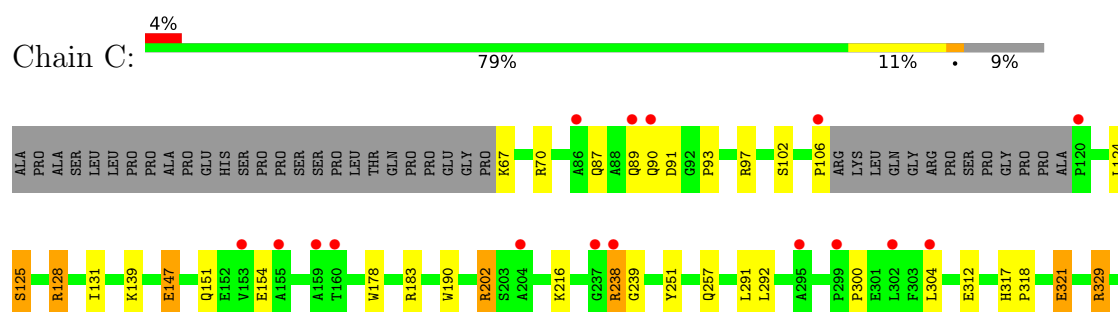
• Molecule 1: Nitric oxide synthase 3

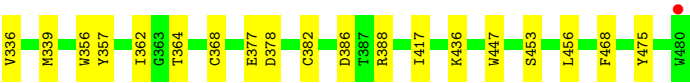


• Molecule 1: Nitric oxide synthase 3

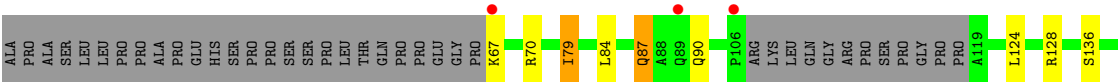
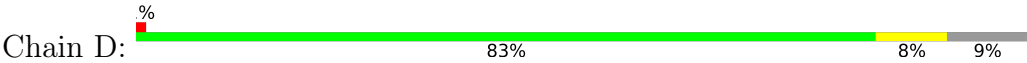


• Molecule 1: Nitric oxide synthase 3





● Molecule 1: Nitric oxide synthase 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.99Å 153.18Å 108.59Å 90.00° 90.75° 90.00°	Depositor
Resolution (Å)	47.23 – 1.80 47.23 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.23-1.80) 98.7 (47.23-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.190 , 0.228 0.184 , 0.223	Depositor DCC
R_{free} test set	8981 reflections (4.22%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14519	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: H4B, HEM, GOL, A1COA, CA, ZN, GD, CL, BTB

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	0.26	0/3309	0.47	0/4509
1	B	0.33	0/3307	0.52	0/4506
1	C	0.25	0/3302	0.46	0/4498
1	D	0.31	0/3321	0.48	0/4525
All	All	0.29	0/13239	0.48	0/18038

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	3214	0	3116	30	0
1	B	3212	0	3116	28	0
1	C	3207	0	3112	32	0
1	D	3220	0	3127	20	0
2	A	43	0	30	3	0
2	B	43	0	30	5	0
2	C	43	0	30	4	0
2	D	43	0	30	5	0
3	A	17	0	15	2	0

Continued on next page...

Continued from previous page...

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	1	0
4	A	25	0	0	1	0
4	B	25	0	0	4	0
4	C	25	0	0	4	0
4	D	25	0	0	1	0
5	A	28	0	37	9	0
5	B	28	0	35	6	0
5	C	28	0	38	6	0
5	D	28	0	36	4	0
6	A	18	0	24	0	0
6	B	6	0	8	0	0
6	C	12	0	16	0	0
6	D	12	0	16	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	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	1	0	0	0	0
9	C	1	0	0	0	0
10	A	1	0	0	0	0
11	A	259	0	0	4	0
11	B	345	0	0	4	1
11	C	218	0	0	5	0
11	D	333	0	0	3	1
All	All	14519	0	12861	140	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 (140) 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)
4:B:503:A1COA:C31	4:B:503:A1COA:C35	2.12	1.21
1:A:119:ALA:HB3	1:A:120:PRO:HD3	1.32	1.09
5:A:504:BTB:O3	11:A:601:HOH:O	1.87	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ALA:HB3	1:A:120:PRO:CD	2.10	0.81
1:B:138:ILE:HD12	1:B:140:ARG:HE	1.50	0.76
1:B:339:MET:SD	4:B:503:A1COA:F23	2.35	0.75
1:D:247:GLN:HB2	1:D:250:ARG:HD3	1.69	0.74
1:A:97:ARG:HG2	1:A:98:ARG:HG2	1.68	0.73
1:C:321:GLU:H	1:C:321:GLU:CD	1.98	0.71
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.70	0.71
1:A:119:ALA:CB	1:A:120:PRO:HD3	2.16	0.71
2:C:501:HEM:HBB2	2:C:501:HEM:HHC	1.73	0.70
1:D:70:ARG:HD2	1:D:79:ILE:HD13	1.74	0.69
1:D:290:PRO:HB3	1:D:304:LEU:HD23	1.76	0.68
1:B:475:TYR:OH	2:B:501:HEM:O1D	2.11	0.68
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.77	0.67
1:C:238:ARG:NH1	1:C:239:GLY:O	2.26	0.65
5:B:505:BTB:H71	5:B:505:BTB:O4	1.97	0.65
1:D:475:TYR:OH	2:D:501:HEM:O1D	2.12	0.65
2:B:501:HEM:HBD1	4:B:503:A1COA:C22	2.26	0.65
5:C:504:BTB:O6	5:C:504:BTB:H32	1.97	0.64
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.78	0.64
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.82	0.61
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.82	0.61
1:C:382:CYS:HA	5:C:504:BTB:H11	1.84	0.60
1:B:290:PRO:HB3	1:B:304:LEU:HD23	1.85	0.59
1:B:474:ARG:HD2	11:B:606:HOH:O	2.03	0.58
1:D:397:LYS:NZ	11:D:603:HOH:O	2.26	0.58
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.85	0.58
1:C:70:ARG:NH2	11:C:604:HOH:O	2.35	0.58
1:C:90:GLN:HB3	1:C:468:PHE:CD2	2.39	0.58
1:B:67:LYS:HG3	1:B:68:PHE:H	1.68	0.57
1:B:336:VAL:HG21	4:B:503:A1COA:C22	2.34	0.57
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.87	0.56
1:D:321:GLU:OE2	5:D:504:BTB:O4	2.24	0.56
1:B:93:PRO:HB3	1:B:106:PRO:HB2	1.89	0.55
1:C:339:MET:SD	4:C:503:A1COA:F23	2.55	0.55
1:A:382:CYS:HA	5:A:504:BTB:H11	1.89	0.55
1:A:88:ALA:O	1:B:97:ARG:NH2	2.39	0.54
5:B:504:BTB:H82	5:B:504:BTB:O4	2.08	0.54
1:C:336:VAL:HG21	4:C:503:A1COA:C22	2.38	0.54
1:C:436:LYS:NZ	11:C:610:HOH:O	2.41	0.54
1:B:321:GLU:OE2	5:B:504:BTB:O4	2.24	0.53
1:C:377:GLU:OE1	5:C:505:BTB:O3	2.18	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:501:HEM:HBD2	4:C:503:A1COA:C22	2.38	0.53
2:D:501:HEM:HBB2	2:D:501:HEM:HHC	1.90	0.53
1:B:81:TYR:HD1	11:B:626:HOH:O	1.92	0.52
5:A:505:BTB:H72	5:A:505:BTB:O4	2.07	0.52
1:A:322:TRP:CD1	5:A:504:BTB:H62	2.44	0.51
2:A:501:HEM:HBD1	4:A:503:A1COA:C22	2.40	0.51
1:C:378:ASP:OD1	11:C:602:HOH:O	2.18	0.51
1:C:386:ASP:OD2	1:C:388:ARG:HG2	2.11	0.51
2:D:501:HEM:HBD2	4:D:503:A1COA:F22	2.01	0.50
1:D:238:ARG:NH2	11:D:611:HOH:O	2.44	0.50
1:A:97:ARG:NH2	1:B:88:ALA:O	2.45	0.50
1:C:93:PRO:HB3	1:C:106:PRO:HB3	1.94	0.50
1:D:149:ARG:NH1	1:D:152:GLU:OE1	2.44	0.50
1:A:306:PRO:HG2	1:A:309:LEU:HB2	1.93	0.50
1:A:233:GLN:HB3	1:A:348:PHE:CE2	2.47	0.49
5:D:504:BTB:O4	5:D:504:BTB:H82	2.12	0.49
1:A:321:GLU:H	1:A:321:GLU:CD	2.21	0.49
1:D:84:LEU:HD12	1:D:87:GLN:HG3	1.94	0.49
1:C:292:LEU:HD22	1:C:300:PRO:HB2	1.95	0.49
1:C:364:THR:O	1:C:368:CYS:HB2	2.13	0.48
1:A:238:ARG:NH1	11:A:607:HOH:O	2.45	0.48
1:D:312:GLU:CD	1:D:329:ARG:HH21	2.22	0.48
1:A:364:THR:O	1:A:368:CYS:HB2	2.14	0.47
1:A:279:TRP:CG	1:A:290:PRO:HG3	2.50	0.47
1:C:329:ARG:NH1	11:C:614:HOH:O	2.48	0.47
1:D:87:GLN:H	1:D:87:GLN:HG2	1.51	0.47
5:A:504:BTB:H72	5:A:504:BTB:H41	1.42	0.47
1:B:364:THR:O	1:B:368:CYS:HB2	2.14	0.47
1:C:257:GLN:HB3	11:C:787:HOH:O	2.13	0.46
1:D:238:ARG:HG2	1:D:296:PRO:HB3	1.98	0.46
1:B:298:GLU:OE1	5:B:505:BTB:O4	2.23	0.46
1:D:90:GLN:HB3	1:D:468:PHE:CD2	2.51	0.46
1:B:447:TRP:HA	3:B:502:H4B:N1	2.31	0.46
1:C:251:TYR:OH	1:C:312:GLU:OE2	2.30	0.46
5:B:505:BTB:H51	5:B:505:BTB:H11	1.49	0.45
1:B:326:LEU:HB3	1:B:328:LEU:HG	1.98	0.45
1:C:183:ARG:HD3	1:C:447:TRP:CD2	2.51	0.45
1:A:90:GLN:HG3	1:A:91:ASP:H	1.81	0.45
1:A:450:PRO:HG2	1:A:457:THR:HG21	1.99	0.45
1:D:447:TRP:HA	3:D:502:H4B:N1	2.32	0.45
1:A:200:ASP:OD1	1:A:200:ASP:N	2.36	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:SER:HB3	1:C:456:LEU:HD12	1.99	0.45
5:C:505:BTB:H72	5:C:505:BTB:H41	1.48	0.45
1:A:233:GLN:NE2	11:A:605:HOH:O	2.29	0.44
5:D:504:BTB:H72	5:D:504:BTB:H11	1.72	0.44
1:B:128:ARG:HH12	1:B:154:GLU:CG	2.31	0.44
1:D:206:GLU:OE2	11:D:601:HOH:O	2.21	0.44
1:B:178:TRP:CE3	1:B:190:TRP:HA	2.53	0.44
1:D:453:SER:HB3	1:D:456:LEU:HD12	2.00	0.44
5:C:505:BTB:H11	5:C:505:BTB:H51	1.58	0.44
1:A:387:THR:HA	1:A:394:TRP:CD1	2.53	0.43
1:C:447:TRP:HA	3:C:502:H4B:N1	2.32	0.43
5:A:505:BTB:H62	5:A:505:BTB:H71	1.52	0.43
1:C:125:SER:HA	1:C:128:ARG:NH1	2.34	0.43
1:C:90:GLN:HG3	1:C:91:ASP:N	2.34	0.43
1:D:124:LEU:HD23	1:D:124:LEU:HA	1.86	0.43
1:A:238:ARG:NH2	11:A:608:HOH:O	2.29	0.43
1:B:470:SER:HA	1:B:471:PRO:C	2.43	0.43
1:A:202:ARG:HD2	1:A:206:GLU:OE2	2.18	0.43
1:A:453:SER:HB3	1:A:456:LEU:HD12	2.01	0.43
1:B:233:GLN:HB3	1:B:348:PHE:CE2	2.54	0.43
1:B:317:HIS:CG	1:B:318:PRO:HD2	2.53	0.43
1:C:102:SER:O	3:C:502:H4B:O10	2.27	0.43
1:A:308:GLU:O	1:A:308:GLU:HG2	2.17	0.43
1:A:377:GLU:OE1	5:A:505:BTB:O3	2.36	0.43
1:B:250:ARG:HA	1:B:250:ARG:HD2	1.90	0.42
1:C:147:GLU:O	1:C:151:GLN:NE2	2.40	0.42
1:C:178:TRP:CE3	1:C:190:TRP:HA	2.54	0.42
1:B:387:THR:HA	1:B:394:TRP:CD1	2.55	0.42
1:D:358:MET:HE3	1:D:360:THR:OG1	2.19	0.42
1:A:170:LEU:HD11	1:A:230:VAL:HG11	2.02	0.42
2:D:501:HEM:HH A	2:D:501:HEM:HBD1	2.01	0.42
2:B:501:HEM:O1D	11:B:601:HOH:O	2.22	0.42
1:A:93:PRO:HB3	1:A:106:PRO:HB2	2.02	0.41
1:A:365:ARG:HH12	3:A:502:H4B:C4	2.33	0.41
1:B:170:LEU:HD11	1:B:230:VAL:HG11	2.01	0.41
1:D:387:THR:HA	1:D:394:TRP:CD1	2.55	0.41
1:B:229:THR:O	1:B:351:ALA:HA	2.20	0.41
1:C:202:ARG:HE	1:C:202:ARG:HB3	1.71	0.41
1:B:81:TYR:N	11:B:626:HOH:O	2.53	0.41
5:D:504:BTB:H32	5:D:504:BTB:H51	1.81	0.41
1:A:447:TRP:HA	3:A:502:H4B:N1	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:504:BTB:H11	5:A:504:BTB:H51	1.82	0.41
1:C:90:GLN:HB3	1:C:468:PHE:CG	2.56	0.41
1:C:357:TYR:CD2	1:C:362:ILE:HD11	2.56	0.41
1:A:204:ALA:HA	1:A:207:MET:HB2	2.02	0.41
1:A:229:THR:O	1:A:351:ALA:HA	2.21	0.41
5:A:505:BTB:H52	5:A:505:BTB:H41	1.84	0.41
5:B:505:BTB:H52	5:B:505:BTB:H81	1.27	0.41
1:C:475:TYR:OH	2:C:501:HEM:O1D	2.39	0.41
1:C:356:TRP:O	4:C:503:A1COA:N02	2.54	0.40
5:C:504:BTB:H41	5:C:504:BTB:H72	1.92	0.40
1:C:131:ILE:HD13	1:C:131:ILE:HA	1.94	0.40
1:D:470:SER:HA	1:D:471:PRO:C	2.46	0.40
1:B:128:ARG:HH12	1:B:154:GLU:HG3	1.87	0.40
1:C:317:HIS:CG	1:C:318:PRO:HD2	2.57	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)
11:B:632:HOH:O	11:D:681:HOH:O[1_456]	2.15	0.05

