



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:59 PM UTC

PDB ID : 9CWD / pdb_00009cwd
Title : Structure of human endothelial nitric oxide synthase heme domain bound with 6-(5-((dimethylamino)methyl)-2,3-difluorophenyl)-4-methylpyridin-2-amine dihydrochloride
Authors : Li, H.; Poulos, T.L.
Deposited on : 2024-07-29
Resolution : 1.92 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

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

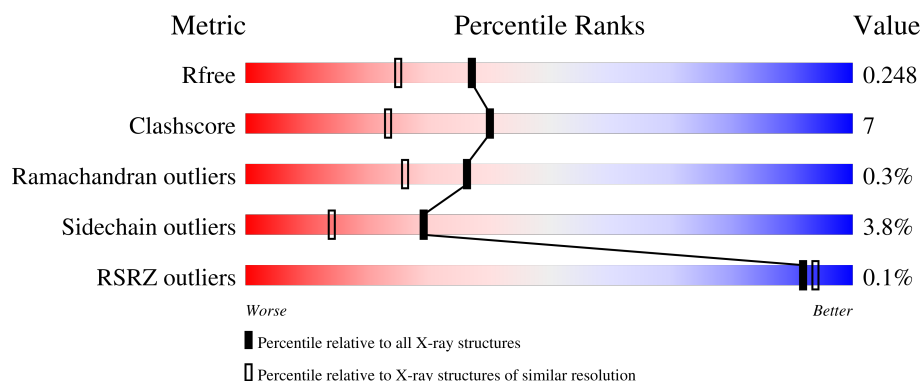
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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
5	BTB	D	505	-	-	X	-
6	GOL	A	512	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14057 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.

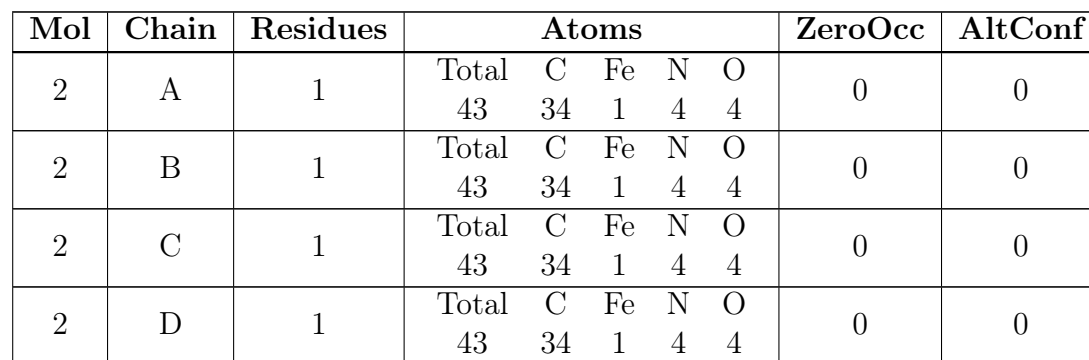
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

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	402	Total	C	N	O	S	0	1	0
			3212	2046	565	585	16			
1	D	402	Total	C	N	O	S	0	0	0
			3211	2044	567	584	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

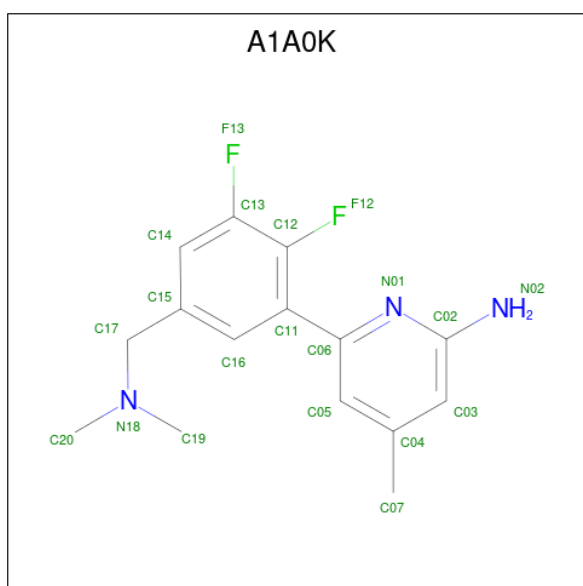
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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- The chemical structure of H4B (Hydroxybenzoylserine) is shown with the following atom labels:
- Hydroxyl group:** O9 (oxygen), H (hydrogen).
 - Chiral center C9(R):** Carbon atom bonded to O9, C10(S), and C6(R).
 - Chiral center C10(S):** Carbon atom bonded to C9(R), C11, and O10 (hydroxyl group).
 - Amino group:** N5 (nitrogen), H (hydrogen).
 - Pyrimidine ring:** N1, N3, N8 (nitrogen atoms); C2, C4A, C6A, C8A (carbon atoms).
 - Carbonyl group:** C4 (carbon), O4 (oxygen).
 - Amino group:** N2 (nitrogen), H2 (hydrogen).

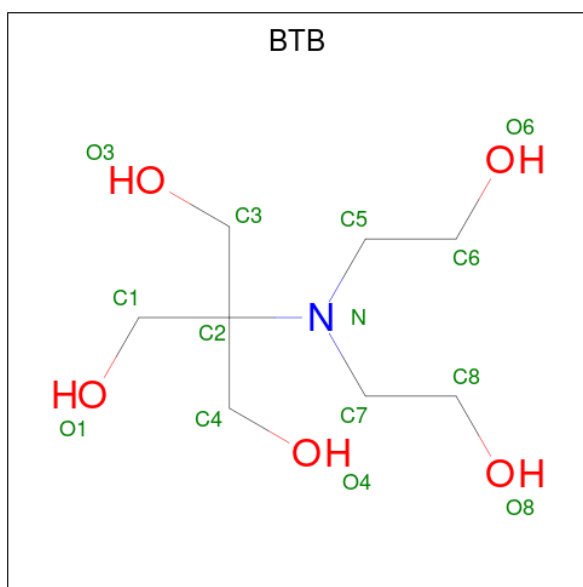
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is (6M)-6-{5-[(dimethylamino)methyl]-2,3-difluorophenyl}-4-methylpyridin-2-amine (CCD ID: A1A0K) (formula: C₁₅H₁₇F₂N₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			20	15	2	3		
4	B	1	Total	C	F	N	0	0
			20	15	2	3		
4	C	1	Total	C	F	N	0	0
			20	15	2	3		
4	D	1	Total	C	F	N	0	0
			20	15	2	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	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	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		
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

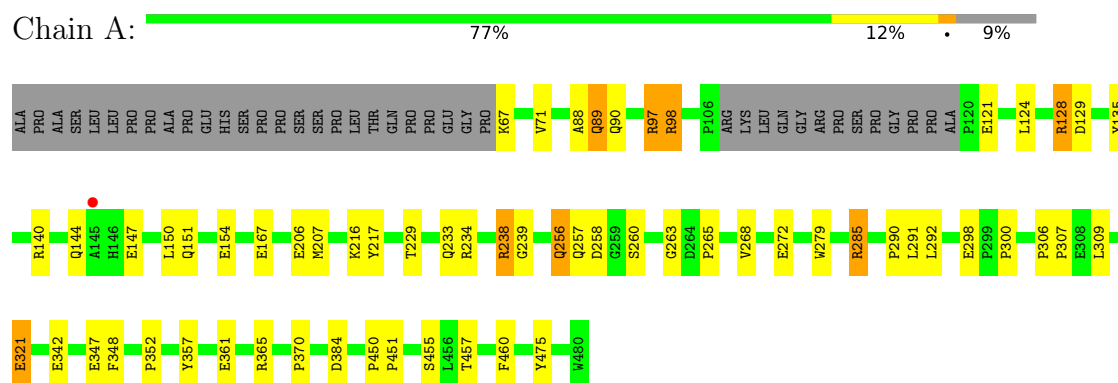
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	125	Total 125	O 125	0	0
10	B	213	Total 213	O 213	0	0
10	C	139	Total 139	O 139	0	0
10	D	209	Total 209	O 209	0	0

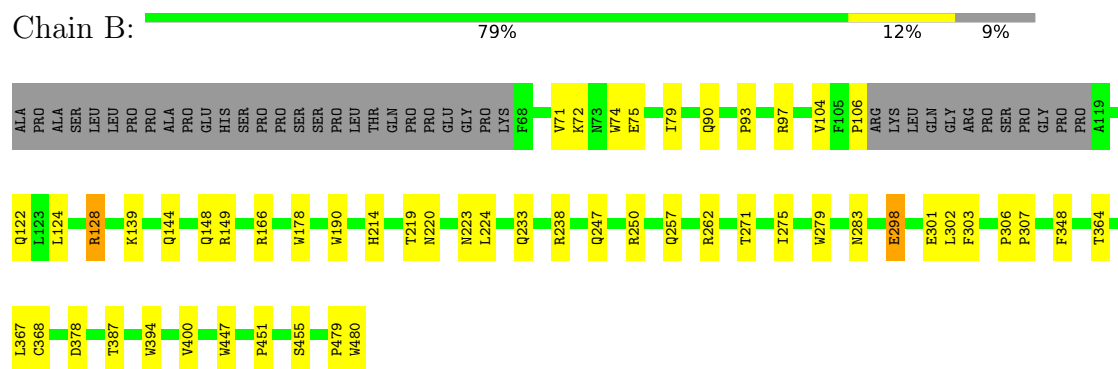
3 Residue-property plots

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.

