



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 2, 2025 – 12:31 PM EDT

PDB ID : 9Q53 / pdb\_00009q53  
Title : Structure of human endothelial nitric oxide synthase heme domain bound with 6-((2,3-difluoro-5-(2-(piperidin-1-yl)ethyl)phenoxy)methyl)-4-methylpyridin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2025-08-20  
Resolution : 1.88 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

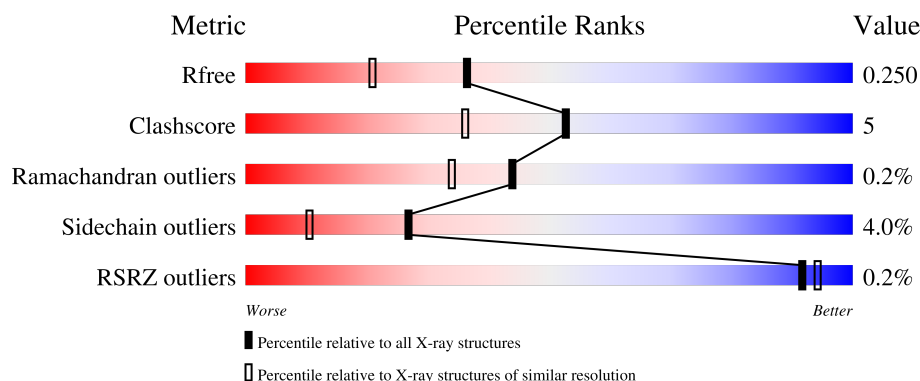
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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))
$R_{free}$	164625	1090 (1.88-1.88)
Clashscore	180529	1144 (1.88-1.88)
Ramachandran outliers	177936	1135 (1.88-1.88)
Sidechain outliers	177891	1135 (1.88-1.88)
RSRZ outliers	164620	1090 (1.88-1.88)

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

Mol	Chain	Length	Quality of chain
1	A	440	<div> <div></div> <div>79%</div> <div>10%</div> <div>•</div> <div>9%</div> </div>
1	B	440	<div> <div></div> <div>81%</div> <div>10%</div> <div></div> <div>9%</div> </div>
1	C	440	<div> <div>%</div> <div>78%</div> <div>12%</div> <div>•</div> <div>9%</div> </div>
1	D	440	<div> <div></div> <div>83%</div> <div>7%</div> <div>•</div> <div>9%</div> </div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14066 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	400	Total	C	N	O	S	0	1	0
			3200	2038	563	583	16			
1	B	402	Total	C	N	O	S	0	2	0
			3215	2048	565	586	16			
1	C	400	Total	C	N	O	S	0	1	0
			3200	2038	563	583	16			
1	D	402	Total	C	N	O	S	0	4	0
			3225	2054	566	589	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

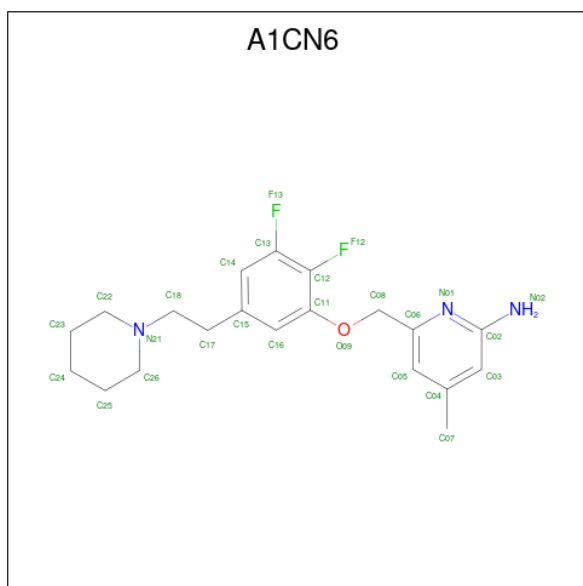
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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- The chemical structure of H4B (Hydroxybutyrate) is shown with the following details:
- Atom Numbering:** Carbons are labeled C7, C6(R), C9(R), C10(S), and C11. Nitrogens are labeled N8, N5, N1, N3, and N2. Oxygen atoms are labeled O9, O4, and O10.
  - Functional Groups:** A carboxylic acid group is attached to C9(R), consisting of C10(S) bonded to O9 (hydroxyl) and O4 (carbonyl). An amine group is attached to C6(R), consisting of N5 bonded to N8 and N3.
  - Stereochemistry:** The hydroxyl group on C10(S) is shown with a red wedge bond. The amine group on C6(R) is shown with a black wedge bond. The carboxylate group on C9(R) is shown with a black wedge bond.
  - Other Labels:** The label "H4B" is at the top. The label "O4" is near the carbonyl oxygen. The label "N2" is near the amine group. The label "C8A" is near the nitrogen N8. The label "C4A" is near the nitrogen N5. The label "C2" is near the nitrogen N1. The label "C7" is near the nitrogen N8. The label "C6(R)" is near the nitrogen N5. The label "C9(R)" is near the nitrogen N5. The label "C10(S)" is near the nitrogen N5. The label "C11" is near the nitrogen N5.

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-(2,3-difluoro-5-[2-(piperidin-1-yl)ethyl]phenoxy)methyl)-4-methylpyridine-2-amine (CCD ID: A1CN6) (formula: C<sub>20</sub>H<sub>25</sub>F<sub>2</sub>N<sub>3</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			26	20	2	3	1		
4	B	1	Total	C	F	N	O	0	0
			26	20	2	3	1		
4	C	1	Total	C	F	N	O	0	0
			26	20	2	3	1		
4	D	1	Total	C	F	N	O	0	0
			26	20	2	3	1		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



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
10	C	1	Total 1	Ca 1	0	0

- Molecule 11 is water.

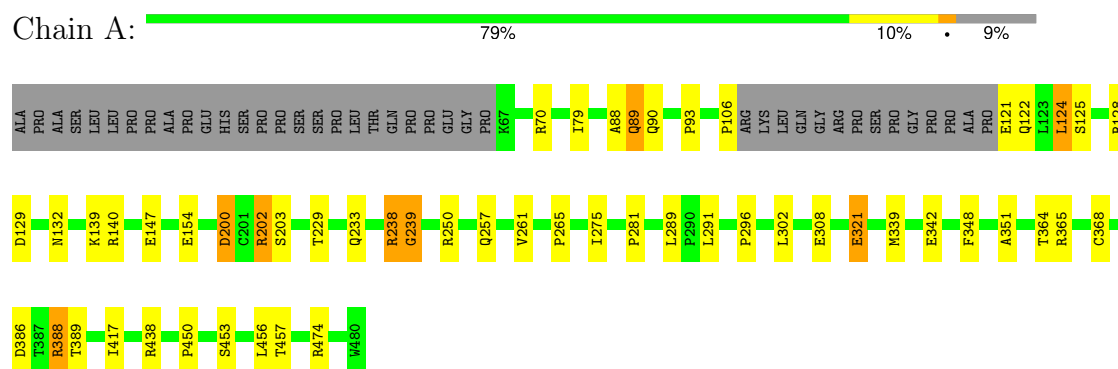
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	151	Total 151	O 151	0	0
11	B	228	Total 228	O 228	0	0
11	C	107	Total 107	O 107	0	0
11	D	224	Total 224	O 224	0	0



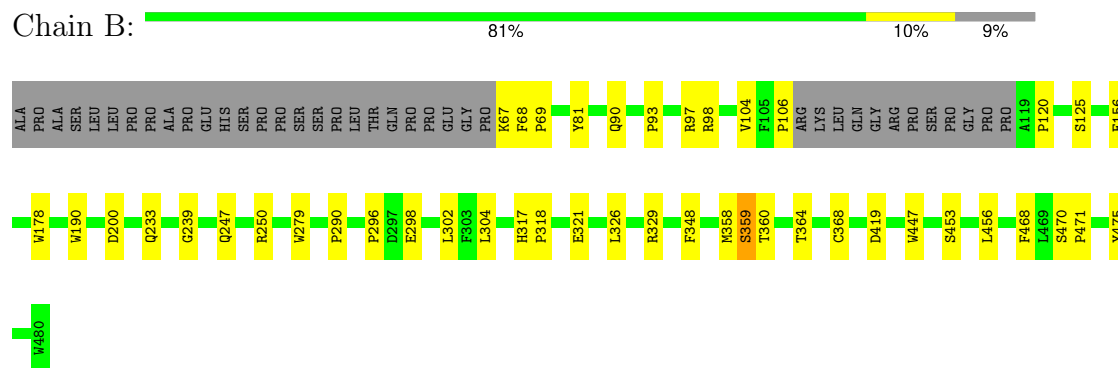
### 3 Residue-property plots

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.