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	399/440 (91%)	388 (97%)	11 (3%)	0	100	100
1	B	399/440 (91%)	390 (98%)	8 (2%)	1 (0%)	36	25
1	C	398/440 (90%)	389 (98%)	8 (2%)	1 (0%)	36	25
1	D	401/440 (91%)	391 (98%)	10 (2%)	0	100	100
All	All	1597/1760 (91%)	1558 (98%)	37 (2%)	2 (0%)	48	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	120	PRO
1	C	89	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/373 (92%)	327 (96%)	15 (4%)	25	13
1	B	342/373 (92%)	338 (99%)	4 (1%)	63	57
1	C	342/373 (92%)	325 (95%)	17 (5%)	22	10
1	D	344/373 (92%)	336 (98%)	8 (2%)	44	33
All	All	1370/1492 (92%)	1326 (97%)	44 (3%)	34	22

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	97	ARG
1	A	122	GLN
1	A	124	LEU
1	A	125	SER
1	A	140	ARG
1	A	149	ARG
1	A	192	LYS
1	A	200	ASP
1	A	203	SER
1	A	258	ASP
1	A	291	LEU
1	A	302	LEU
1	A	308	GLU
1	A	438	ARG
1	B	125	SER
1	B	200	ASP
1	B	326	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	436	LYS
1	C	67	LYS
1	C	87	GLN
1	C	97	ARG
1	C	124	LEU
1	C	125	SER
1	C	128	ARG
1	C	139	LYS
1	C	147	GLU
1	C	154	GLU
1	C	202	ARG
1	C	216	LYS
1	C	238	ARG
1	C	291	LEU
1	C	304	LEU
1	C	321	GLU
1	C	329	ARG
1	C	417	ILE
1	D	67	LYS
1	D	79	ILE
1	D	87	GLN
1	D	128	ARG
1	D	136	SER
1	D	144	GLN
1	D	213[A]	ASN
1	D	213[B]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	233	GLN
1	C	89	GLN
1	C	126	GLN
1	C	276	GLN
1	D	176	GLN

5.3.3 RNA ⓘ

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 39 ligands modelled in this entry, 11 are monoatomic - leaving 28 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$
4	A1COA	D	503	-	26,26,26	0.39	0	33,35,35	1.34	2 (6%)
4	A1COA	C	503	-	26,26,26	0.31	0	33,35,35	1.34	2 (6%)
3	H4B	A	502	-	17,18,18	1.06	1 (5%)	14,26,26	2.07	5 (35%)
5	BTB	B	505	-	13,13,13	0.58	0	7,16,16	1.55	1 (14%)
5	BTB	D	504	8	13,13,13	0.51	0	7,16,16	0.37	0
6	GOL	C	506	-	5,5,5	0.32	0	5,5,5	0.67	0
4	A1COA	A	503	-	26,26,26	0.31	0	33,35,35	1.33	3 (9%)
6	GOL	A	506	-	5,5,5	0.40	0	5,5,5	0.78	0
2	HEM	B	501	1	50,50,50	1.49	10 (20%)	67,82,82	1.26	6 (8%)
2	HEM	C	501	1	50,50,50	1.74	7 (14%)	67,82,82	1.32	7 (10%)
6	GOL	D	506	-	5,5,5	0.34	0	5,5,5	0.42	0
6	GOL	C	507	-	5,5,5	0.36	0	5,5,5	0.42	0
5	BTB	B	504	8	13,13,13	0.44	0	7,16,16	0.67	0
4	A1COA	B	503	-	26,26,26	0.37	0	33,35,35	1.43	4 (12%)
6	GOL	B	506	-	5,5,5	0.39	0	5,5,5	0.37	0
5	BTB	A	504	8	13,13,13	0.53	0	7,16,16	1.07	1 (14%)
3	H4B	C	502	-	17,18,18	0.94	0	14,26,26	2.06	5 (35%)
5	BTB	C	505	-	13,13,13	0.58	0	7,16,16	1.12	1 (14%)
5	BTB	A	505	-	13,13,13	1.34	1 (7%)	7,16,16	1.15	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BTB	D	505	-	13,13,13	0.56	0	7,16,16	1.45	1 (14%)
6	GOL	A	508	-	5,5,5	0.43	0	5,5,5	0.14	0
6	GOL	A	507	-	5,5,5	0.35	0	5,5,5	0.35	0
6	GOL	D	507	-	5,5,5	0.29	0	5,5,5	0.37	0
2	HEM	A	501	1	50,50,50	1.66	7 (14%)	67,82,82	1.38	8 (11%)
5	BTB	C	504	8	13,13,13	0.41	0	7,16,16	0.59	0
3	H4B	B	502	-	17,18,18	0.92	0	14,26,26	1.69	3 (21%)
2	HEM	D	501	1	50,50,50	1.67	8 (16%)	67,82,82	1.37	10 (14%)
3	H4B	D	502	-	17,18,18	0.92	0	14,26,26	2.15	6 (42%)

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
4	A1COA	D	503	-	-	8/14/14/14	0/2/2/2
4	A1COA	C	503	-	-	5/14/14/14	0/2/2/2
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
5	BTB	B	505	-	-	13/21/21/21	-
5	BTB	D	504	8	-	3/21/21/21	-
6	GOL	C	506	-	-	3/4/4/4	-
4	A1COA	A	503	-	-	4/14/14/14	0/2/2/2
6	GOL	A	506	-	-	2/4/4/4	-
2	HEM	B	501	1	-	3/14/54/54	-
2	HEM	C	501	1	-	3/14/54/54	-
6	GOL	D	506	-	-	3/4/4/4	-
6	GOL	C	507	-	-	2/4/4/4	-
5	BTB	B	504	8	-	6/21/21/21	-
4	A1COA	B	503	-	-	6/14/14/14	0/2/2/2
6	GOL	B	506	-	-	2/4/4/4	-
5	BTB	A	504	8	-	6/21/21/21	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
5	BTB	C	505	-	-	11/21/21/21	-
5	BTB	A	505	-	-	7/21/21/21	-
5	BTB	D	505	-	-	10/21/21/21	-
6	GOL	A	508	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	507	-	-	4/4/4/4	-
6	GOL	D	507	-	-	2/4/4/4	-
2	HEM	A	501	1	-	5/14/54/54	-
5	BTB	C	504	8	-	8/21/21/21	-
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
2	HEM	D	501	1	-	1/14/54/54	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	FE-NB	6.71	2.15	1.94
2	D	501	HEM	FE-NB	6.10	2.13	1.94
2	A	501	HEM	FE-NB	4.98	2.10	1.94
2	B	501	HEM	FE-NB	4.94	2.10	1.94
2	C	501	HEM	FE-NC	4.68	2.10	1.95
2	A	501	HEM	FE-NC	4.58	2.10	1.95
2	D	501	HEM	FE-NC	4.54	2.10	1.95
2	A	501	HEM	FE-NA	4.33	2.09	1.95
2	A	501	HEM	FE-ND	4.32	2.08	1.94
2	C	501	HEM	FE-NA	4.20	2.09	1.95
5	A	505	BTB	C2-N	-4.16	1.40	1.48
2	D	501	HEM	FE-NA	3.41	2.06	1.95
2	C	501	HEM	CAC-C3C	3.06	1.55	1.47
2	B	501	HEM	FE-NC	3.06	2.05	1.95
2	C	501	HEM	CAB-C3B	3.05	1.55	1.47
2	B	501	HEM	CAB-C3B	3.05	1.55	1.47
2	D	501	HEM	CAB-C3B	3.01	1.55	1.47
2	B	501	HEM	CMC-C2C	2.96	1.56	1.50
2	D	501	HEM	CAC-C3C	2.94	1.55	1.47
2	A	501	HEM	CAB-C3B	2.94	1.55	1.47
2	A	501	HEM	CAC-C3C	2.86	1.55	1.47
2	B	501	HEM	CAC-C3C	2.74	1.54	1.47
2	B	501	HEM	CMD-C2D	2.50	1.55	1.50
2	D	501	HEM	CMB-C2B	2.44	1.55	1.50
2	A	501	HEM	CMC-C2C	2.36	1.55	1.50
2	C	501	HEM	FE-ND	2.36	2.02	1.94
3	A	502	H4B	C4-N3	-2.33	1.34	1.38
2	B	501	HEM	FE-ND	2.30	2.02	1.94
2	D	501	HEM	CMA-C3A	2.27	1.55	1.50
2	C	501	HEM	CMC-C2C	2.26	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	CMB-C2B	2.21	1.55	1.50
2	B	501	HEM	C3D-C2D	-2.15	1.32	1.36
2	D	501	HEM	FE-ND	2.14	2.01	1.94
2	B	501	HEM	CMA-C3A	2.06	1.55	1.50