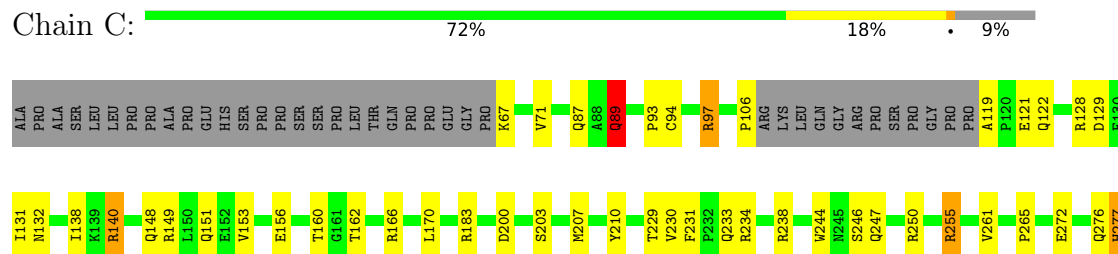
- Molecule 1: Nitric oxide synthase, endothelial

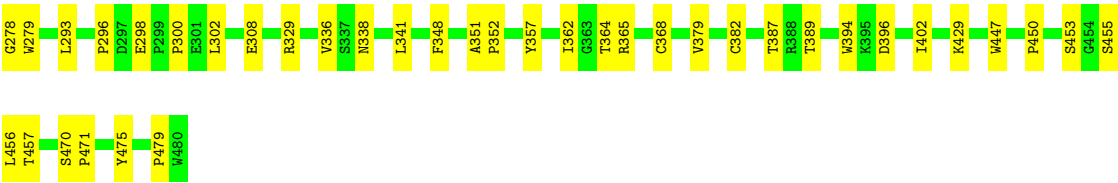


- Molecule 1: Nitric oxide synthase, endothelial

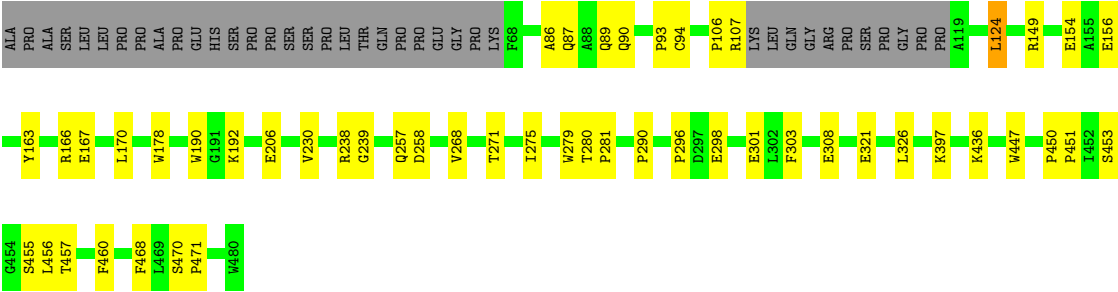
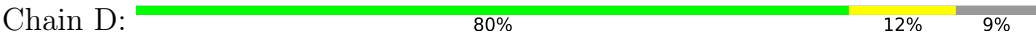


- Molecule 1: Nitric oxide synthase, endothelial





● 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	59.40Å 152.57Å 108.31Å 90.00° 90.73° 90.00°	Depositor
Resolution (Å)	49.52 – 1.92 49.52 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.52-1.92) 94.6 (49.52-1.92)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.208 , 0.252 0.203 , 0.248	Depositor DCC
R_{free} test set	7265 reflections (3.83%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.667	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	0.167 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14057	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GD3, ZN, HEM, A1A0K, H4B, BTB, CL

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	0/3302	0.49	0/4498
1	B	0.36	0/3312	0.52	0/4514
1	C	0.28	0/3307	0.47	0/4506
1	D	0.37	0/3303	0.55	0/4501
All	All	0.33	0/13224	0.51	0/18019

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	40	0
1	B	3211	0	3114	34	0
1	C	3212	0	3116	49	0
1	D	3211	0	3111	34	1
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	2	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	1	0
4	A	20	0	0	1	0
4	B	20	0	0	0	0
4	C	20	0	0	2	0
4	D	20	0	0	0	0
5	A	42	0	56	8	0
5	B	28	0	36	5	1
5	C	42	0	55	7	0
5	D	28	0	38	8	0
6	A	18	0	24	1	0
6	B	12	0	16	0	0
6	C	18	0	24	0	0
6	D	12	0	16	0	0
7	A	1	0	0	1	0
7	B	1	0	0	0	0
7	C	1	0	0	1	0
7	D	1	0	0	0	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	125	0	0	0	0
10	B	213	0	0	0	0
10	C	139	0	0	3	0
10	D	209	0	0	3	0
All	All	14057	0	12898	173	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 7.

The worst 5 of 173 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:D:275:ILE:HD12	1:D:281:PRO:HG3	1.65	0.79
1:A:97:ARG:HG2	1:A:98:ARG:HG2	1.64	0.78
1:B:124:LEU:HB3	1:B:128:ARG:HH12	1.48	0.77
1:C:234:ARG:HA	1:C:238:ARG:HH21	1.53	0.71
1:B:247:GLN:HB2	1:B:250:ARG:HD3	1.75	0.68

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:D:167:GLU:OE1	5:B:505:BTB:O1[1_554]	2.09	0.11

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%)	381 (96%)	15 (4%)	2 (0%)	24	14
1	B	400/440 (91%)	391 (98%)	9 (2%)	0	100	100
1	C	399/440 (91%)	387 (97%)	10 (2%)	2 (0%)	24	14
1	D	398/440 (90%)	390 (98%)	8 (2%)	0	100	100
All	All	1595/1760 (91%)	1549 (97%)	42 (3%)	4 (0%)	36	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	257	GLN
1	C	89	GLN
1	C	277	HIS

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%)	325 (95%)	17 (5%)	22	8
1	B	343/373 (92%)	332 (97%)	11 (3%)	34	18
1	C	342/373 (92%)	327 (96%)	15 (4%)	25	10
1	D	341/373 (91%)	332 (97%)	9 (3%)	40	24
All	All	1368/1492 (92%)	1316 (96%)	52 (4%)	29	14

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	67	LYS
1	C	153	VAL
1	D	268	VAL
1	C	71	VAL
1	C	121	GLU