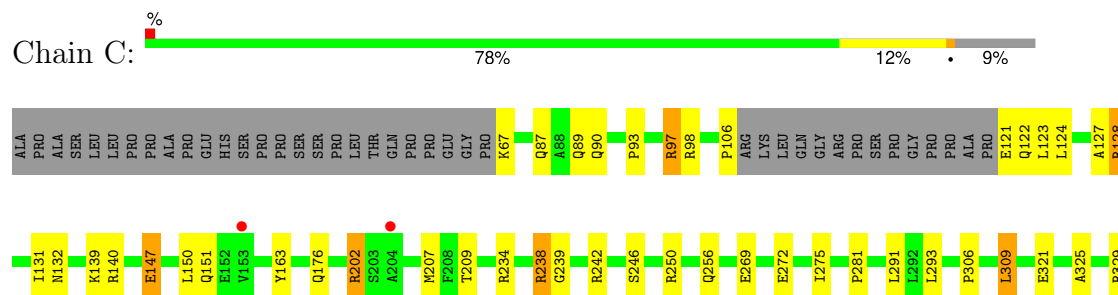
#### • Molecule 1: Nitric oxide synthase 3

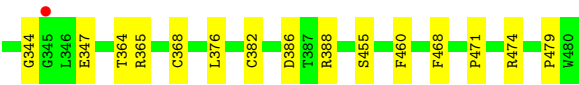


#### • Molecule 1: Nitric oxide synthase 3

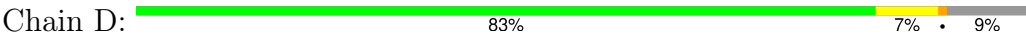


#### • Molecule 1: Nitric oxide synthase 3





● 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, $\alpha$ , $\beta$ , $\gamma$	59.99Å 153.66Å 109.19Å 90.00° 90.63° 90.00°	Depositor
Resolution (Å)	47.28 – 1.88 47.28 – 1.88	Depositor EDS
% Data completeness (in resolution range)	96.7 (47.28-1.88) 93.6 (47.28-1.88)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 1.88Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.211 , 0.253 0.208 , 0.250	Depositor DCC
$R_{free}$ test set	7801 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.158 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: A1CN6, CL, H4B, GD, BTB, CA, ZN, GOL, 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	0.28	0/3294	0.48	0/4487
1	B	0.35	0/3313	0.53	0/4514
1	C	0.28	0/3294	0.48	0/4487
1	D	0.34	0/3329	0.51	0/4536
All	All	0.32	0/13230	0.50	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	3200	0	3104	27	0
1	B	3215	0	3121	26	1
1	C	3200	0	3104	29	0
1	D	3225	0	3131	20	1
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	5	0
3	A	17	0	15	1	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	1	0
3	D	17	0	15	2	0
4	A	26	0	0	1	0
4	B	26	0	0	2	0
4	C	26	0	0	0	0
4	D	26	0	0	1	0
5	A	28	0	38	4	0
5	B	28	0	37	6	0
5	C	28	0	38	6	0
5	D	28	0	37	7	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
10	C	1	0	0	0	0
11	A	151	0	0	2	0
11	B	228	0	0	2	0
11	C	107	0	0	1	0
11	D	224	0	0	5	0
All	All	14066	0	12854	129	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.

The worst 5 of 129 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLN:NE2	11:B:601:HOH:O	2.11	0.82
1:D:247:GLN:HB2	1:D:250:ARG:HD3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.73	0.71
1:A:88:ALA:O	1:B:97:ARG:NH2	2.24	0.70
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.75	0.69

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:B:200:ASP:O	1:D:140:ARG:NH2[1_456]	2.19	0.01

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/440 (90%)	383 (96%)	13 (3%)	1 (0%)	37	26
1	B	400/440 (91%)	393 (98%)	6 (2%)	1 (0%)	37	26
1	C	397/440 (90%)	380 (96%)	16 (4%)	1 (0%)	37	26
1	D	402/440 (91%)	392 (98%)	10 (2%)	0	100	100
All	All	1596/1760 (91%)	1548 (97%)	45 (3%)	3 (0%)	44	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	GLN
1	B	120	PRO
1	A	239	GLY

### 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	341/373 (91%)	319 (94%)	22 (6%)	14	4
1	B	343/373 (92%)	338 (98%)	5 (2%)	60	49
1	C	341/373 (91%)	324 (95%)	17 (5%)	20	7
1	D	345/373 (92%)	333 (96%)	12 (4%)	31	15
All	All	1370/1492 (92%)	1314 (96%)	56 (4%)	27	10

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	87	GLN
1	D	417	ILE
1	C	139	LYS
1	D	378	ASP
1	D	213[A]	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	276	GLN
1	D	126	GLN
1	D	151	GLN
1	B	151	GLN
1	B	403	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 12 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
5	BTB	A	504	8	13,13,13	0.38	0	7,16,16	0.54	0
2	HEM	D	501	1	42,50,50	1.53	5 (11%)	46,82,82	1.80	14 (30%)
4	A1CN6	D	503	-	28,28,28	0.39	0	36,38,38	1.57	6 (16%)
6	GOL	B	506	-	5,5,5	0.34	0	5,5,5	0.33	0
5	BTB	D	504	8	13,13,13	0.41	0	7,16,16	0.65	0
3	H4B	C	502	-	16,18,18	0.92	0	14,26,26	2.36	5 (35%)
6	GOL	A	508	-	5,5,5	0.42	0	5,5,5	0.14	0
2	HEM	B	501	1	42,50,50	1.59	6 (14%)	46,82,82	1.74	10 (21%)
4	A1CN6	A	503	-	28,28,28	0.40	0	36,38,38	1.67	6 (16%)
2	HEM	C	501	1	42,50,50	1.53	6 (14%)	46,82,82	1.66	11 (23%)
5	BTB	C	505	-	13,13,13	0.46	0	7,16,16	0.90	0
5	BTB	B	505	-	13,13,13	0.49	0	7,16,16	1.21	0
6	GOL	A	506	-	5,5,5	0.36	0	5,5,5	0.34	0
3	H4B	A	502	-	16,18,18	0.84	0	14,26,26	2.48	5 (35%)
5	BTB	B	504	8	13,13,13	0.45	0	7,16,16	0.70	0
5	BTB	D	505	-	13,13,13	0.39	0	7,16,16	0.76	0
5	BTB	A	505	-	13,13,13	0.62	0	7,16,16	0.89	0
3	H4B	B	502	-	16,18,18	0.89	0	14,26,26	2.35	5 (35%)
6	GOL	C	506	-	5,5,5	0.33	0	5,5,5	0.41	0
6	GOL	A	507	-	5,5,5	0.37	0	5,5,5	0.27	0
6	GOL	D	506	-	5,5,5	0.34	0	5,5,5	0.34	0
2	HEM	A	501	1	42,50,50	1.54	8 (19%)	46,82,82	1.84	12 (26%)
4	A1CN6	B	503	-	28,28,28	0.45	0	36,38,38	1.36	5 (13%)
6	GOL	C	507	-	5,5,5	0.39	0	5,5,5	0.27	0
3	H4B	D	502	-	16,18,18	0.90	0	14,26,26	2.69	5 (35%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BTB	C	504	8	13,13,13	0.39	0	7,16,16	0.42	0
4	A1CN6	C	503	-	28,28,28	0.32	0	36,38,38	1.38	5 (13%)
6	GOL	D	507	-	5,5,5	0.27	0	5,5,5	0.43	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	A	504	8	-	3/21/21/21	-
2	HEM	D	501	1	-	3/12/54/54	-
4	A1CN6	D	503	-	-	4/10/18/18	0/3/3/3
6	GOL	B	506	-	-	2/4/4/4	-
5	BTB	D	504	8	-	7/21/21/21	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
6	GOL	A	508	-	-	2/4/4/4	-
2	HEM	B	501	1	-	3/12/54/54	-
4	A1CN6	A	503	-	-	7/10/18/18	0/3/3/3
2	HEM	C	501	1	-	4/12/54/54	-
5	BTB	C	505	-	-	12/21/21/21	-
5	BTB	B	505	-	-	13/21/21/21	-
6	GOL	A	506	-	-	4/4/4/4	-
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
5	BTB	B	504	8	-	5/21/21/21	-
5	BTB	D	505	-	-	11/21/21/21	-
5	BTB	A	505	-	-	6/21/21/21	-
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
6	GOL	C	506	-	-	4/4/4/4	-
6	GOL	A	507	-	-	2/4/4/4	-
6	GOL	D	506	-	-	2/4/4/4	-
2	HEM	A	501	1	-	2/12/54/54	-
4	A1CN6	B	503	-	-	5/10/18/18	0/3/3/3
6	GOL	C	507	-	-	4/4/4/4	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
5	BTB	C	504	8	-	7/21/21/21	-
4	A1CN6	C	503	-	-	5/10/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	D	507	-	-	2/4/4/4	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3C-C2C	-4.25	1.34	1.40
2	B	501	HEM	C3C-C4C	3.89	1.47	1.41
2	B	501	HEM	C3C-CAC	3.71	1.56	1.47
2	D	501	HEM	C3C-C2C	-3.67	1.35	1.40
2	A	501	HEM	C3C-C2C	-3.63	1.35	1.40

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	H4B	C8A-C4A-C4	6.08	120.03	114.50
3	A	502	H4B	C8A-C4A-C4	5.98	119.94	114.50
3	B	502	H4B	C8A-C4A-C4	5.91	119.88	114.50
2	B	501	HEM	CBA-CAA-C2A	-5.83	102.73	112.54
3	D	502	H4B	C8A-C4A-C4	5.79	119.77	114.50

There are no chirality outliers.