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	A1COA	C02-N01-C06	4.57	121.49	118.07
4	C	503	A1COA	C02-N01-C06	4.49	121.43	118.07
4	D	503	A1COA	C02-N01-C06	4.43	121.38	118.07
3	D	502	H4B	C2-N1-C8A	4.33	121.00	113.36
4	B	503	A1COA	C02-N01-C06	4.22	121.22	118.07
2	D	501	HEM	CBA-CAA-C2A	-4.17	101.00	112.53
3	C	502	H4B	C2-N1-C8A	4.08	120.56	113.36
3	A	502	H4B	C2-N1-C8A	4.00	120.42	113.36
3	B	502	H4B	C2-N1-C8A	3.73	119.94	113.36
2	B	501	HEM	CBA-CAA-C2A	-3.49	102.87	112.53
5	B	505	BTB	O4-C4-C2	3.44	119.50	111.40
3	C	502	H4B	O4-C4-C4A	-3.39	119.09	127.26
2	A	501	HEM	C3B-C4B-NB	-3.35	107.06	109.47
4	D	503	A1COA	O09-C21-C22	3.18	120.72	115.92
2	A	501	HEM	C2A-C1A-NA	-3.18	106.63	110.15
2	C	501	HEM	C3B-C4B-NB	-3.14	107.21	109.47
4	B	503	A1COA	C31-C25-C24	-3.12	115.29	120.54
2	A	501	HEM	CAD-CBD-CGD	-2.98	105.77	113.67
5	D	505	BTB	O1-C1-C2	-2.97	104.42	111.40
3	D	502	H4B	C11-C10-C9	-2.95	108.51	112.11
3	D	502	H4B	C2-N3-C4	-2.88	119.89	125.11
2	C	501	HEM	CBD-CAD-C3D	-2.86	104.63	112.53
3	D	502	H4B	O4-C4-C4A	-2.83	120.43	127.26
3	D	502	H4B	C4A-C4-N3	2.82	119.87	112.13
2	C	501	HEM	C3D-C4D-ND	-2.82	107.08	110.17
2	C	501	HEM	C3B-C2B-C1B	2.81	108.52	106.41
3	A	502	H4B	O10-C10-C9	-2.81	105.12	109.77
2	C	501	HEM	C1B-NB-C4B	2.79	108.51	105.21
3	A	502	H4B	C11-C10-C9	-2.78	108.71	112.11
2	A	501	HEM	CBA-CAA-C2A	-2.77	104.86	112.53
3	C	502	H4B	C11-C10-C9	-2.74	108.77	112.11
3	A	502	H4B	O4-C4-C4A	-2.73	120.67	127.26
2	C	501	HEM	C4D-ND-C1D	2.73	108.44	105.21
2	D	501	HEM	C3B-C2B-C1B	2.73	108.46	106.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C1B-NB-C4B	2.72	108.43	105.21
4	B	503	A1COA	F23-C23-C22	2.70	121.98	118.32
4	C	503	A1COA	O09-C21-C22	2.66	119.94	115.92
3	C	502	H4B	C4A-C4-N3	2.64	119.37	112.13
2	D	501	HEM	CBD-CAD-C3D	-2.64	105.25	112.53
2	D	501	HEM	C2A-C1A-NA	-2.62	107.24	110.15
2	D	501	HEM	CHC-C1C-NC	2.57	127.25	124.45
5	A	504	BTB	O3-C3-C2	2.51	117.31	111.40
2	A	501	HEM	C3D-C4D-ND	-2.50	107.43	110.17
3	A	502	H4B	C4A-C4-N3	2.41	118.76	112.13
2	B	501	HEM	CHC-C1C-NC	2.41	127.08	124.45
5	C	505	BTB	O3-C3-C2	-2.38	105.79	111.40
2	A	501	HEM	C4D-ND-C1D	2.37	108.01	105.21
3	B	502	H4B	O4-C4-C4A	-2.36	121.56	127.26
5	A	505	BTB	O3-C3-C2	-2.36	105.86	111.40
2	B	501	HEM	CHB-C4A-NA	2.35	128.12	123.86
2	A	501	HEM	C3B-C2B-C1B	2.35	108.17	106.41
2	B	501	HEM	C3B-C2B-C1B	2.33	108.16	106.41
2	C	501	HEM	C2A-C1A-NA	-2.28	107.62	110.15
2	D	501	HEM	C3D-C4D-ND	-2.27	107.68	110.17
2	D	501	HEM	C3B-C4B-NB	-2.27	107.84	109.47
2	D	501	HEM	CHD-C1D-ND	2.26	126.86	124.42
3	B	502	H4B	C4A-C4-N3	2.26	118.34	112.13
4	A	503	A1COA	C32-C31-C25	-2.22	105.89	112.15
4	A	503	A1COA	O09-C21-C22	2.21	119.26	115.92
3	C	502	H4B	C2-N3-C4	-2.21	121.11	125.11
4	B	503	A1COA	C26-C25-C24	2.19	121.99	119.01
3	D	502	H4B	O9-C9-C6	2.13	114.38	109.28
2	D	501	HEM	C1B-NB-C4B	2.10	107.69	105.21
2	B	501	HEM	C1A-CHA-C4D	-2.09	121.34	126.25
2	D	501	HEM	C4C-NC-C1C	2.07	109.19	105.82
2	B	501	HEM	C2A-C1A-NA	-2.02	107.92	110.15

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	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	504	BTB	C3-C2-C4-O4
5	B	504	BTB	N-C2-C4-O4
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-C4-O4
5	B	505	BTB	C3-C2-C4-O4
5	B	505	BTB	N-C2-C4-O4
5	B	505	BTB	C8-C7-N-C5
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-C3-O3
5	C	504	BTB	C4-C2-C3-O3
5	C	504	BTB	N-C2-C3-O3
5	C	505	BTB	C1-C2-C4-O4
5	C	505	BTB	C3-C2-C4-O4
5	C	505	BTB	C1-C2-N-C5
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
5	C	505	BTB	C4-C2-N-C7
5	D	504	BTB	C1-C2-C4-O4
5	D	504	BTB	C3-C2-C4-O4
5	D	504	BTB	N-C2-C4-O4
5	D	505	BTB	O1-C1-C2-C3
5	D	505	BTB	O1-C1-C2-C4
5	D	505	BTB	O1-C1-C2-N
5	D	505	BTB	C1-C2-C3-O3
5	D	505	BTB	C4-C2-C3-O3
5	D	505	BTB	N-C2-C3-O3
5	D	505	BTB	C1-C2-C4-O4
5	D	505	BTB	C3-C2-C4-O4
5	D	505	BTB	N-C2-C4-O4
6	A	506	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	507	GOL	C1-C2-C3-O3
6	B	506	GOL	O1-C1-C2-C3
6	C	506	GOL	C1-C2-C3-O3
6	D	506	GOL	O1-C1-C2-C3
6	D	507	GOL	O1-C1-C2-C3
4	D	503	A1COA	C31-C32-N33-C36
2	A	501	HEM	C2A-CAA-CBA-CGA
5	B	505	BTB	N-C5-C6-O6
6	D	507	GOL	O1-C1-C2-O2
2	C	501	HEM	C2A-CAA-CBA-CGA
5	D	505	BTB	N-C5-C6-O6
5	A	505	BTB	N-C7-C8-O8
6	A	507	GOL	O1-C1-C2-C3
6	C	506	GOL	O1-C1-C2-C3
6	C	507	GOL	O1-C1-C2-C3
4	C	503	A1COA	C35-C34-N33-C32
5	C	504	BTB	N-C7-C8-O8
5	C	505	BTB	N-C7-C8-O8
5	B	504	BTB	C1-C2-C4-O4
6	A	506	GOL	O1-C1-C2-O2
6	A	507	GOL	O2-C2-C3-O3
6	C	506	GOL	O2-C2-C3-O3
6	D	506	GOL	O1-C1-C2-O2
2	A	501	HEM	C3D-CAD-CBD-CGD
5	A	505	BTB	C6-C5-N-C7
5	A	504	BTB	N-C5-C6-O6
4	B	503	A1COA	C35-C34-N33-C32
4	D	503	A1COA	C35-C34-N33-C32
2	A	501	HEM	C4B-C3B-CAB-CBB
5	B	505	BTB	N-C7-C8-O8
4	A	503	A1COA	C35-C34-N33-C32
6	B	506	GOL	O1-C1-C2-O2
4	C	503	A1COA	C24-C25-C31-C32
4	C	503	A1COA	C35-C34-N33-C36
4	B	503	A1COA	C35-C34-N33-C36
4	D	503	A1COA	C35-C34-N33-C36
4	C	503	A1COA	C26-C25-C31-C32
4	B	503	A1COA	C37-C36-N33-C34
4	D	503	A1COA	C37-C36-N33-C34
4	D	503	A1COA	C24-C25-C31-C32
4	D	503	A1COA	C26-C25-C31-C32
4	A	503	A1COA	C24-C25-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	507	GOL	O1-C1-C2-O2
6	D	506	GOL	O2-C2-C3-O3
4	B	503	A1COA	C22-C21-O09-C08
2	C	501	HEM	C4B-C3B-CAB-CBB
2	D	501	HEM	C4B-C3B-CAB-CBB
4	A	503	A1COA	C26-C25-C31-C32
5	C	504	BTB	C3-C2-C4-O4
2	C	501	HEM	C1A-C2A-CAA-CBA
5	B	505	BTB	C1-C2-N-C5
5	B	505	BTB	C1-C2-N-C7
5	B	505	BTB	C4-C2-N-C7
6	A	507	GOL	O1-C1-C2-O2
4	D	503	A1COA	C37-C36-N33-C32
4	A	503	A1COA	C35-C34-N33-C36
5	A	504	BTB	O1-C1-C2-C3
5	C	505	BTB	O1-C1-C2-C4
4	C	503	A1COA	C25-C31-C32-N33
4	B	503	A1COA	C31-C32-N33-C34
2	A	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O1D
4	D	503	A1COA	C25-C31-C32-N33
2	B	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	CAD-CBD-CGD-O1D
4	B	503	A1COA	C37-C36-N33-C32
5	A	505	BTB	N-C2-C3-O3
5	B	505	BTB	C3-C2-N-C7
5	C	505	BTB	N-C2-C4-O4

There are no ring outliers.