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

Mol	Chain	Res	Type
1	B	122	GLN
1	C	233	GLN
1	C	277	HIS
1	D	126	GLN
1	D	466	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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$
6	GOL	A	508	-	5,5,5	0.39	0	5,5,5	0.75	0
4	A1A0K	B	503	-	21,21,21	0.49	0	30,30,30	1.58	7 (23%)
5	BTB	C	504	8	13,13,13	0.39	0	7,16,16	1.29	1 (14%)
2	HEM	A	501	1	50,50,50	1.67	7 (14%)	67,82,82	1.39	9 (13%)
6	GOL	A	512	-	5,5,5	0.78	0	5,5,5	2.02	2 (40%)
4	A1A0K	C	503	-	21,21,21	0.49	0	30,30,30	2.06	6 (20%)
5	BTB	B	505	-	13,13,13	0.67	0	7,16,16	1.08	0
5	BTB	D	505	-	13,13,13	0.73	0	7,16,16	1.39	1 (14%)
6	GOL	D	506	-	5,5,5	0.36	0	5,5,5	0.39	0
5	BTB	C	506	-	13,13,13	0.48	0	7,16,16	0.59	0
6	GOL	D	507	-	5,5,5	0.43	0	5,5,5	0.18	0
3	H4B	A	502	-	17,18,18	0.81	0	14,26,26	1.86	4 (28%)
5	BTB	D	504	8	13,13,13	0.36	0	7,16,16	0.42	0
5	BTB	A	504	8	13,13,13	0.64	0	7,16,16	1.93	1 (14%)
2	HEM	D	501	1	50,50,50	1.78	9 (18%)	67,82,82	1.55	11 (16%)
6	GOL	C	507	-	5,5,5	0.44	0	5,5,5	0.26	0
6	GOL	C	508	-	5,5,5	0.32	0	5,5,5	0.47	0
3	H4B	D	502	-	17,18,18	0.92	1 (5%)	14,26,26	1.75	4 (28%)
4	A1A0K	A	503	-	21,21,21	0.43	0	30,30,30	1.62	5 (16%)
2	HEM	C	501	1	50,50,50	1.64	9 (18%)	67,82,82	1.46	8 (11%)
5	BTB	A	506	-	13,13,13	0.42	0	7,16,16	0.50	0
4	A1A0K	D	503	-	21,21,21	0.59	0	30,30,30	1.64	7 (23%)
6	GOL	C	509	-	5,5,5	0.37	0	5,5,5	0.22	0
3	H4B	C	502	-	17,18,18	1.02	1 (5%)	14,26,26	1.84	4 (28%)
5	BTB	A	505	-	13,13,13	0.43	0	7,16,16	0.62	0
6	GOL	B	507	-	5,5,5	0.37	0	5,5,5	0.30	0
5	BTB	C	505	-	13,13,13	0.73	0	7,16,16	1.01	0
3	H4B	B	502	-	17,18,18	0.84	0	14,26,26	2.15	5 (35%)
5	BTB	B	504	8	13,13,13	0.44	0	7,16,16	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	A	507	-	5,5,5	0.41	0	5,5,5	0.25	0
6	GOL	B	506	-	5,5,5	0.35	0	5,5,5	0.30	0
2	HEM	B	501	1	50,50,50	1.73	8 (16%)	67,82,82	1.42	10 (14%)

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
6	GOL	A	508	-	-	4/4/4/4	-
4	A1A0K	B	503	-	-	1/8/8/8	0/2/2/2
5	BTB	C	504	8	-	6/21/21/21	-
2	HEM	A	501	1	-	1/14/54/54	-
6	GOL	A	512	-	-	4/4/4/4	-
4	A1A0K	C	503	-	-	0/8/8/8	0/2/2/2
5	BTB	B	505	-	-	14/21/21/21	-
5	BTB	D	505	-	-	8/21/21/21	-
6	GOL	D	506	-	-	0/4/4/4	-
5	BTB	C	506	-	-	8/21/21/21	-
6	GOL	D	507	-	-	0/4/4/4	-
3	H4B	A	502	-	-	2/8/17/17	0/2/2/2
5	BTB	D	504	8	-	3/21/21/21	-
5	BTB	A	504	8	-	4/21/21/21	-
2	HEM	D	501	1	-	0/14/54/54	-
6	GOL	C	507	-	-	2/4/4/4	-
6	GOL	C	508	-	-	2/4/4/4	-
3	H4B	D	502	-	-	0/8/17/17	0/2/2/2
4	A1A0K	A	503	-	-	2/8/8/8	0/2/2/2
2	HEM	C	501	1	-	0/14/54/54	-
5	BTB	A	506	-	-	10/21/21/21	-
4	A1A0K	D	503	-	-	2/8/8/8	0/2/2/2
6	GOL	C	509	-	-	2/4/4/4	-
3	H4B	C	502	-	-	0/8/17/17	0/2/2/2
5	BTB	A	505	-	-	14/21/21/21	-
6	GOL	B	507	-	-	2/4/4/4	-
5	BTB	C	505	-	-	13/21/21/21	-
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTB	B	504	8	-	3/21/21/21	-
6	GOL	A	507	-	-	4/4/4/4	-
6	GOL	B	506	-	-	4/4/4/4	-
2	HEM	B	501	1	-	1/14/54/54	-

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	FE-NC	7.10	2.18	1.95
2	B	501	HEM	FE-NB	5.99	2.13	1.94
2	B	501	HEM	FE-NC	4.97	2.11	1.95
2	A	501	HEM	FE-NC	4.76	2.10	1.95
2	A	501	HEM	FE-NA	4.68	2.10	1.95

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	A1A0K	C06-N01-C02	6.89	122.80	118.52
4	A	503	A1A0K	C06-N01-C02	5.00	121.62	118.52
4	C	503	A1A0K	C06-C11-C12	-4.97	118.31	124.24
3	B	502	H4B	C2-N1-C8A	4.59	121.47	113.36
5	A	504	BTB	O3-C3-C2	4.51	122.02	111.40

There are no chirality outliers.

5 of 116 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
5	A	505	BTB	C4-C2-C3-O3

There are no ring outliers.

20 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	504	BTB	4	0
2	A	501	HEM	3	0
4	C	503	A1A0K	2	0