5 of 119 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	HEM	C2A-CAA-CBA-CGA
4	A	503	A1CN6	C12-C11-O09-C08
4	D	503	A1CN6	C12-C11-O09-C08
5	A	504	BTB	O1-C1-C2-N
5	A	505	BTB	O1-C1-C2-C3

There are no ring outliers.

19 monomers are involved in 43 short contacts:

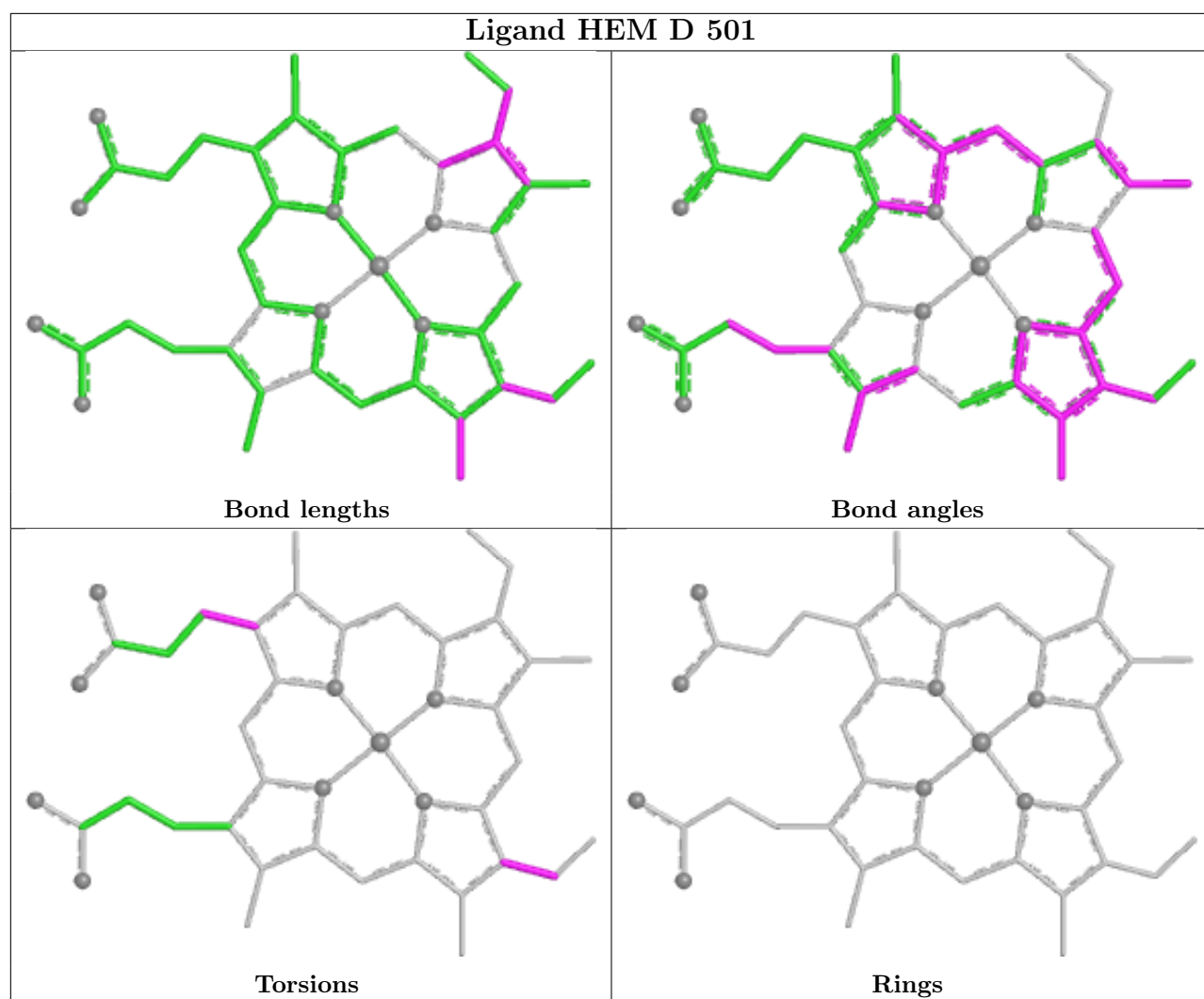
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	504	BTB	1	0
2	D	501	HEM	5	0
4	D	503	A1CN6	1	0
5	D	504	BTB	4	0
3	C	502	H4B	1	0
2	B	501	HEM	3	0
4	A	503	A1CN6	1	0

*Continued on next page...*

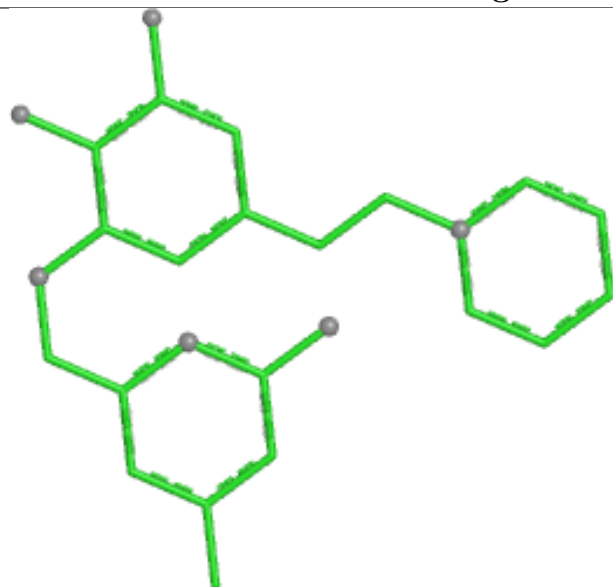
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	2	0
5	C	505	BTB	3	0
5	B	505	BTB	5	0
3	A	502	H4B	1	0
5	B	504	BTB	1	0
5	D	505	BTB	3	0
5	A	505	BTB	3	0
3	B	502	H4B	1	0
2	A	501	HEM	2	0
4	B	503	A1CN6	2	0
3	D	502	H4B	2	0
5	C	504	BTB	3	0

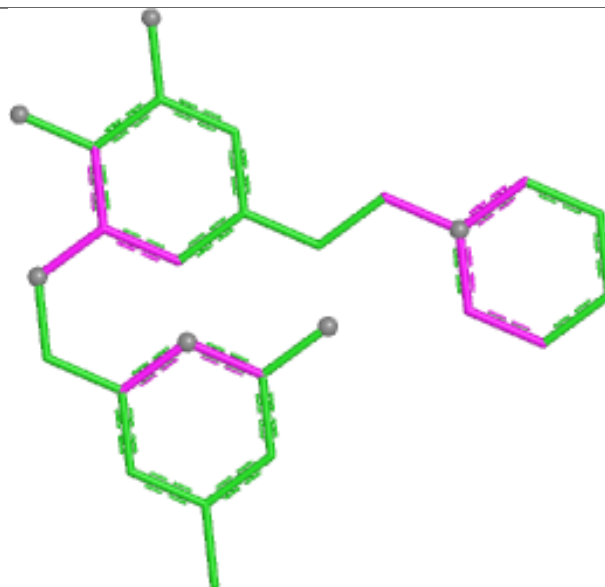
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