19 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	503	A1COA	1	0
4	C	503	A1COA	4	0
3	A	502	H4B	2	0
5	B	505	BTB	4	0
5	D	504	BTB	4	0
4	A	503	A1COA	1	0
2	B	501	HEM	5	0
2	C	501	HEM	4	0
5	B	504	BTB	2	0

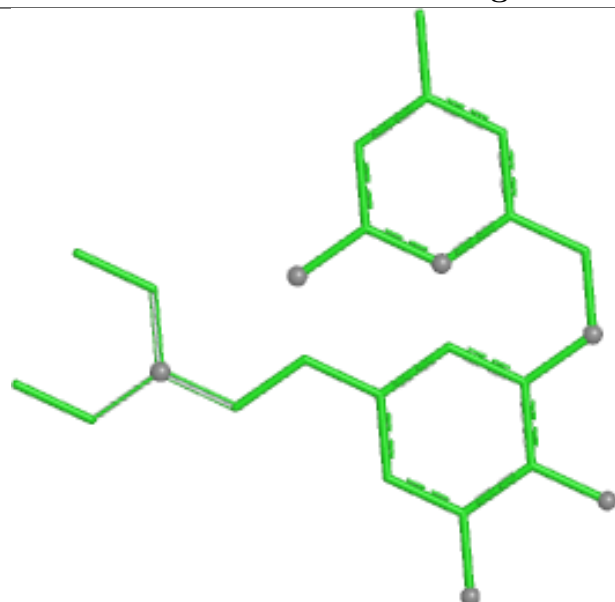
Continued on next page...

Continued from previous page...

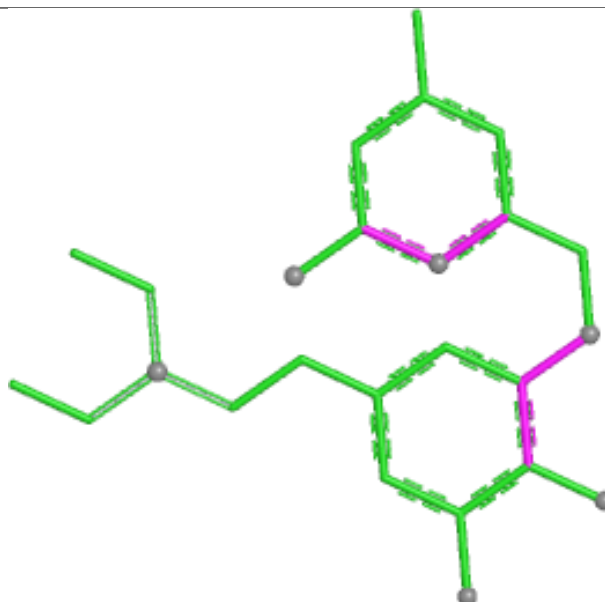
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	A1COA	4	0
5	A	504	BTB	5	0
3	C	502	H4B	2	0
5	C	505	BTB	3	0
5	A	505	BTB	4	0
2	A	501	HEM	3	0
5	C	504	BTB	3	0
3	B	502	H4B	1	0
2	D	501	HEM	5	0
3	D	502	H4B	1	0

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.