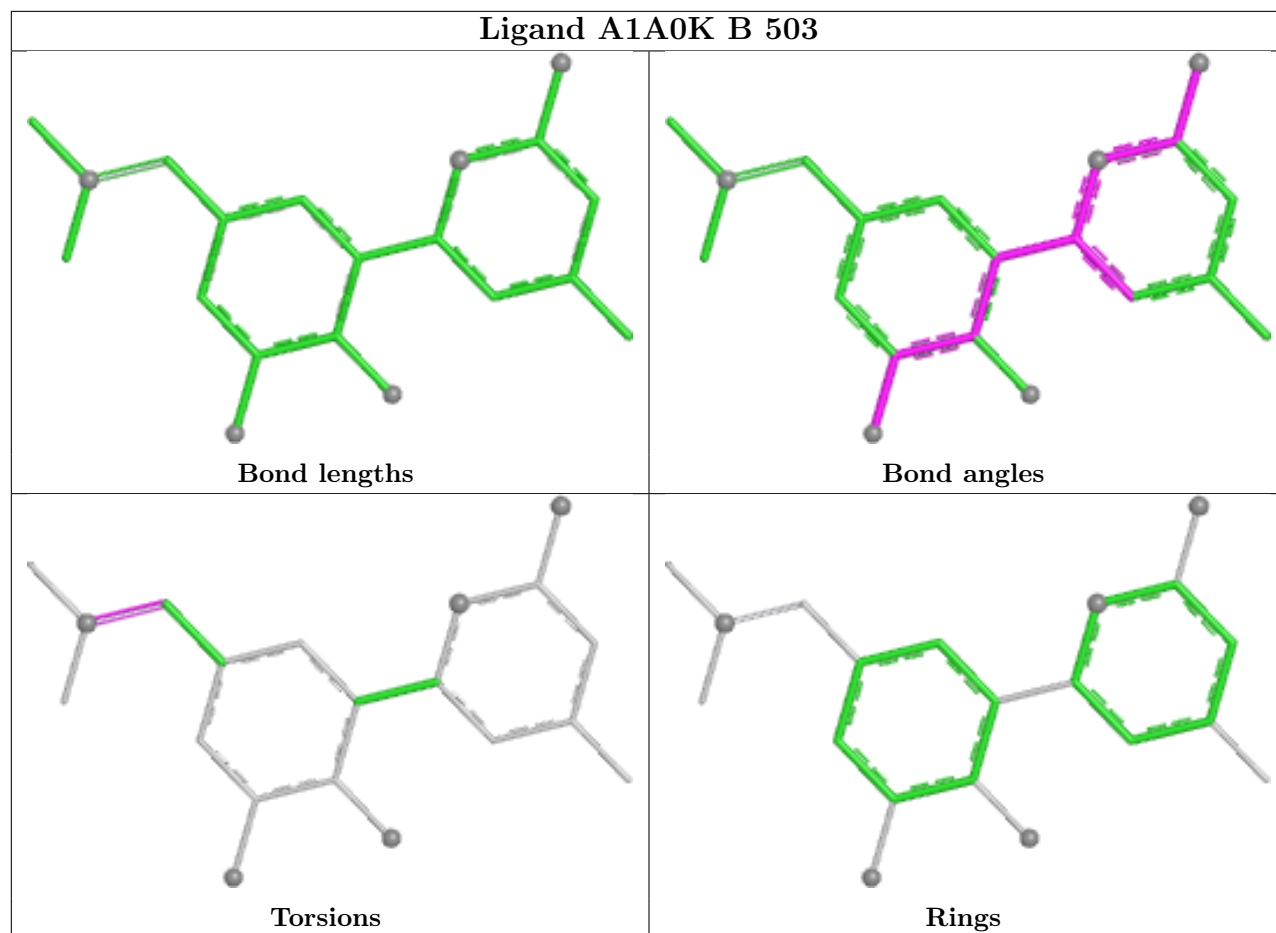
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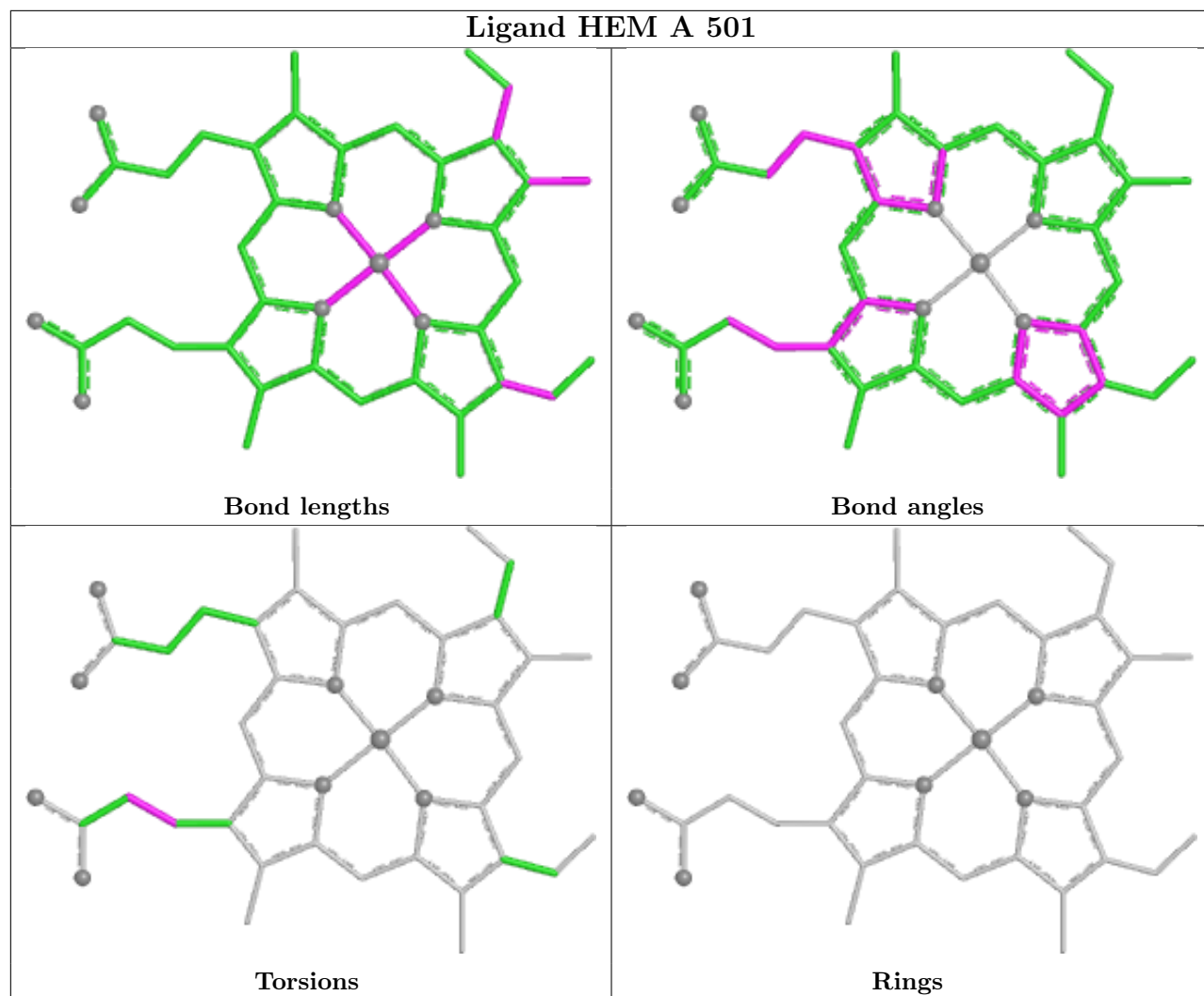
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	BTB	5	1
5	D	505	BTB	7	0
5	C	506	BTB	1	0
3	A	502	H4B	1	0
5	D	504	BTB	1	0
5	A	504	BTB	2	0
2	D	501	HEM	2	0
3	D	502	H4B	1	0
4	A	503	A1A0K	1	0
2	C	501	HEM	3	0
5	A	506	BTB	3	0
3	C	502	H4B	1	0
5	A	505	BTB	3	0
5	C	505	BTB	2	0
3	B	502	H4B	1	0
6	A	507	GOL	1	0
2	B	501	HEM	2	0

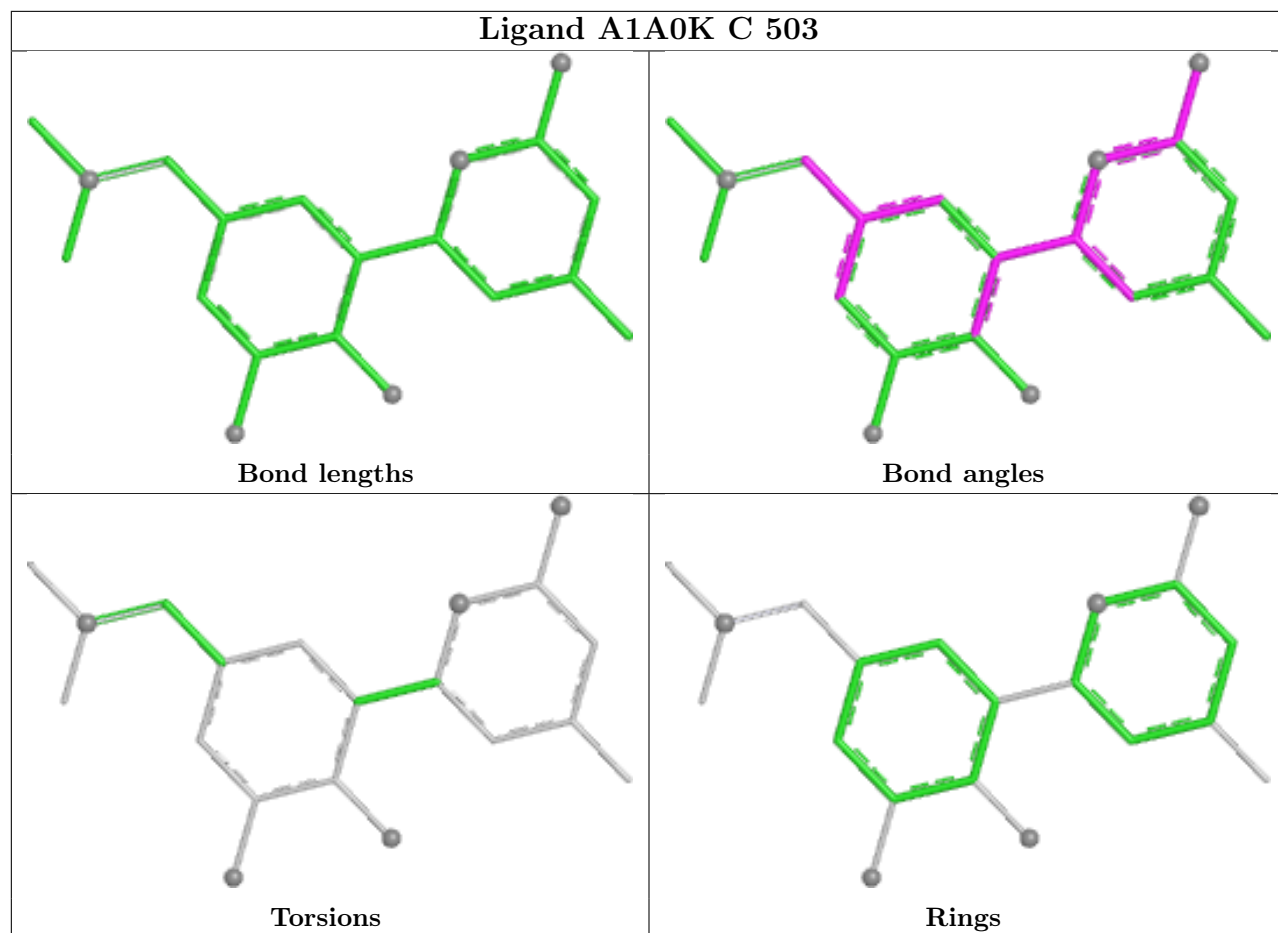
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