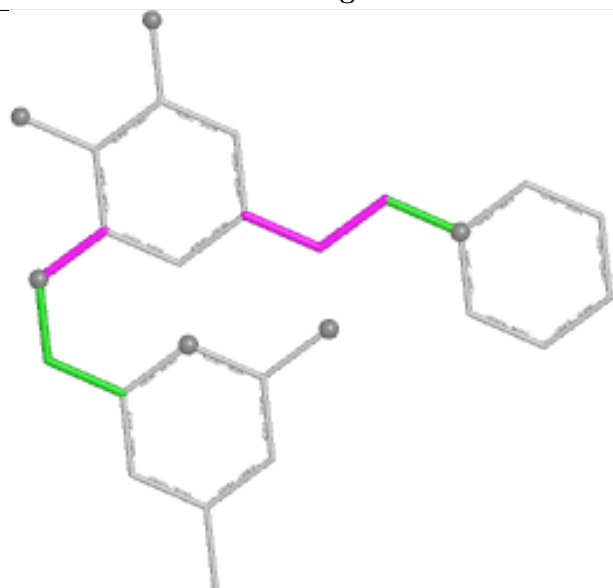
## Ligand A1CN6 D 503



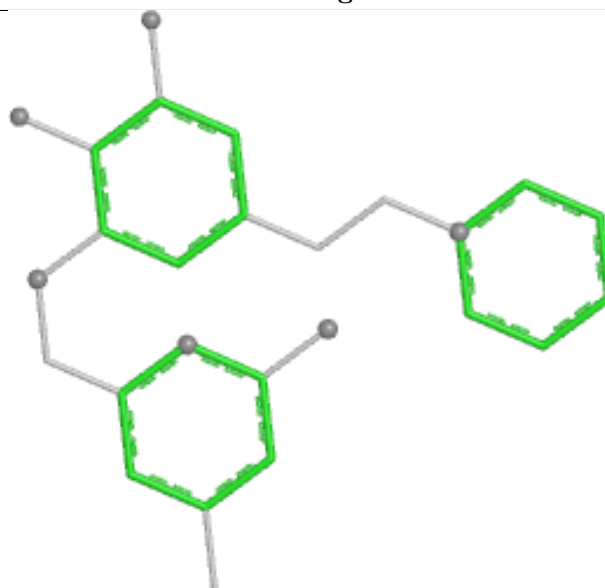
Bond lengths



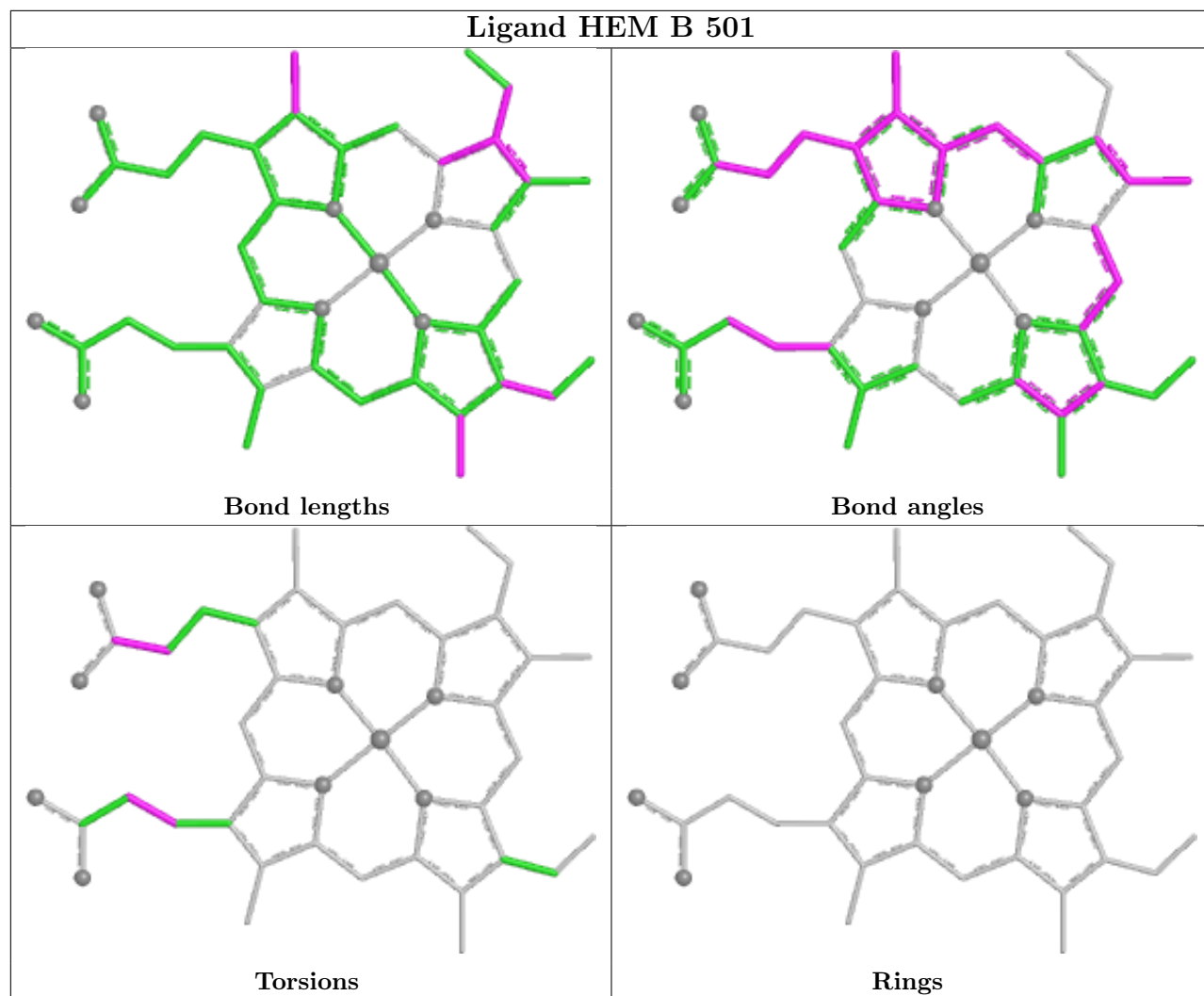
Bond angles



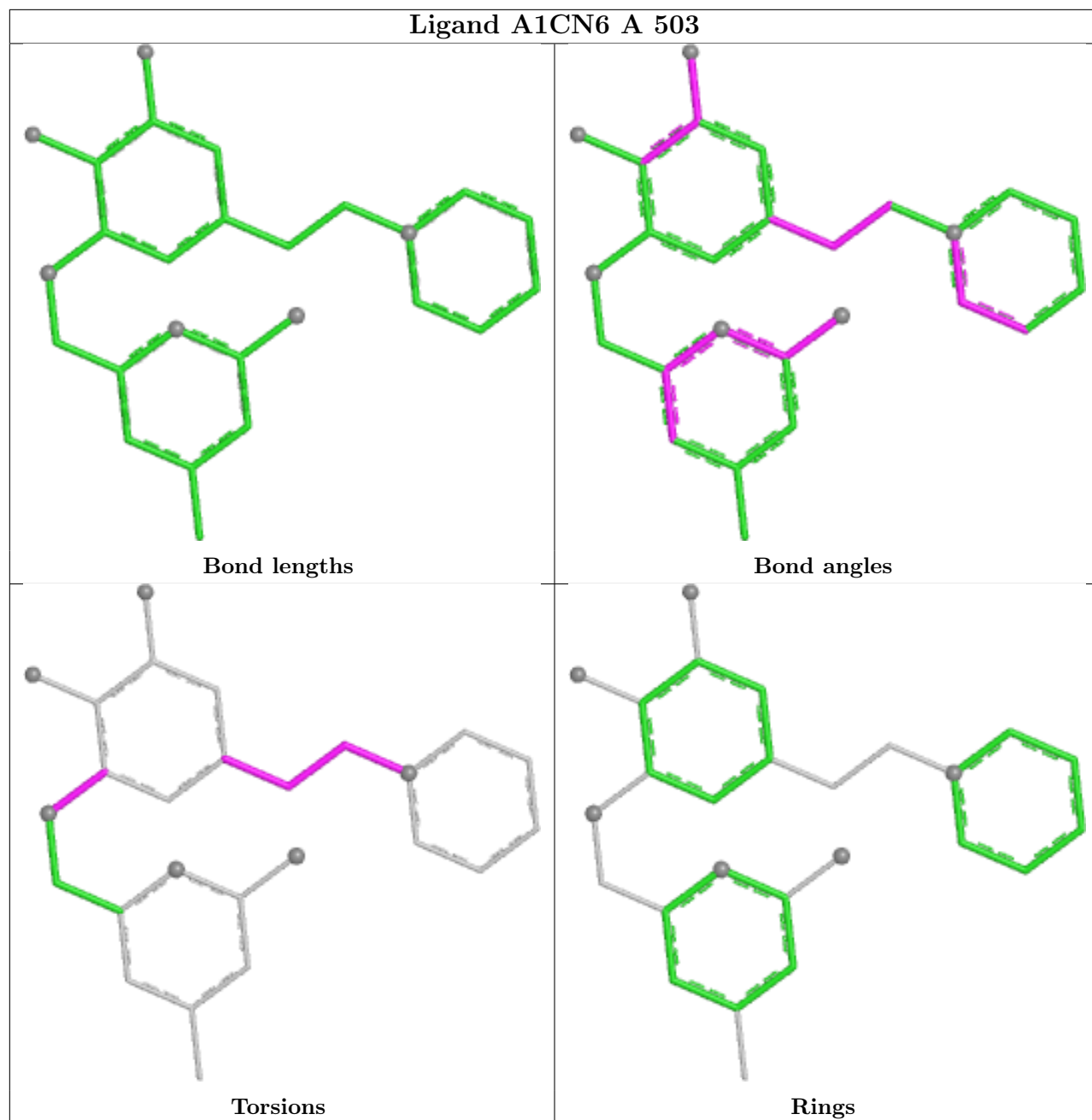
Torsions

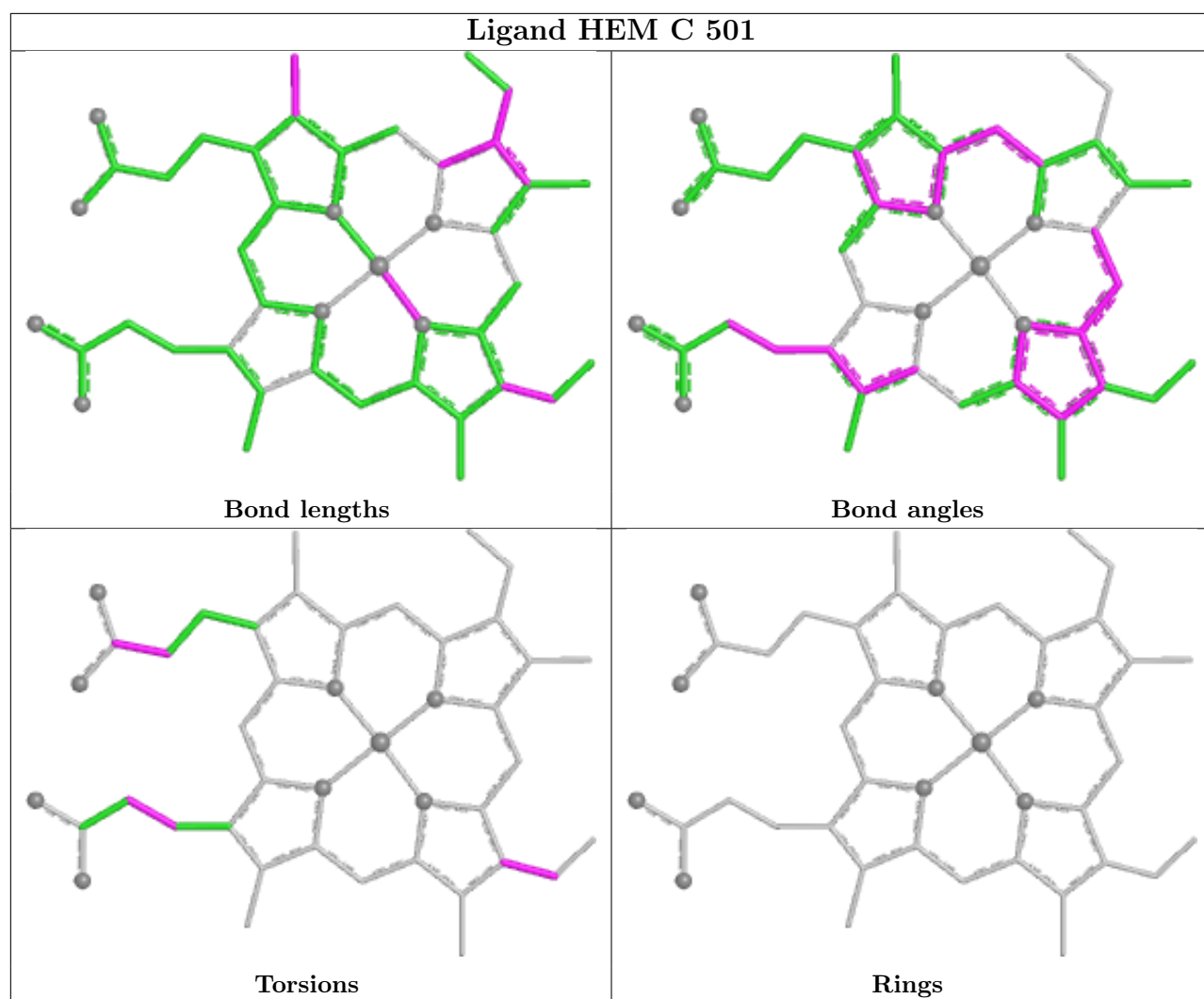


Rings

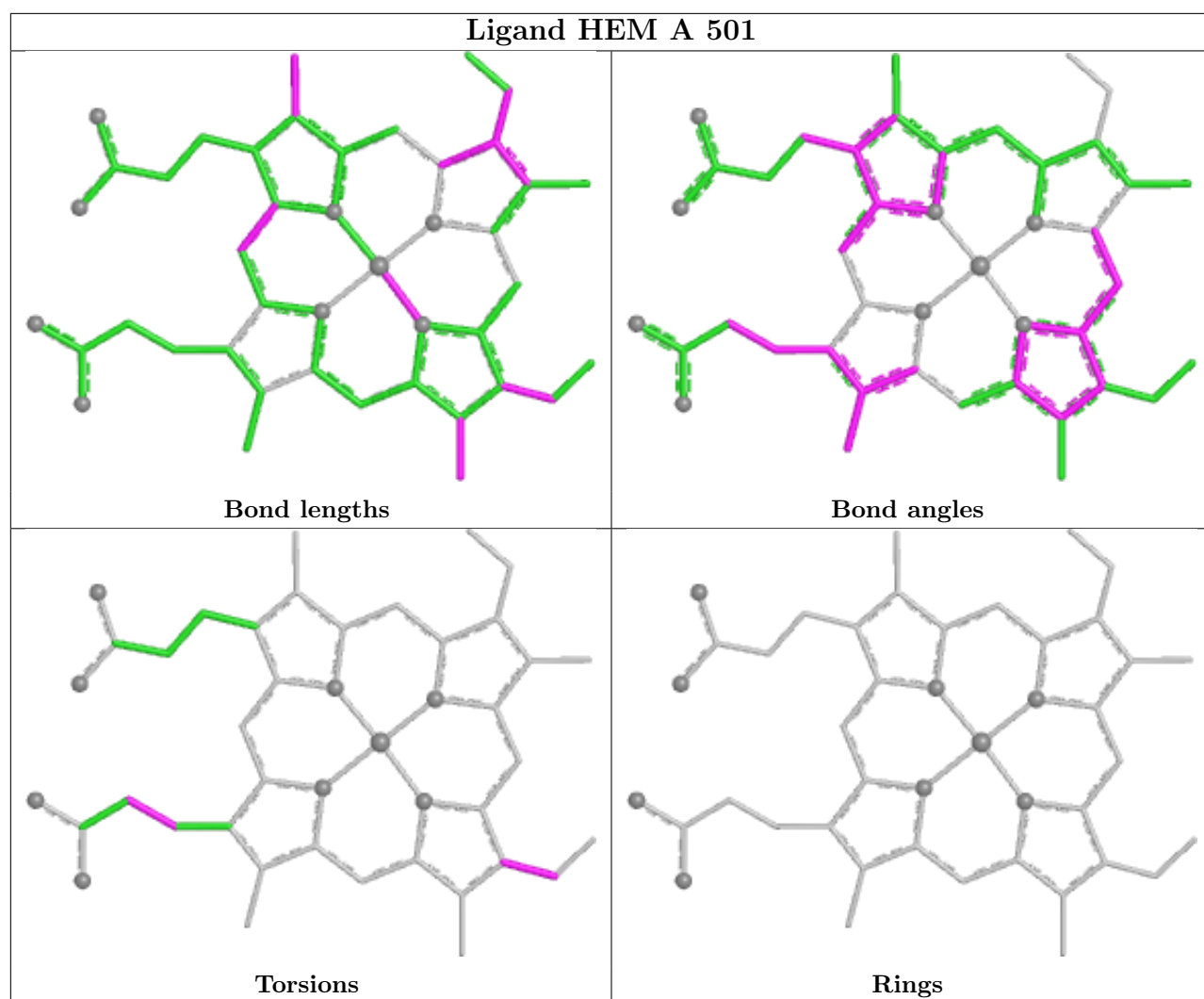


## Ligand A1CN6 A 503

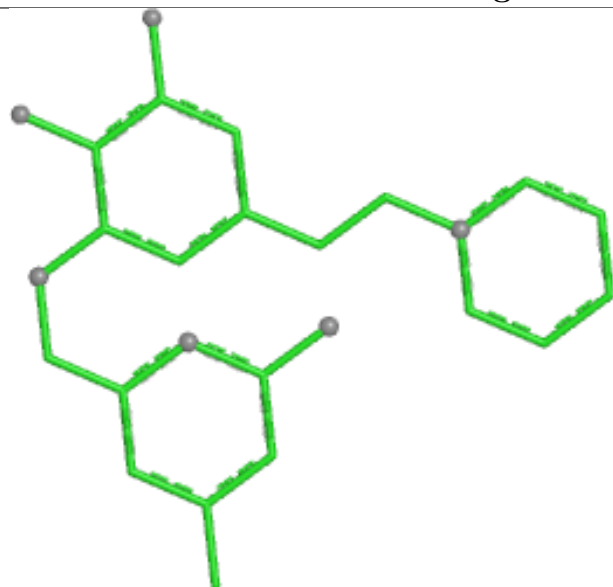




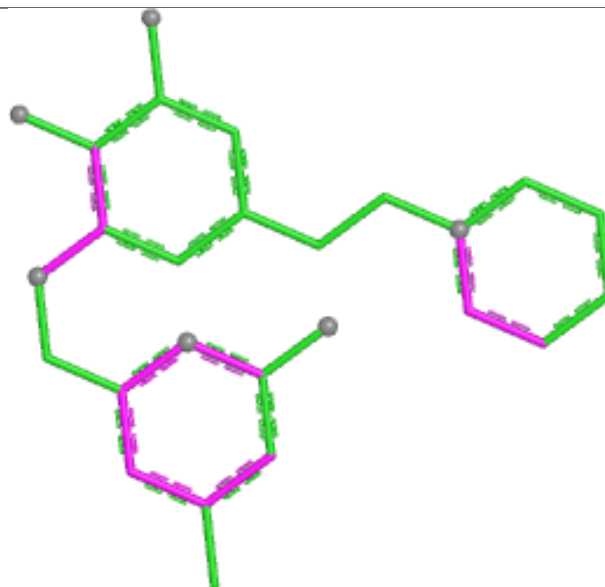