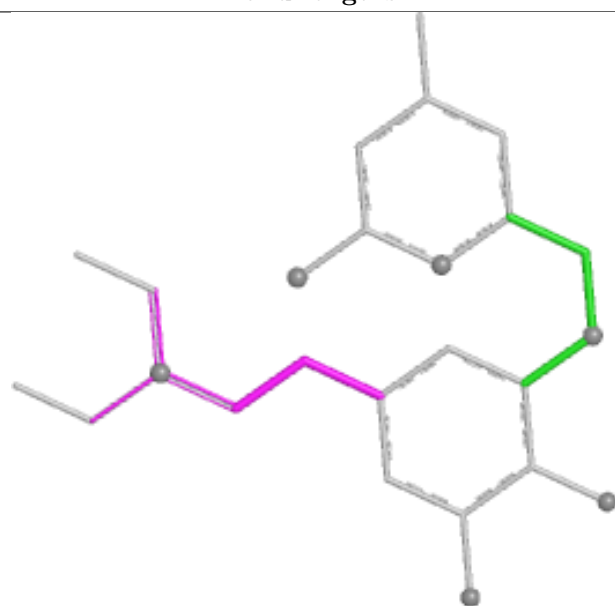
Ligand A1COA D 503



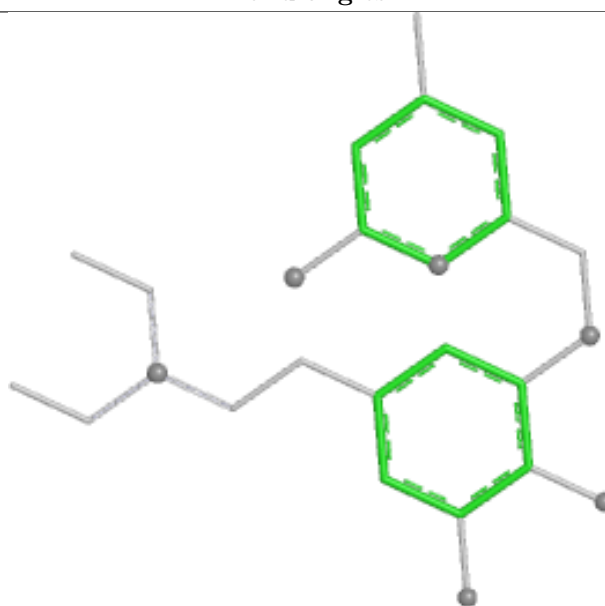
Bond lengths



Bond angles

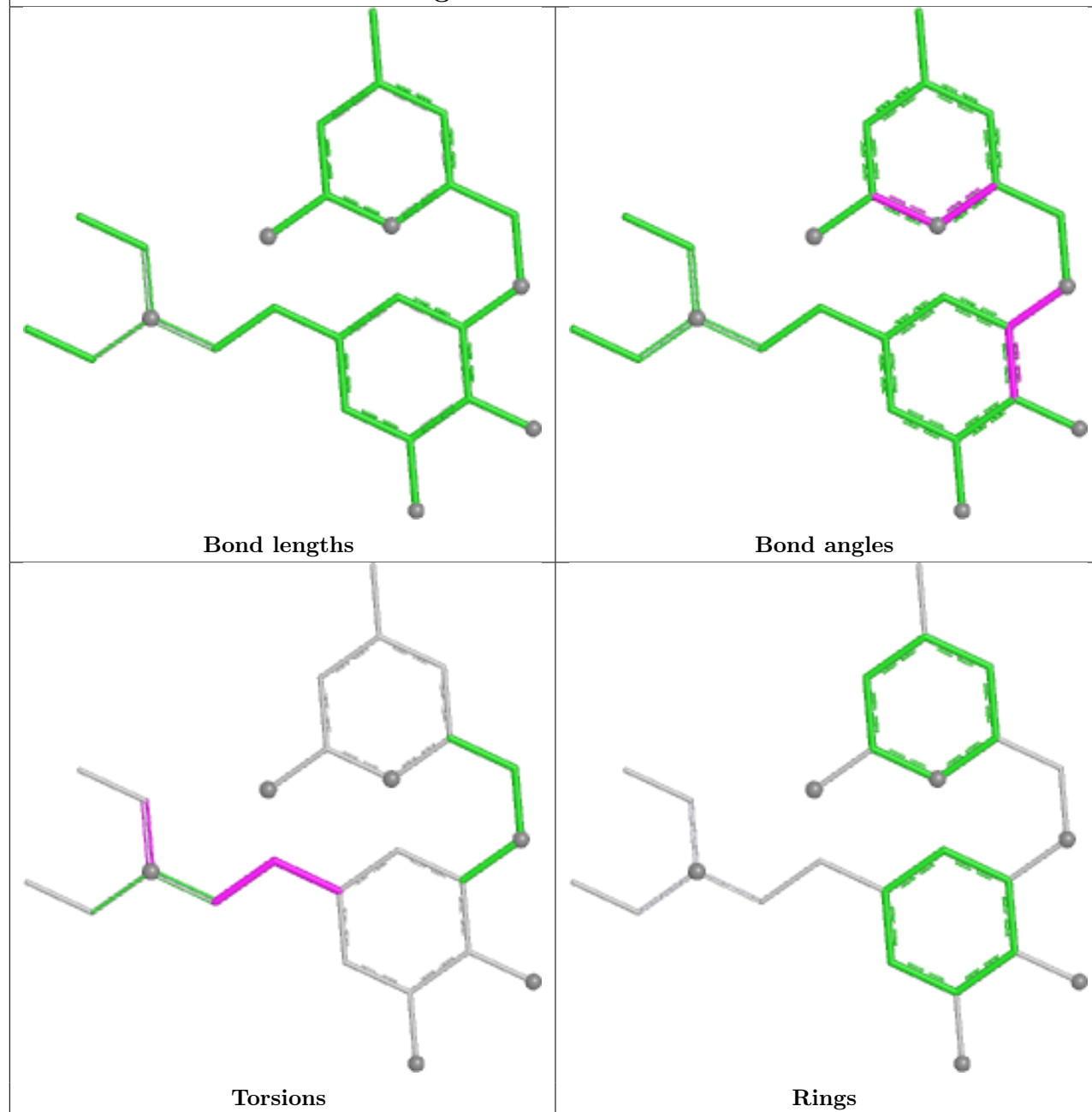


Torsions

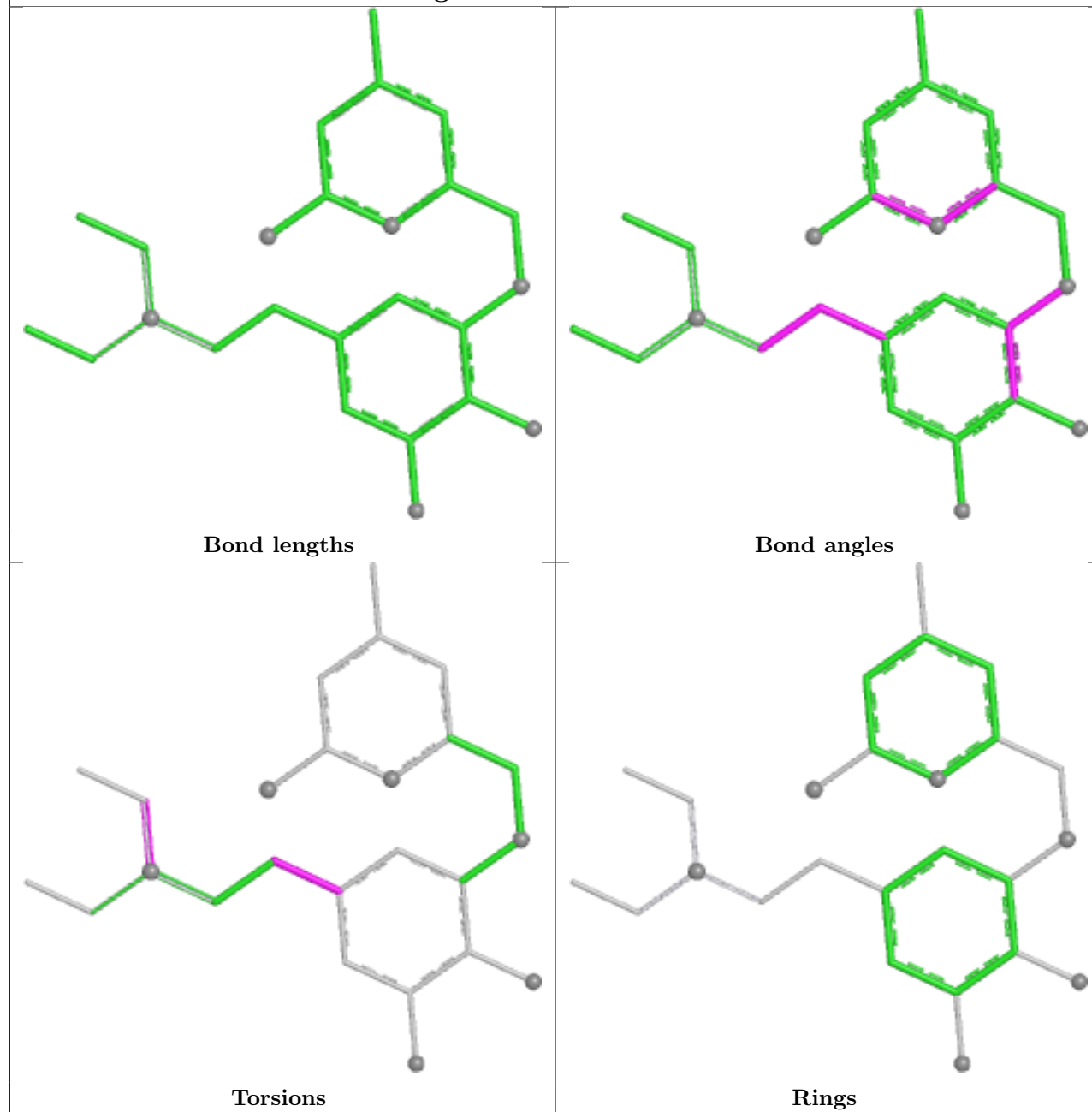


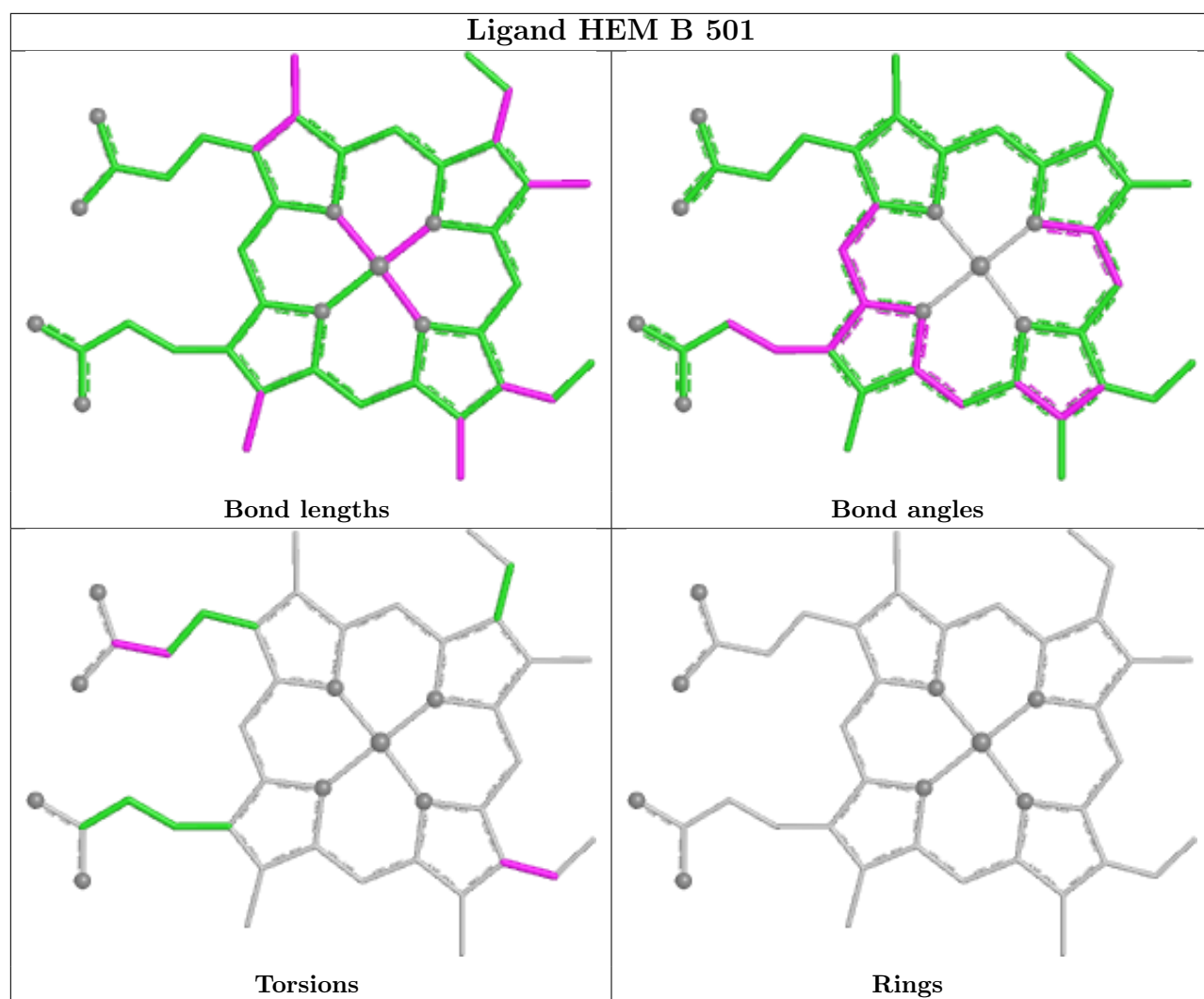
Rings

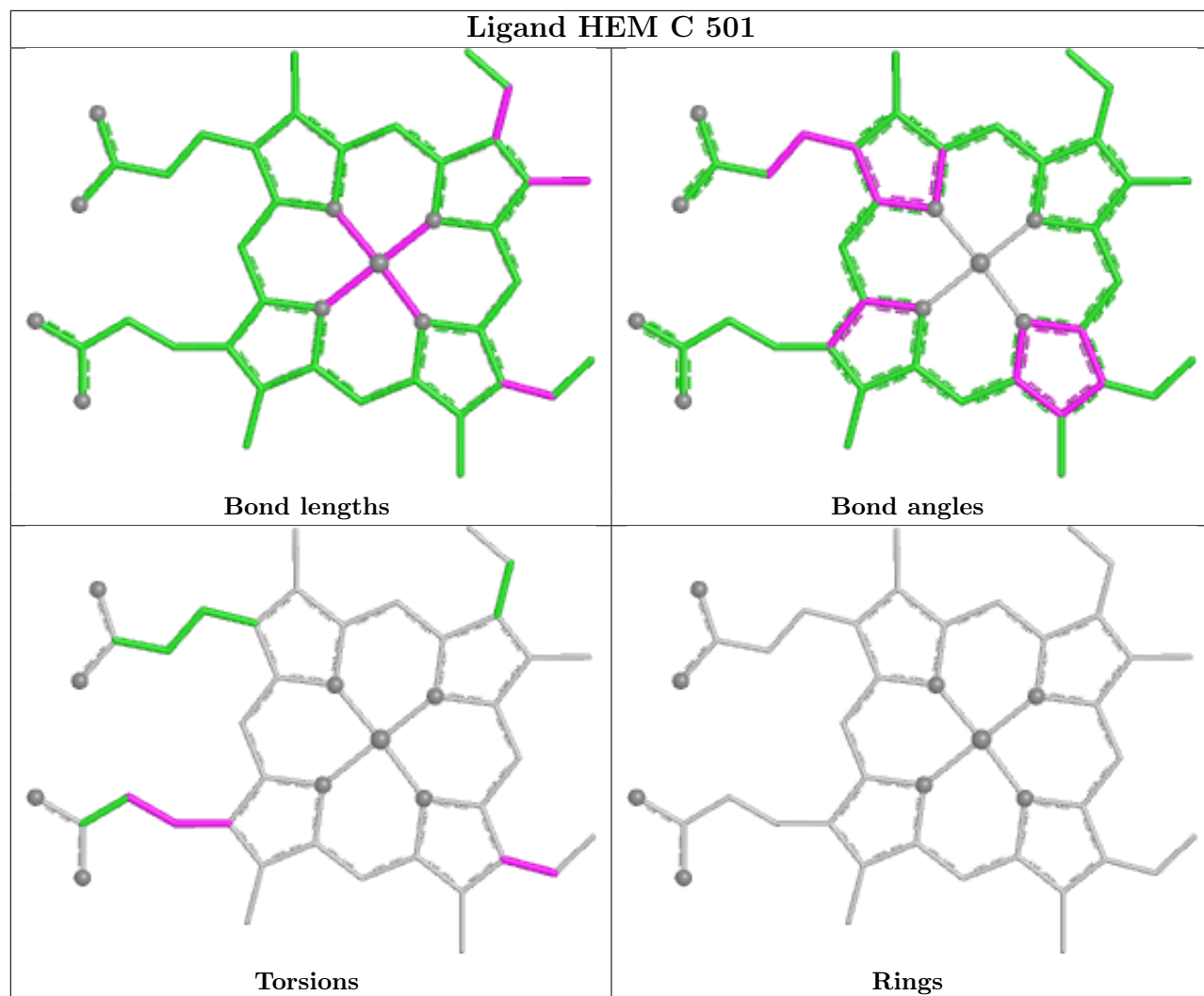
Ligand A1COA C 503



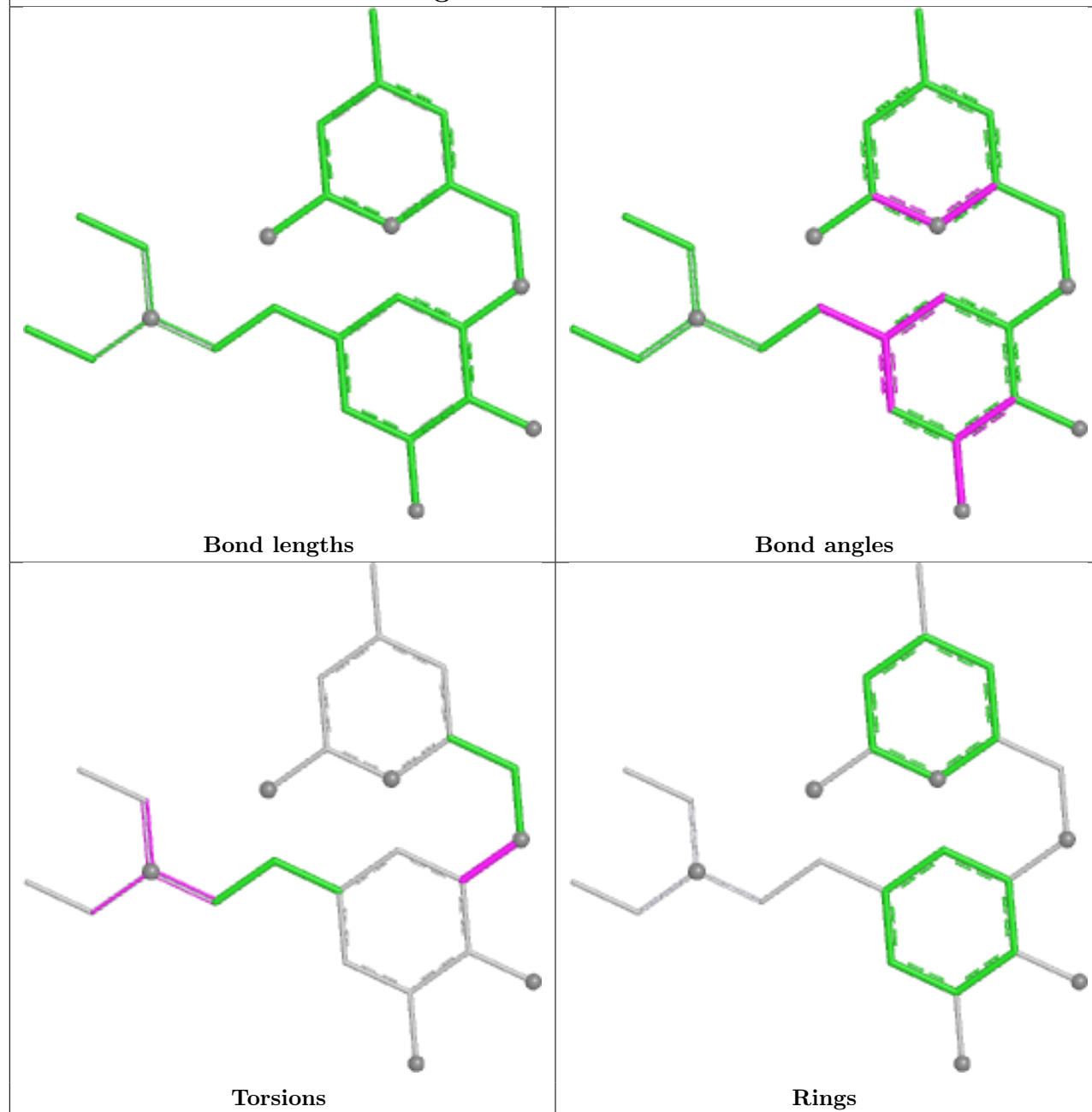
Ligand A1COA A 503

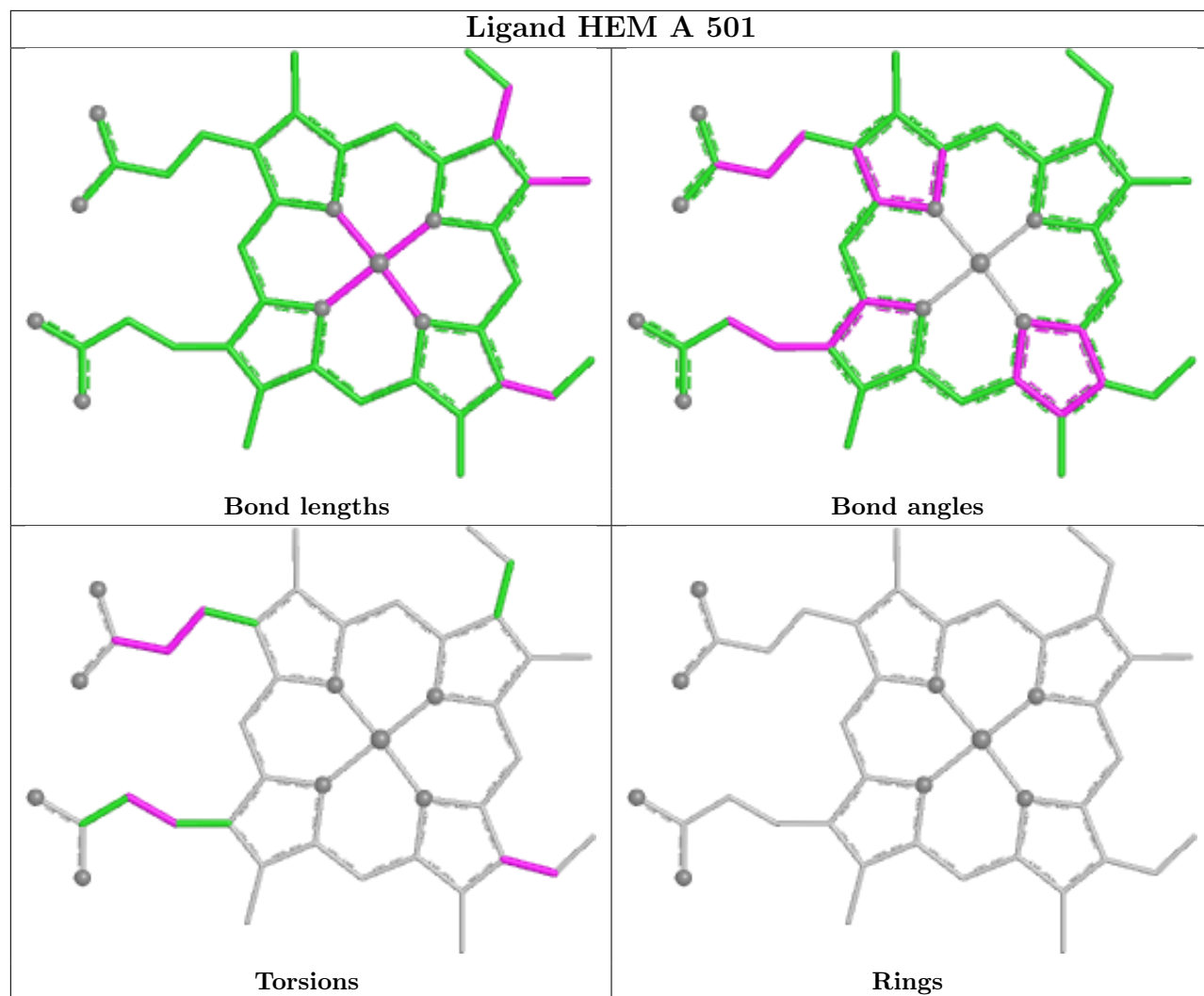


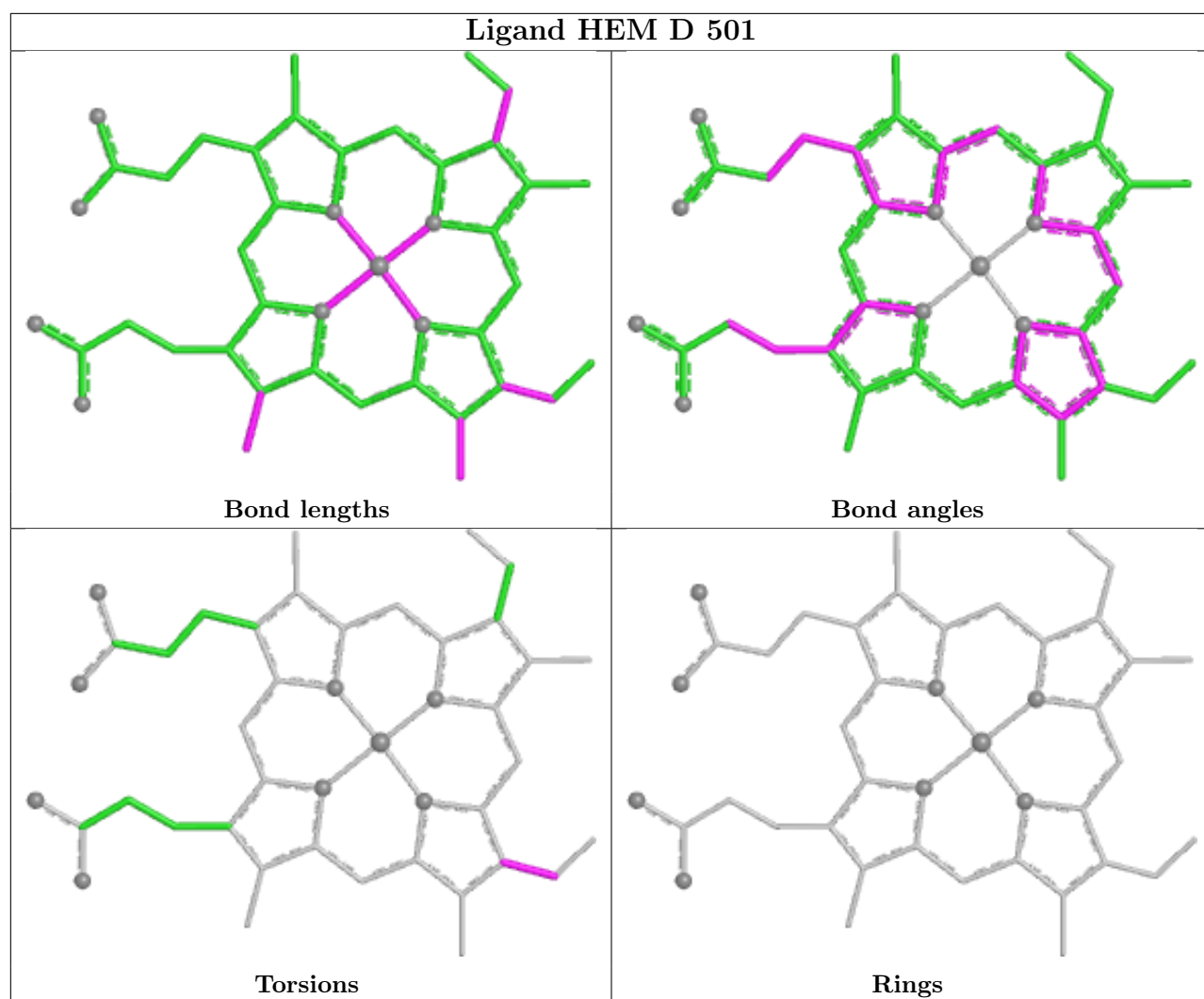




Ligand A1COA B 503







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	402/440 (91%)	0.31	16 (3%) 42 41	20, 43, 81, 110	1 (0%)
1	B	402/440 (91%)	-0.17	7 (1%) 69 69	19, 29, 52, 107	1 (0%)
1	C	401/440 (91%)	0.46	17 (4%) 40 40	18, 44, 81, 106	1 (0%)
1	D	402/440 (91%)	-0.07	5 (1%) 76 77	17, 32, 65, 108	3 (0%)