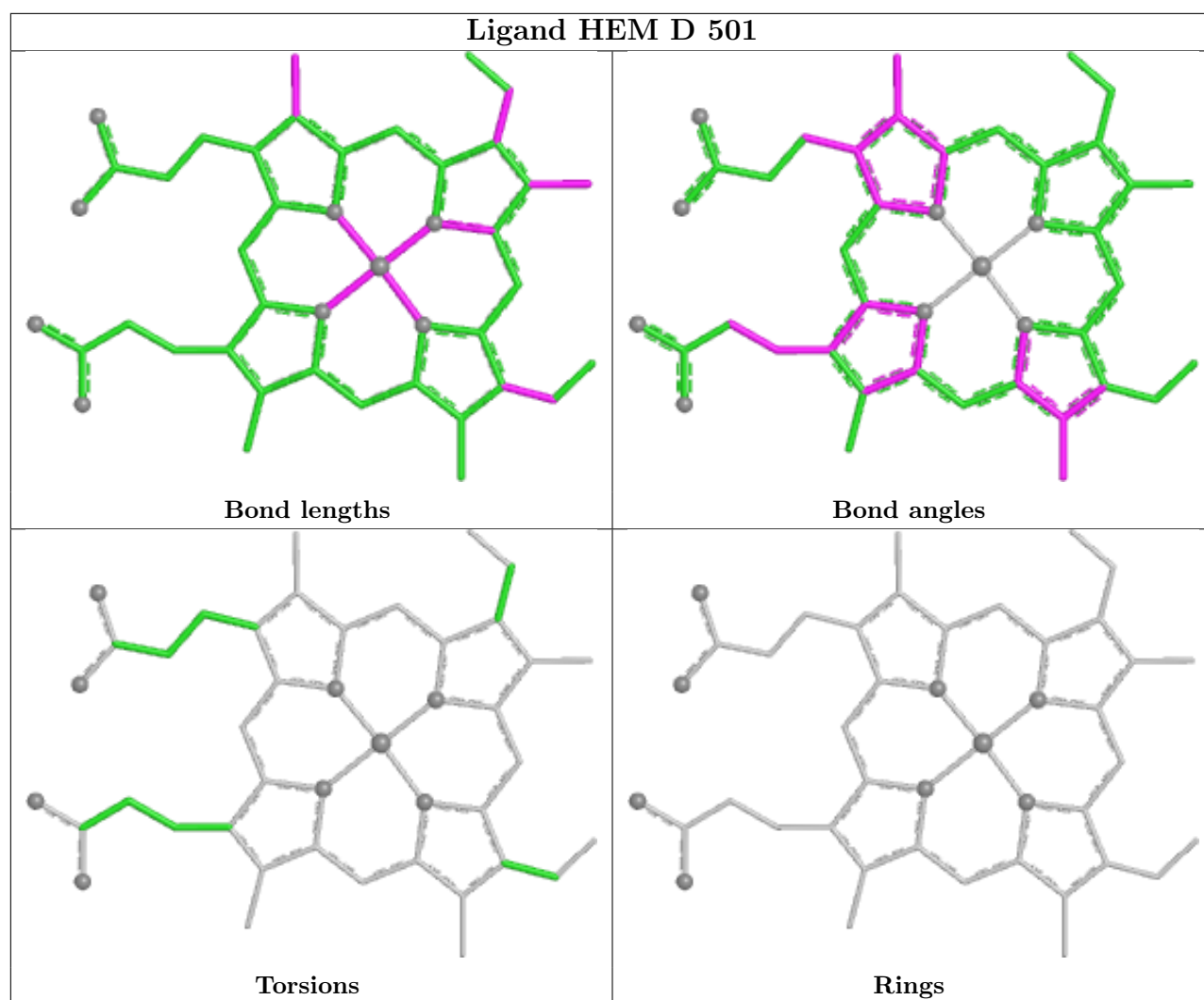
Ligand A1A0K B 503



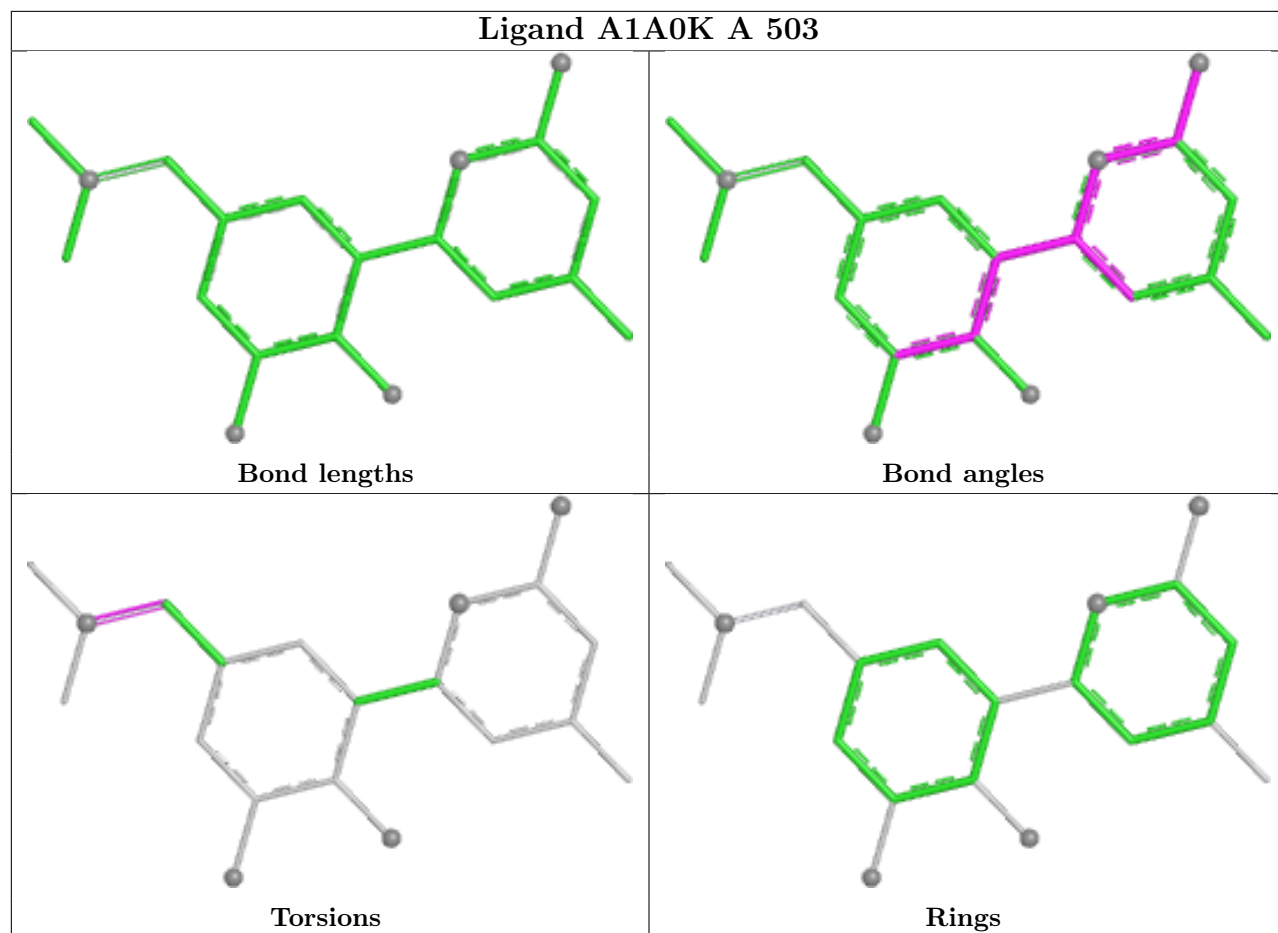


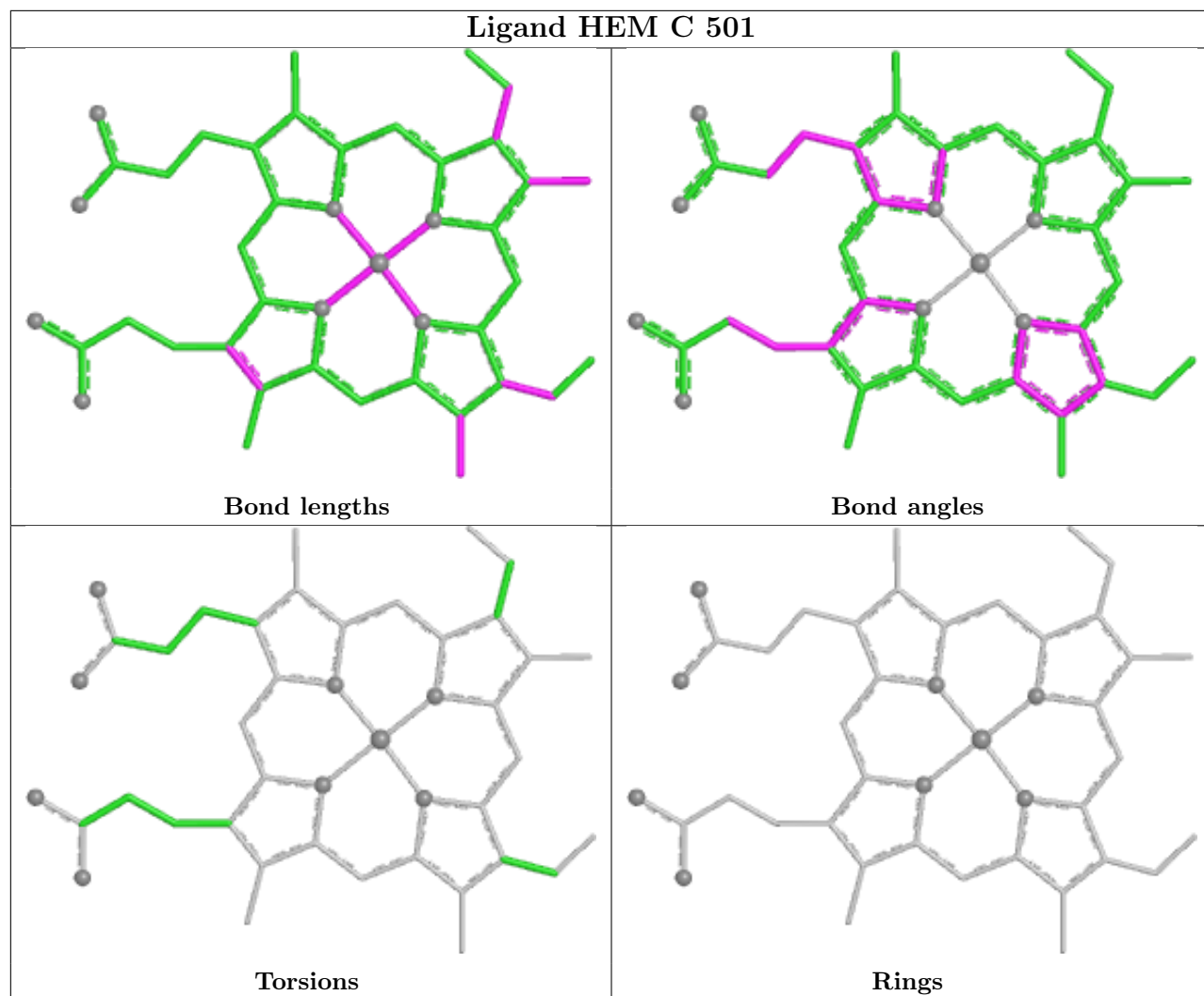
Ligand A1A0K C 503



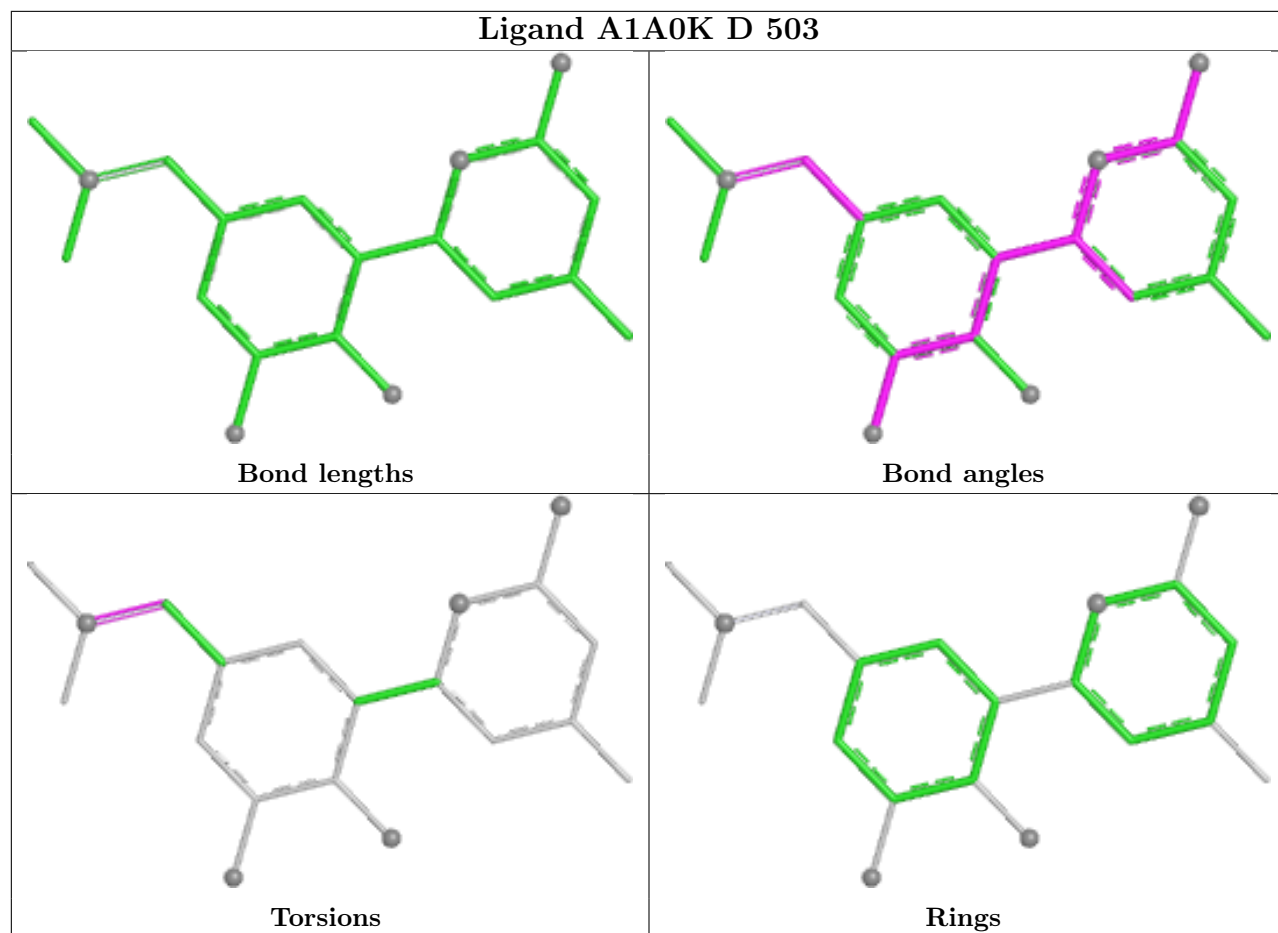


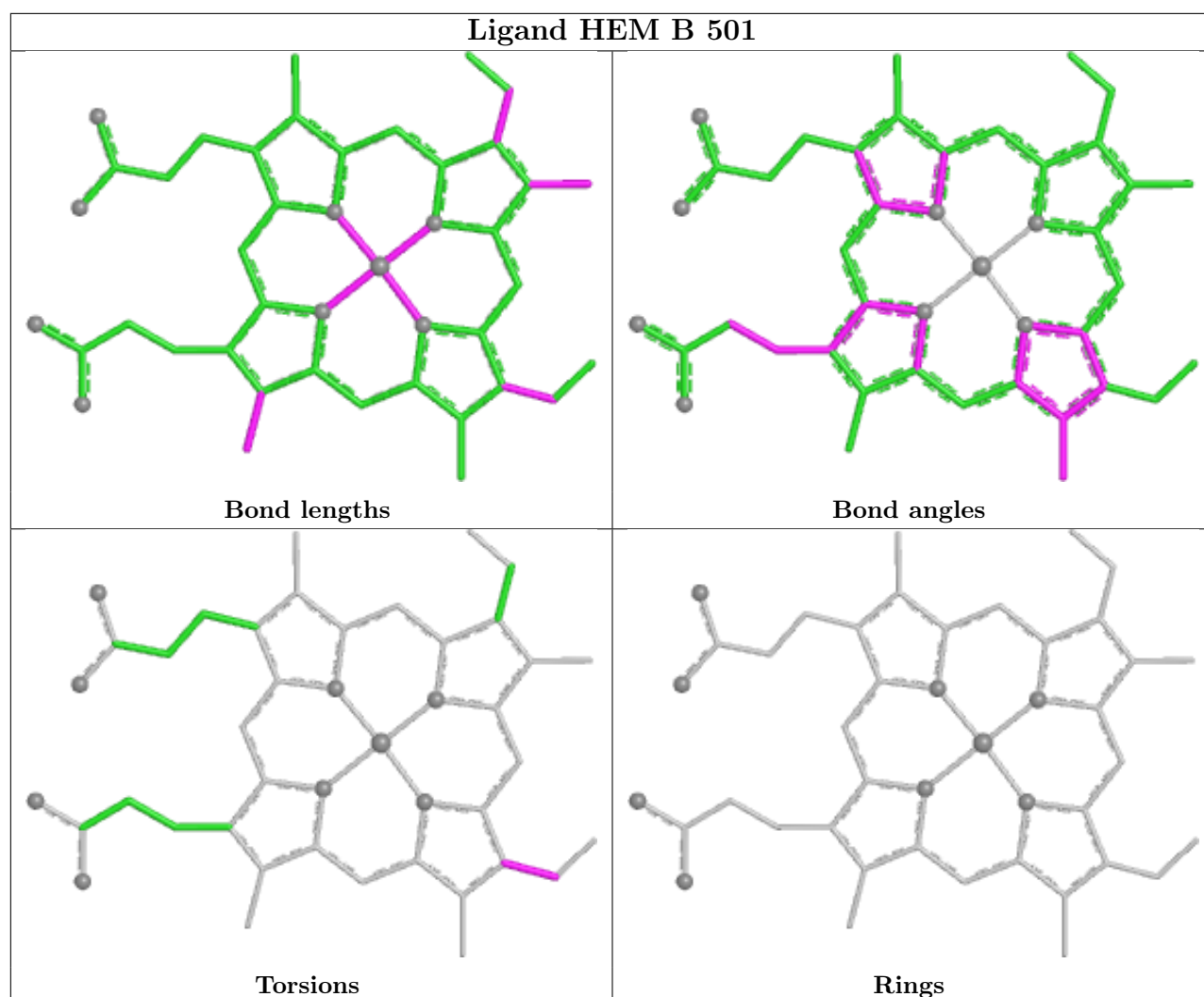
Ligand A1A0K A 503





Ligand A1A0K D 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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	401/440 (91%)	-0.56	1 (0%) 91 93	28, 58, 101, 129	1 (0%)
1	B	401/440 (91%)	-0.94	0 100 100	21, 41, 77, 116	3 (0%)
1	C	402/440 (91%)	-0.68	0 100 100	26, 56, 99, 127	1 (0%)
1	D	402/440 (91%)	-1.01	0 100 100	26, 39, 67, 122	0
All	All	1606/1760 (91%)	-0.80	1 (0%) 92 94	21, 48, 94, 129	5 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	ALA	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	B	506	6/6	0.92	0.05	69,74,78,80	0

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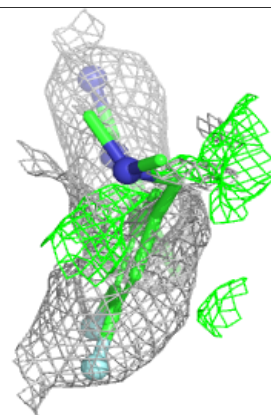