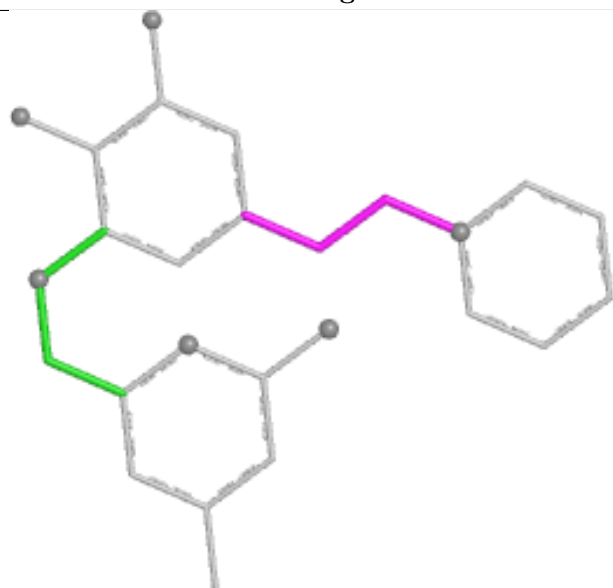
## Ligand A1CN6 B 503



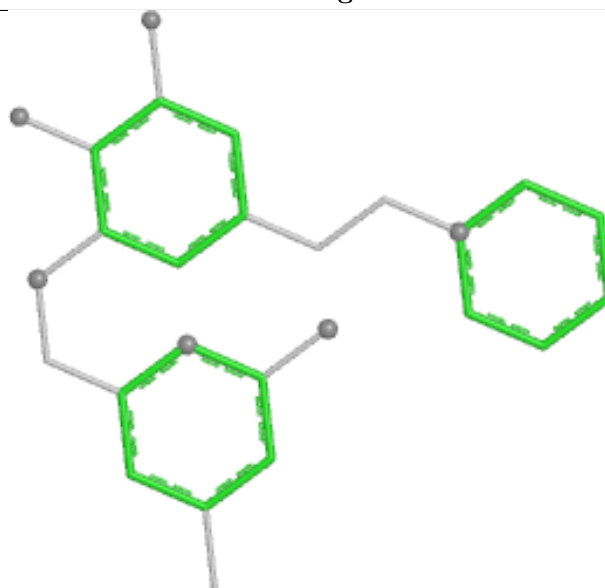
Bond lengths



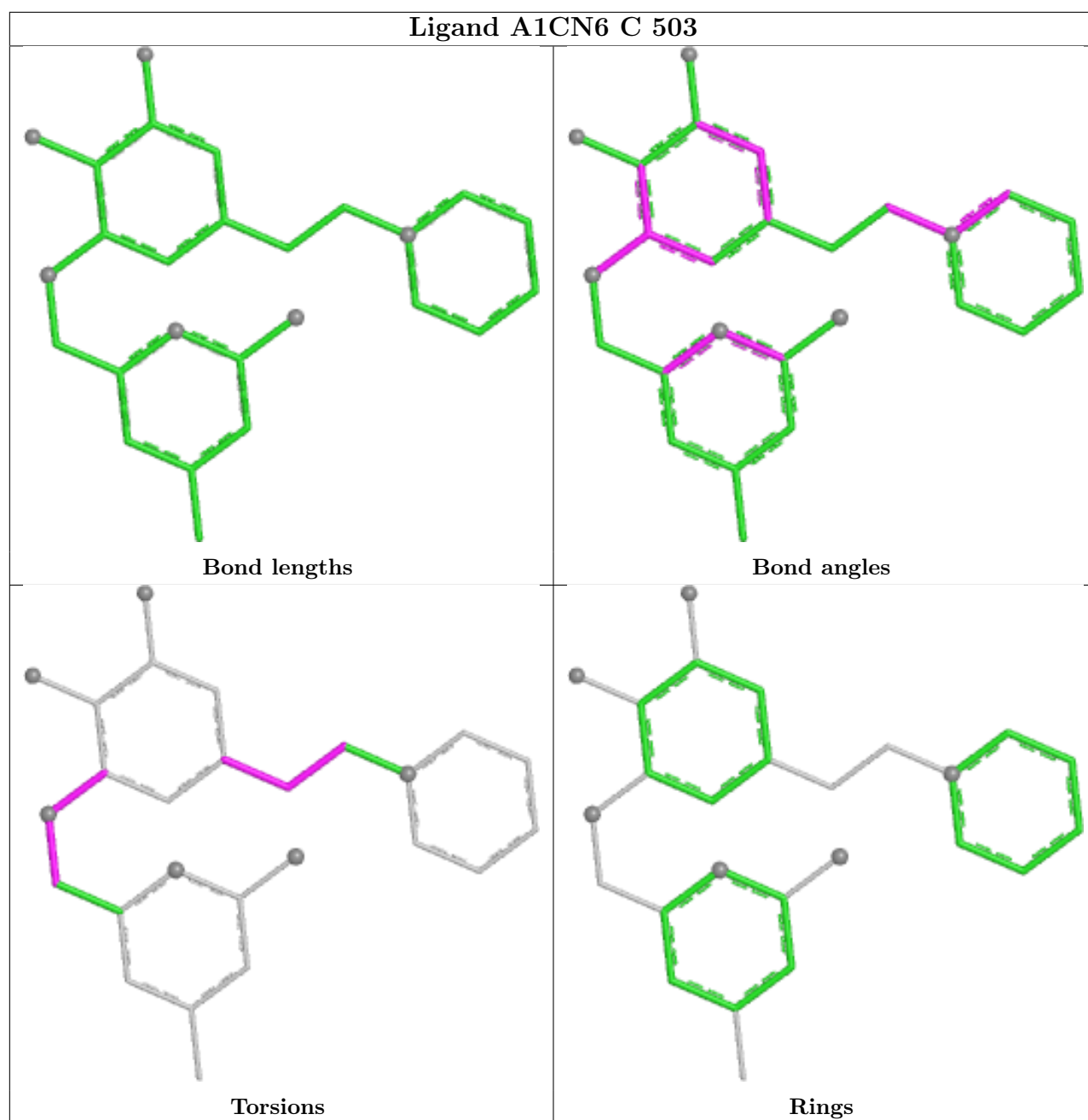
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	400/440 (90%)	-0.91	0	100   100	25, 53, 99, 134	1 (0%)
1	B	402/440 (91%)	-1.23	0	100   100	22, 38, 67, 117	2 (0%)
1	C	400/440 (90%)	-0.61	3 (0%)	82   86	25, 60, 114, 147	1 (0%)
1	D	402/440 (91%)	-1.17	0	100   100	24, 38, 78, 127	4 (0%)
All	All	1604/1760 (91%)	-0.98	3 (0%)	92   94	22, 46, 99, 147	8 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	ALA	3.5
1	C	345	GLY	2.6
1	C	153	VAL	2.4

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

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

### 6.3 Carbohydrates [i](#)

There are no 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, 95<sup>th</sup> 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.