All	All	1607/1760 (91%)	0.13	45 (2%) 55 55	17, 36, 77, 110	6 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	106	PRO	6.2
1	A	106	PRO	4.7
1	D	106	PRO	4.0
1	C	120	PRO	4.0
1	B	106	PRO	3.9
1	B	119	ALA	3.7
1	A	120	PRO	3.6
1	D	257	GLN	3.4
1	B	257	GLN	3.3
1	C	204	ALA	3.3
1	D	259	GLY	3.1
1	D	67	LYS	3.0
1	A	119	ALA	2.7
1	A	107	ARG	2.7
1	B	89	GLN	2.6
1	B	258	ASP	2.6
1	A	155	ALA	2.6
1	C	295	ALA	2.6
1	A	158	ALA	2.5
1	C	86	ALA	2.5
1	A	141	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	89	GLN	2.4
1	C	153	VAL	2.4
1	A	304	LEU	2.4
1	C	238	ARG	2.4
1	C	299	PRO	2.4
1	C	159	ALA	2.3
1	C	90	GLN	2.3
1	A	142	GLY	2.2
1	C	155	ALA	2.2
1	C	480	TRP	2.2
1	A	280	THR	2.2
1	C	160	THR	2.2
1	A	257	GLN	2.2
1	B	122	GLN	2.2
1	C	237	GLY	2.2
1	C	304	LEU	2.1
1	D	89	GLN	2.1
1	A	153	VAL	2.1
1	A	480	TRP	2.1
1	B	67	LYS	2.0
1	A	160	THR	2.0
1	C	302	LEU	2.0
1	A	239	GLY	2.0
1	A	344	GLY	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](#)