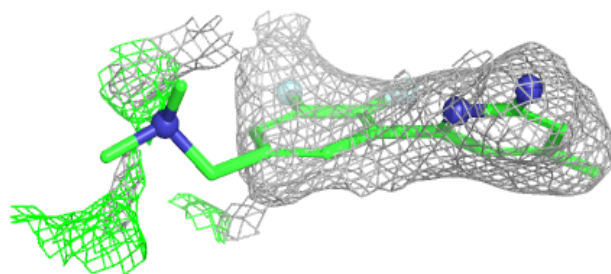
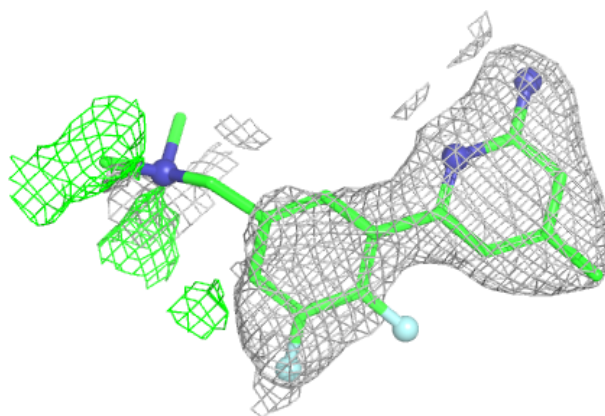
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	A1A0K	C	503	20/20	0.96	0.09	47,90,101,101	0
6	GOL	C	508	6/6	0.96	0.06	48,67,68,81	0
5	BTB	A	506	14/14	0.97	0.05	79,90,96,97	0
5	BTB	C	506	14/14	0.97	0.04	71,78,85,87	0
6	GOL	A	507	6/6	0.97	0.04	47,54,67,73	0
4	A1A0K	A	503	20/20	0.97	0.07	36,72,85,87	0
5	BTB	A	505	14/14	0.97	0.05	56,75,85,85	0
6	GOL	D	507	6/6	0.97	0.04	69,70,74,74	0
5	BTB	D	505	14/14	0.98	0.04	52,63,78,81	0
3	H4B	C	502	17/17	0.98	0.04	39,43,48,59	0
5	BTB	B	505	14/14	0.98	0.04	49,65,76,77	0
6	GOL	C	507	6/6	0.98	0.04	45,52,55,55	0
4	A1A0K	B	503	20/20	0.98	0.05	31,64,79,82	0
6	GOL	C	509	6/6	0.98	0.04	69,71,74,74	0
6	GOL	D	506	6/6	0.98	0.06	55,72,76,79	0
5	BTB	D	504	14/14	0.98	0.06	43,66,78,81	0
5	BTB	C	505	14/14	0.99	0.04	31,61,74,74	0
2	HEM	C	501	43/43	0.99	0.05	37,44,63,86	0
2	HEM	D	501	43/43	0.99	0.04	19,30,47,64	0