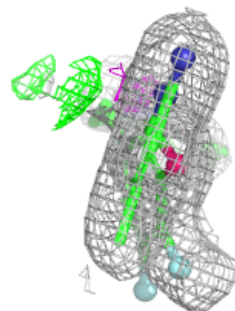
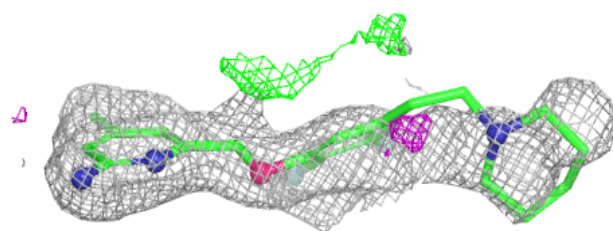
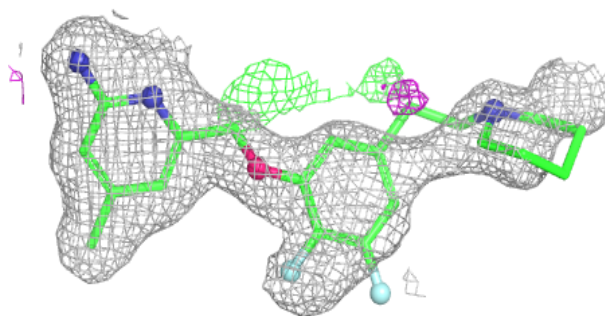
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	C	507	6/6	0.93	0.06	84,88,89,90	0
6	GOL	A	507	6/6	0.94	0.07	103,107,107,108	0
6	GOL	B	506	6/6	0.95	0.05	70,71,77,81	0
6	GOL	D	506	6/6	0.95	0.05	68,70,72,74	0
5	BTB	C	504	14/14	0.96	0.10	99,111,128,135	0
6	GOL	C	506	6/6	0.96	0.06	56,75,83,83	0
5	BTB	D	505	14/14	0.96	0.05	51,73,83,86	0
5	BTB	A	504	14/14	0.96	0.08	65,88,96,103	0
5	BTB	B	505	14/14	0.97	0.05	57,80,83,87	0
5	BTB	D	504	14/14	0.98	0.05	32,58,74,75	0
4	A1CN6	D	503	26/26	0.98	0.08	22,96,110,111	0
6	GOL	A	506	6/6	0.98	0.04	45,61,64,69	0
3	H4B	B	502	17/17	0.98	0.04	28,40,46,48	0
5	BTB	A	505	14/14	0.98	0.04	36,65,75,76	0
4	A1CN6	A	503	26/26	0.98	0.09	35,90,122,127	0
4	A1CN6	C	503	26/26	0.98	0.08	40,90,132,135	0
5	BTB	C	505	14/14	0.98	0.04	66,74,87,92	0
8	GD	C	509	1/1	0.98	0.03	177,177,177,177	0
3	H4B	D	502	17/17	0.99	0.04	30,40,49,54	0
5	BTB	B	504	14/14	0.99	0.05	35,76,88,88	0
6	GOL	A	508	6/6	0.99	0.07	66,78,82,85	0
2	HEM	C	501	43/43	0.99	0.05	42,57,88,105	0
4	A1CN6	B	503	26/26	0.99	0.07	19,101,110,115	0
3	H4B	A	502	17/17	0.99	0.04	35,49,58,59	0
2	HEM	A	501	43/43	0.99	0.04	32,45,75,93	0
6	GOL	D	507	6/6	0.99	0.04	60,63,65,68	0
7	CL	B	507	1/1	0.99	0.04	53,53,53,53	0
7	CL	C	508	1/1	0.99	0.07	57,57,57,57	0
7	CL	D	508	1/1	0.99	0.09	47,47,47,47	0
8	GD	A	510	1/1	0.99	0.04	149,149,149,149	0
3	H4B	C	502	17/17	0.99	0.04	46,53,61,72	0
7	CL	A	509	1/1	1.00	0.05	47,47,47,47	0
2	HEM	B	501	43/43	1.00	0.03	14,26,51,79	0
8	GD	B	508	1/1	1.00	0.01	48,48,48,48	0
2	HEM	D	501	43/43	1.00	0.03	19,27,65,90	0
8	GD	D	509	1/1	1.00	0.01	46,46,46,46	0
9	ZN	A	511	1/1	1.00	0.01	35,35,35,35	0
9	ZN	C	510	1/1	1.00	0.01	39,39,39,39	0
10	CA	A	512	1/1	1.00	0.01	41,41,41,41	0
10	CA	C	511	1/1	1.00	0.02	46,46,46,46	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.

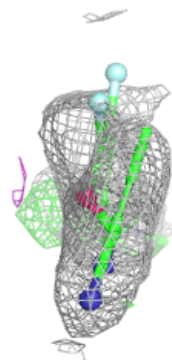
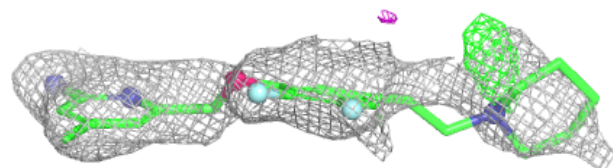
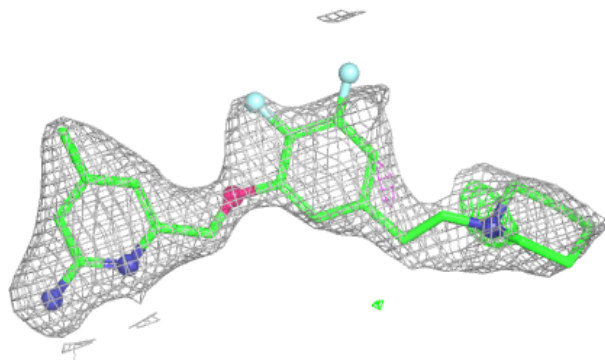
**Electron density around A1CN6 D 503:**

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



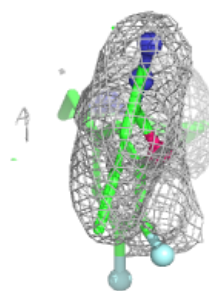
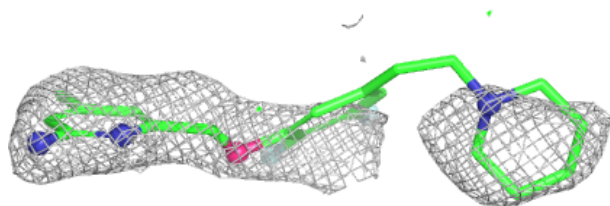
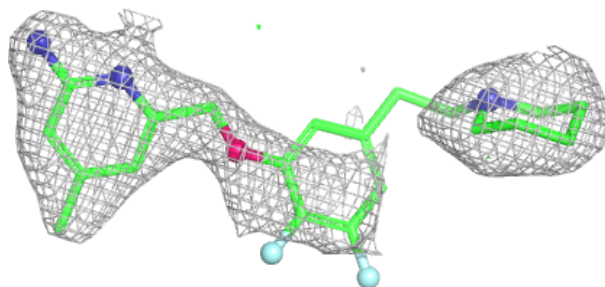
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and green (positive)



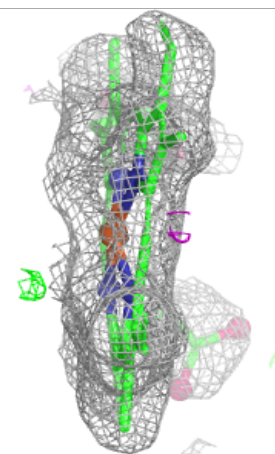
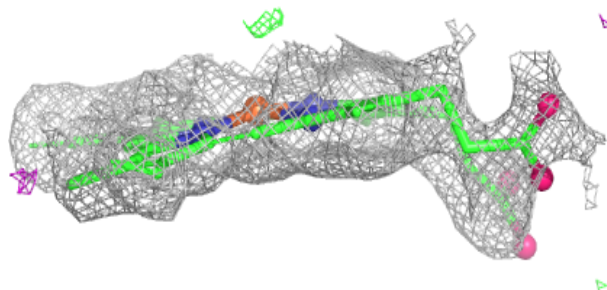
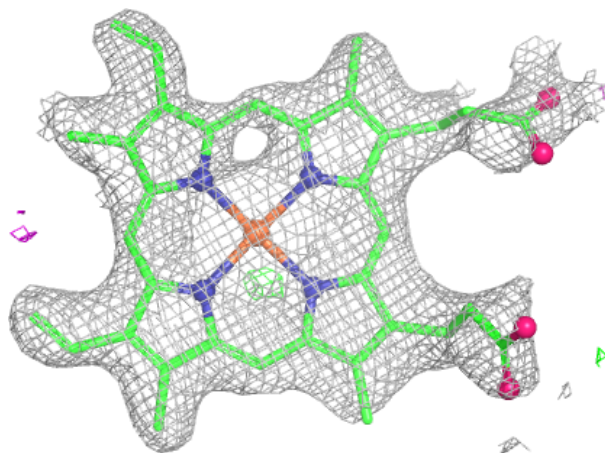
**Electron density around A1CN6 C 503:**