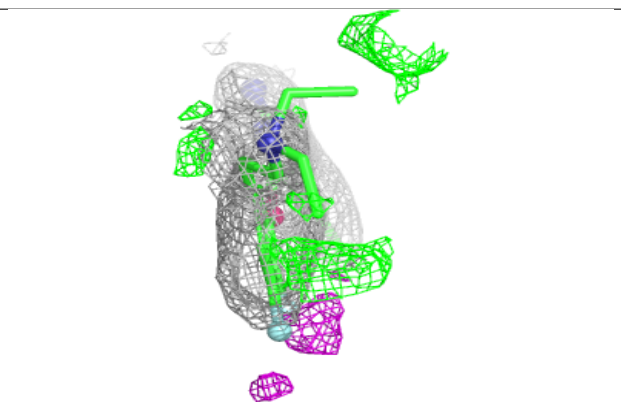
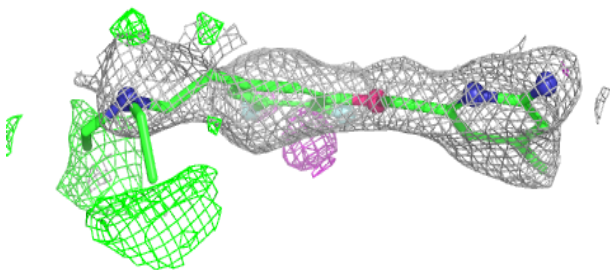
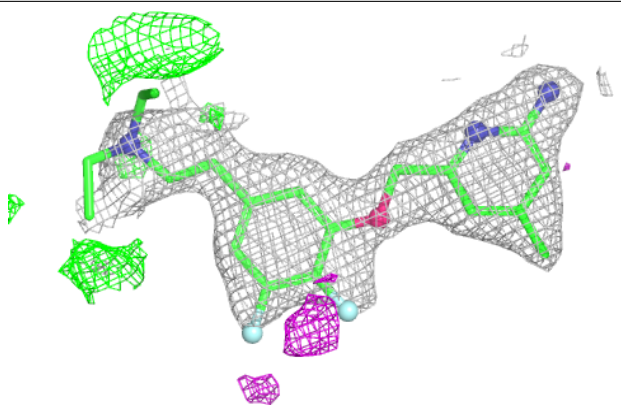
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BTB	B	505	14/14	0.60	0.22	63,68,79,84	0
6	GOL	A	507	6/6	0.60	0.17	83,85,87,89	0
6	GOL	D	506	6/6	0.62	0.18	65,72,72,73	0
6	GOL	B	506	6/6	0.67	0.16	64,69,72,72	0
5	BTB	D	505	14/14	0.72	0.17	39,64,71,71	0
4	A1COA	A	503	25/25	0.74	0.23	37,83,93,98	0
5	BTB	C	504	14/14	0.78	0.18	60,91,98,100	0
5	BTB	C	505	14/14	0.82	0.19	32,58,70,74	0
6	GOL	C	507	6/6	0.82	0.10	78,80,85,85	0
6	GOL	A	508	6/6	0.82	0.18	52,62,67,70	0
4	A1COA	C	503	25/25	0.83	0.21	41,83,99,107	0
4	A1COA	D	503	25/25	0.83	0.21	22,82,97,98	0
5	BTB	B	504	14/14	0.83	0.15	46,52,71,73	0
4	A1COA	B	503	25/25	0.85	0.20	24,80,92,95	0
5	BTB	D	504	14/14	0.87	0.14	37,47,57,58	0
5	BTB	A	505	14/14	0.89	0.17	10,49,64,65	0
6	GOL	C	506	6/6	0.89	0.14	39,60,72,73	0
6	GOL	D	507	6/6	0.89	0.15	53,59,60,63	0
5	BTB	A	504	14/14	0.90	0.15	17,65,74,78	0
3	H4B	A	502	17/17	0.91	0.10	29,39,45,49	0
6	GOL	A	506	6/6	0.92	0.10	36,40,55,57	0
3	H4B	C	502	17/17	0.92	0.09	35,44,50,50	0
8	GD	C	509	1/1	0.92	0.12	121,121,121,121	0
3	H4B	D	502	17/17	0.93	0.07	25,32,38,41	0
3	H4B	B	502	17/17	0.95	0.07	26,32,37,37	0
2	HEM	C	501	43/43	0.96	0.10	29,39,74,82	0
7	CL	C	508	1/1	0.97	0.09	48,48,48,48	0
8	GD	A	510	1/1	0.97	0.16	72,72,72,72	0
8	GD	B	508	1/1	0.97	0.04	37,37,37,37	0
2	HEM	A	501	43/43	0.97	0.08	25,34,63,72	0
7	CL	D	508	1/1	0.98	0.08	33,33,33,33	0
2	HEM	D	501	43/43	0.98	0.07	18,24,59,85	0
7	CL	B	507	1/1	0.98	0.06	37,37,37,37	0
2	HEM	B	501	43/43	0.98	0.07	15,22,49,71	0
9	ZN	C	510	1/1	0.98	0.03	30,30,30,30	0
8	GD	D	509	1/1	0.99	0.04	35,35,35,35	0
7	CL	A	509	1/1	0.99	0.09	43,43,43,43	0
10	CA	A	512	1/1	0.99	0.04	31,31,31,31	0
9	ZN	A	511	1/1	1.00	0.02	27,27,27,27	0

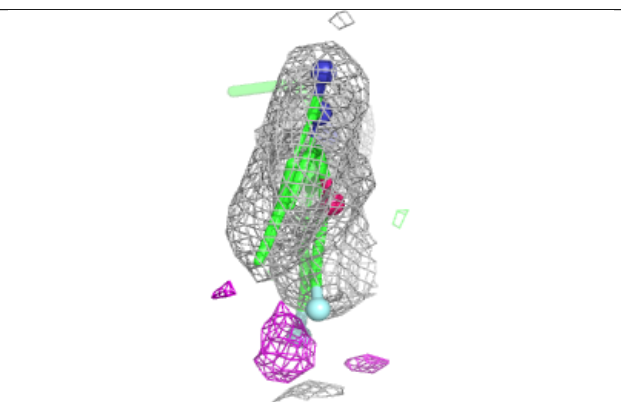
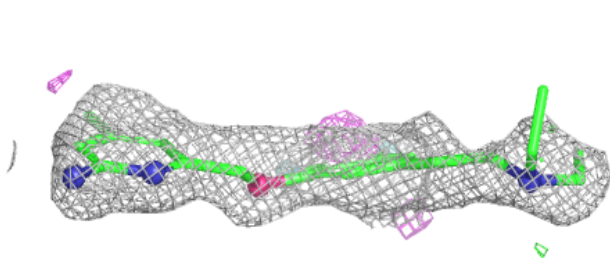
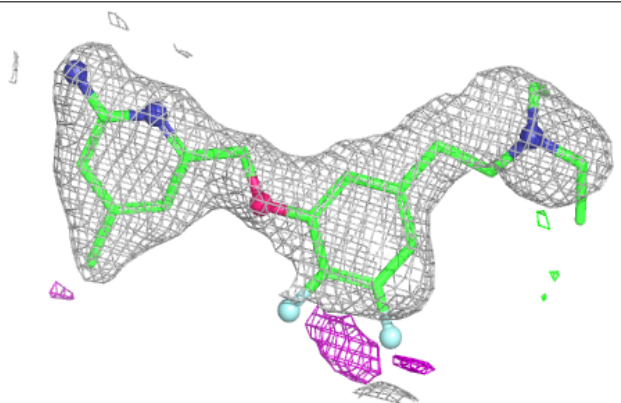
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1COA 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)

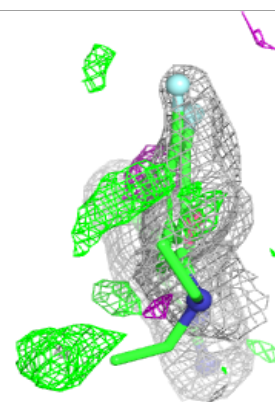
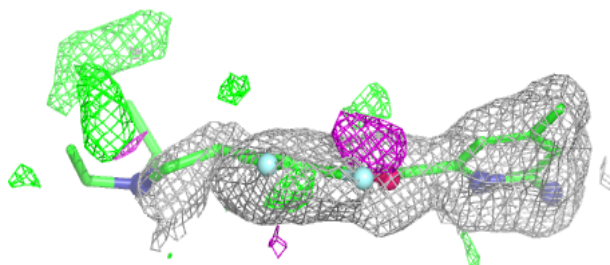
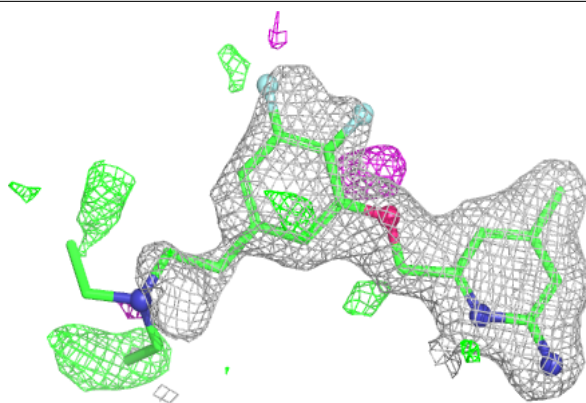
**Electron density around A1COA C 503:**

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



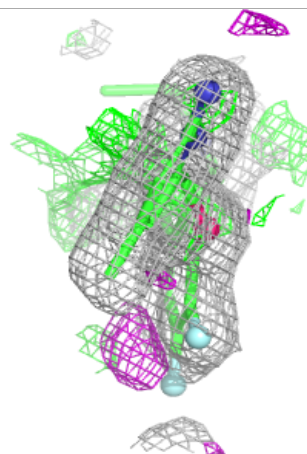
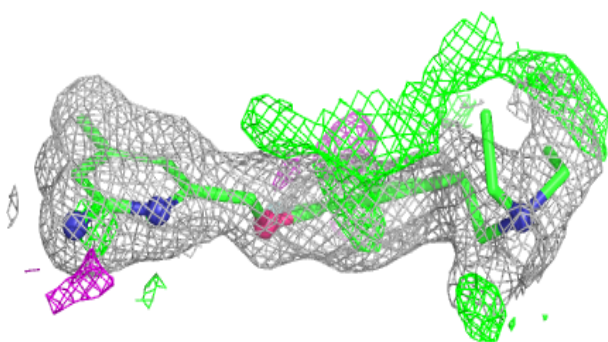
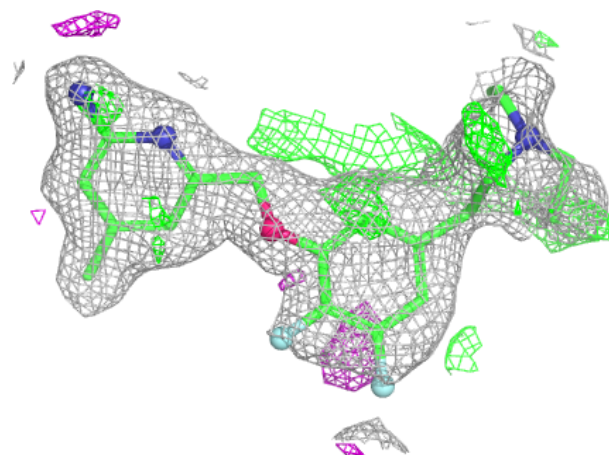
Electron density around A1COA D 503:

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



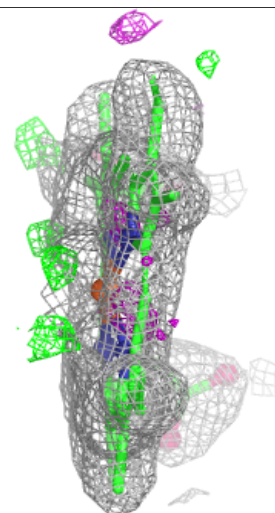
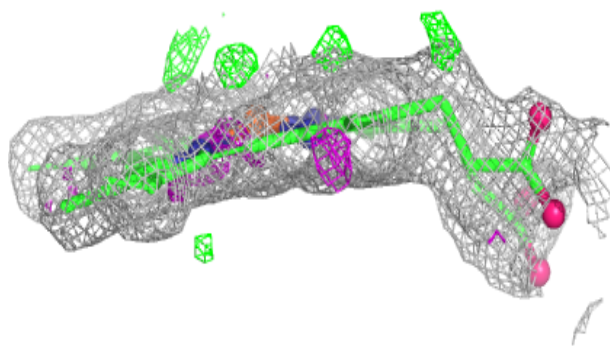
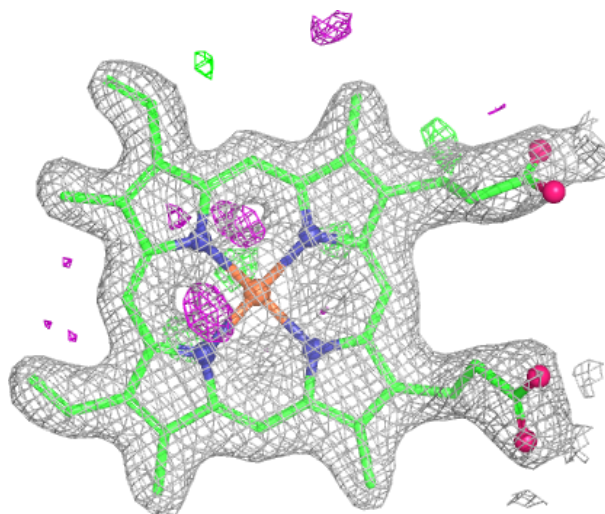
Electron density around A1COA B 503:

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



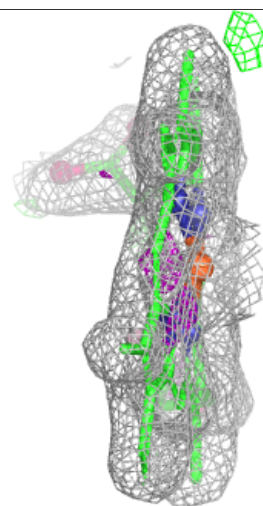
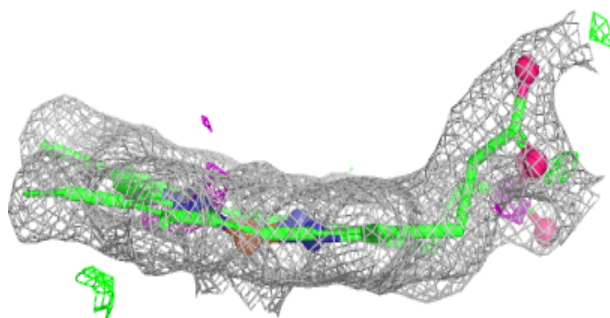
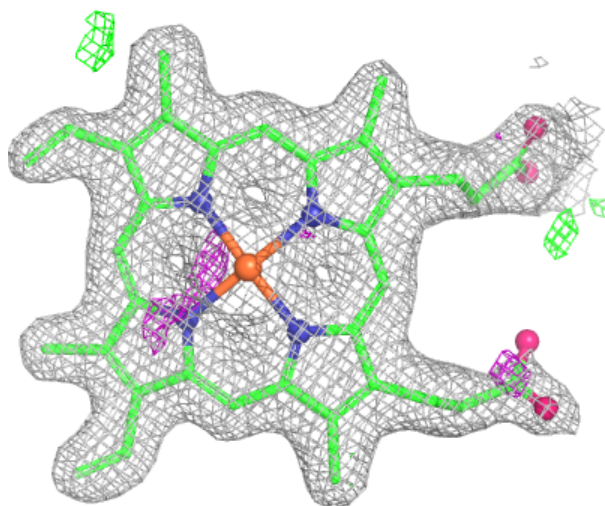
Electron density around HEM C 501:

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



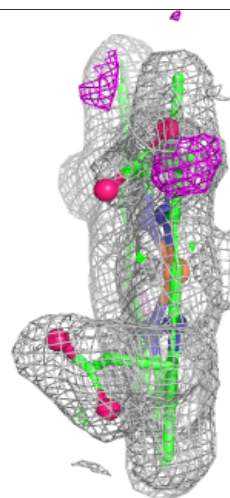
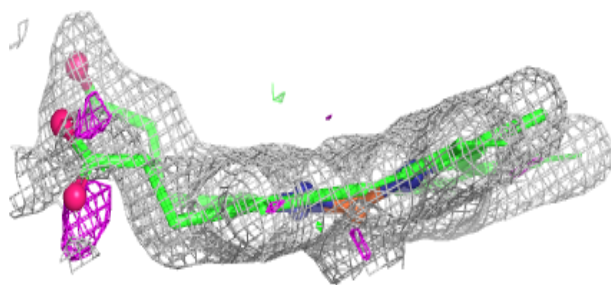
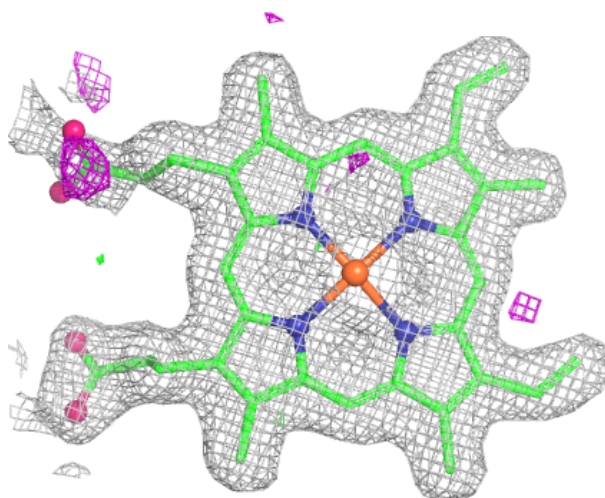
Electron density around HEM A 501:

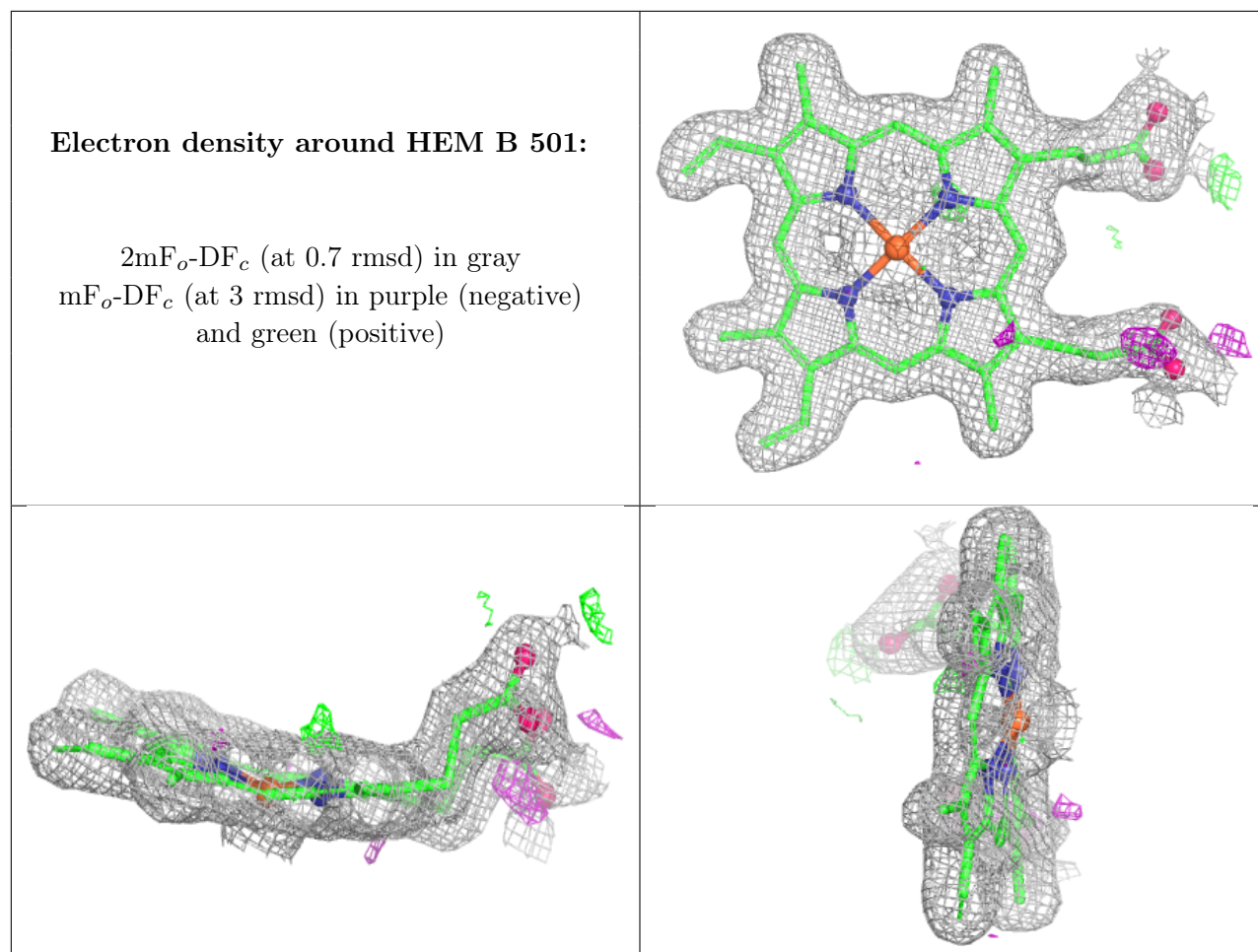
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM D 501:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.