3	H4B	A	502	17/17	0.99	0.04	44,50,55,60	0
4	A1A0K	D	503	20/20	0.99	0.05	27,54,77,81	0
6	GOL	A	508	6/6	0.99	0.05	51,59,71,74	0
6	GOL	A	512	6/6	0.99	0.05	20,42,60,61	0
5	BTB	A	504	14/14	0.99	0.04	41,72,82,88	0
6	GOL	B	507	6/6	0.99	0.06	55,65,73,77	0
3	H4B	B	502	17/17	0.99	0.04	34,41,46,47	0
2	HEM	A	501	43/43	0.99	0.06	38,55,72,87	0
5	BTB	B	504	14/14	0.99	0.04	32,47,64,65	0
3	H4B	D	502	17/17	0.99	0.04	36,41,46,52	0
5	BTB	C	504	14/14	0.99	0.04	21,60,75,86	0
7	CL	A	509	1/1	0.99	0.04	50,50,50,50	0
7	CL	C	510	1/1	0.99	0.05	52,52,52,52	0
7	CL	D	508	1/1	0.99	0.03	41,41,41,41	0
2	HEM	B	501	43/43	1.00	0.03	25,34,54,62	0
7	CL	B	508	1/1	1.00	0.04	42,42,42,42	0
8	GD3	A	510	1/1	1.00	0.01	72,72,72,72	1
8	GD3	B	509	1/1	1.00	0.01	45,45,45,45	0
8	GD3	B	510	1/1	1.00	0.02	52,52,52,52	1
8	GD3	D	509	1/1	1.00	0.01	46,46,46,46	0
9	ZN	A	511	1/1	1.00	0.01	40,40,40,40	0
9	ZN	C	511	1/1	1.00	0.01	36,36,36,36	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.