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and green (positive)



**Electron density around HEM C 501:**

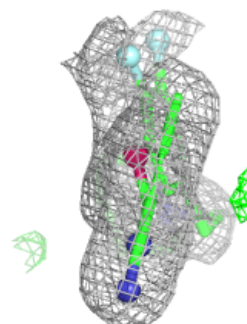
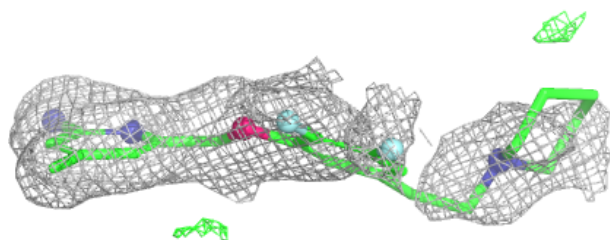
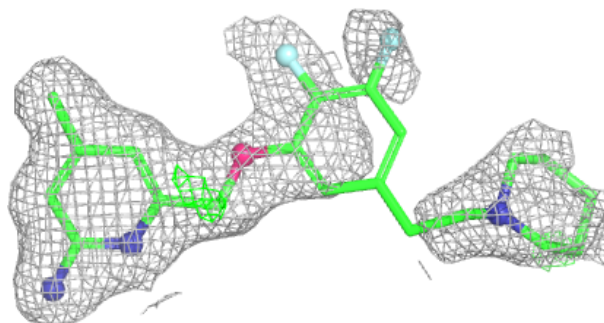
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





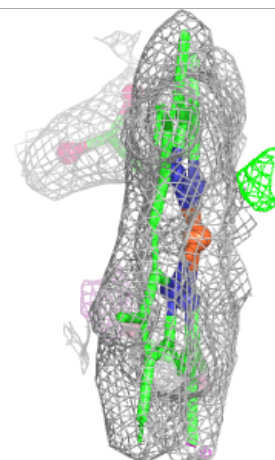
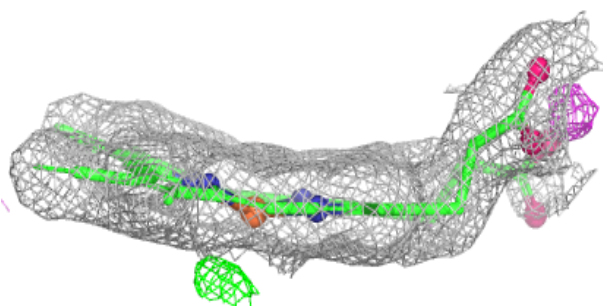
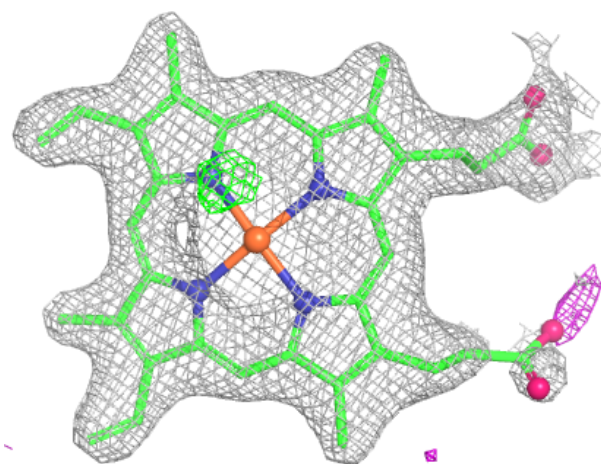
**Electron density around A1CN6 B 503:**

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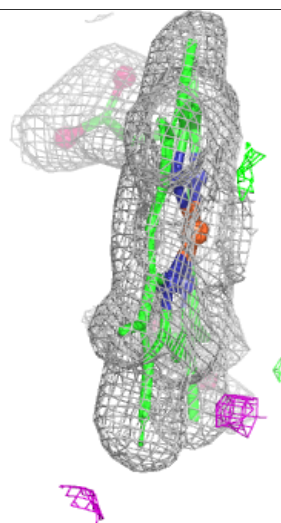
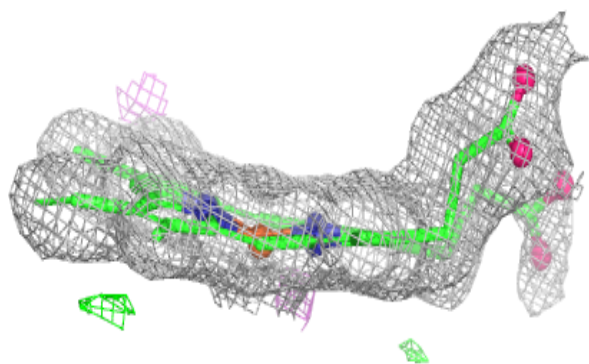
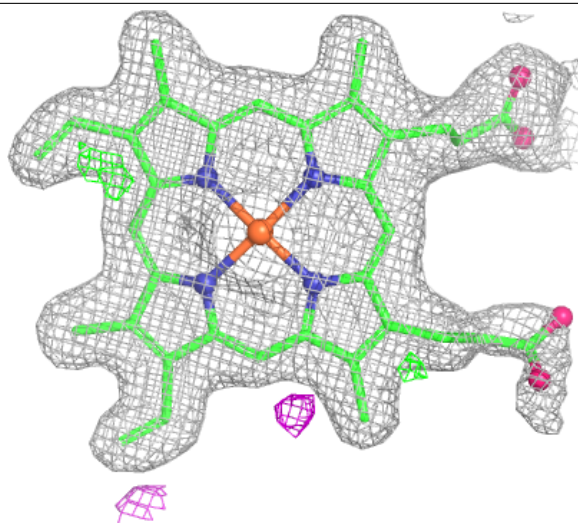
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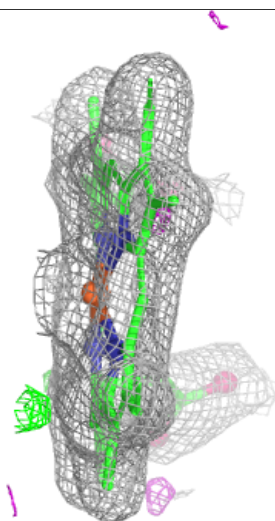
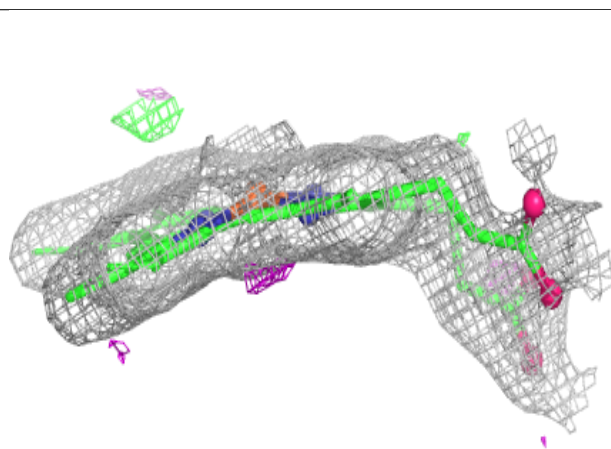
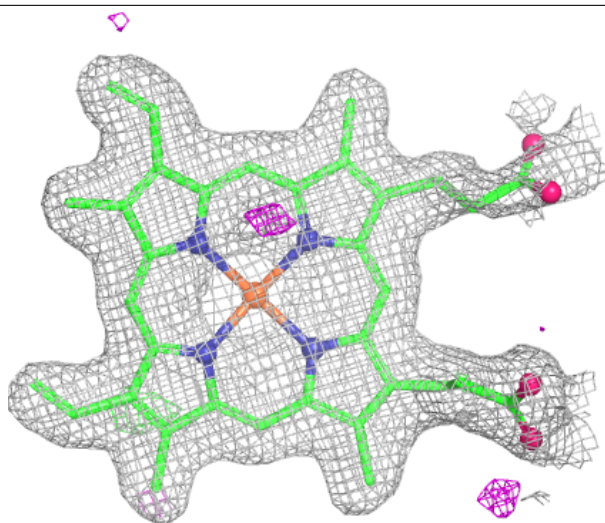
**Electron density around HEM B 501:**

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



**Electron density around HEM D 501:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.