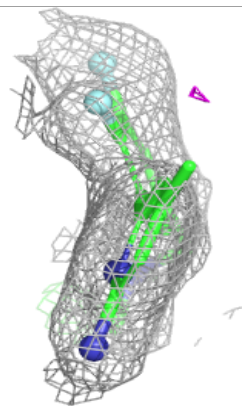
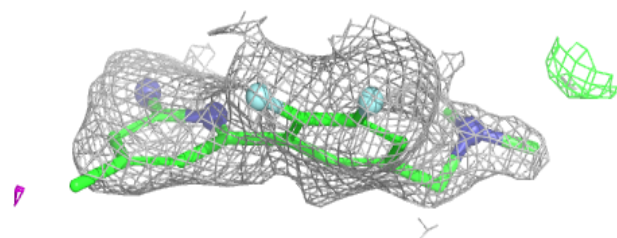
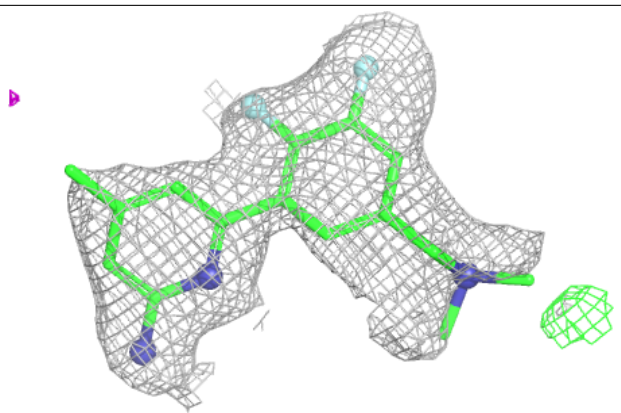
Electron density around A1A0K C 503:

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



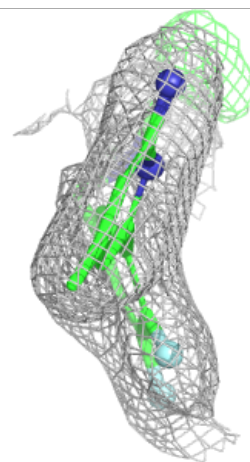
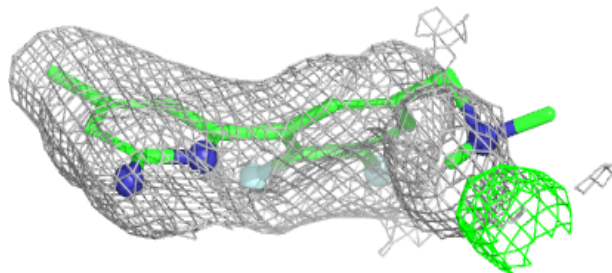
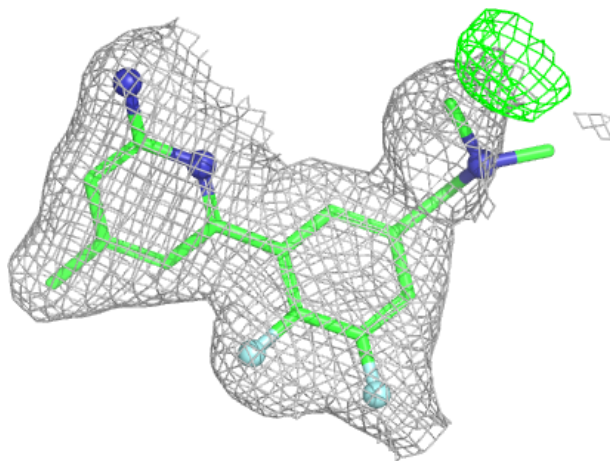
Electron density around A1A0K A 503:

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



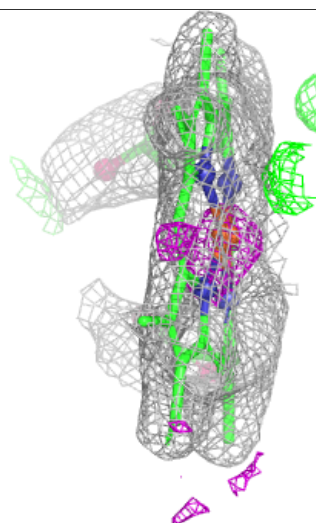
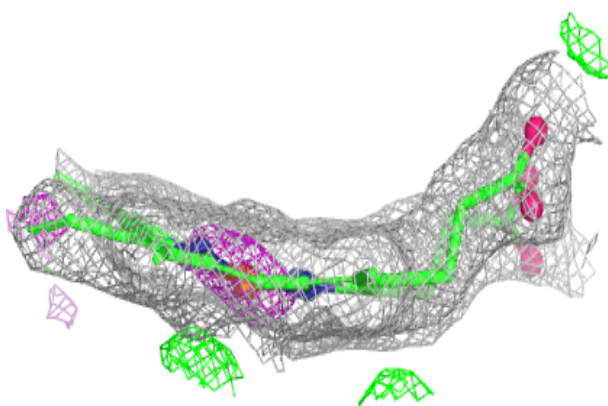
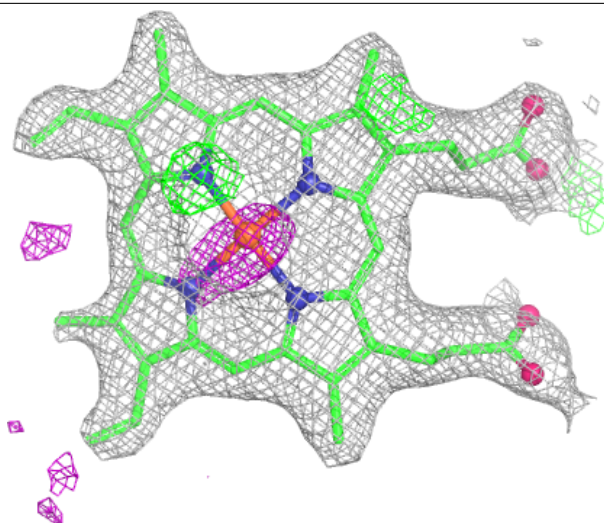
Electron density around A1A0K B 503:

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



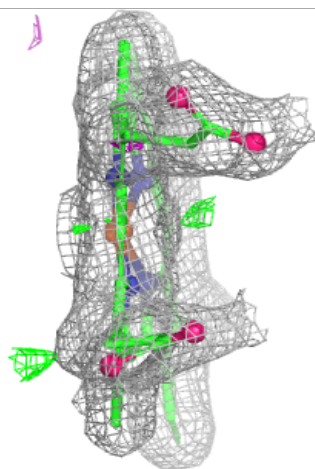
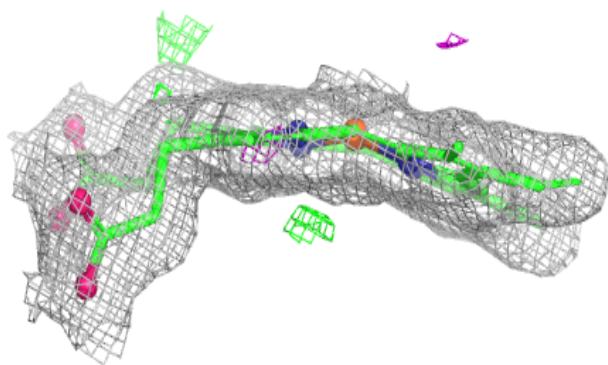
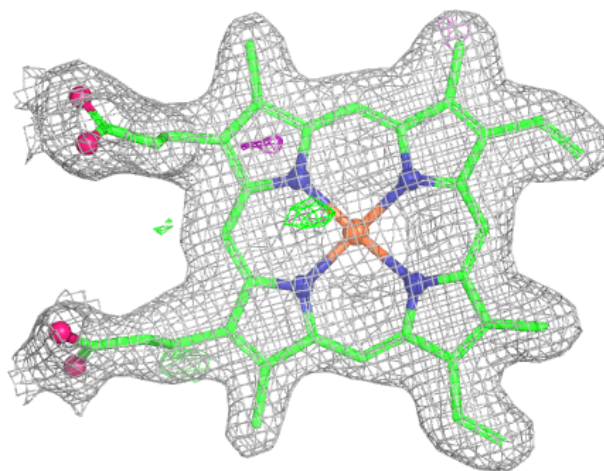
Electron density around HEM C 501:

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



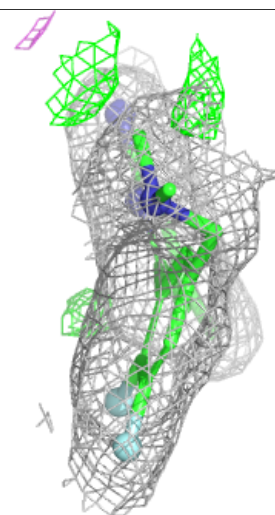
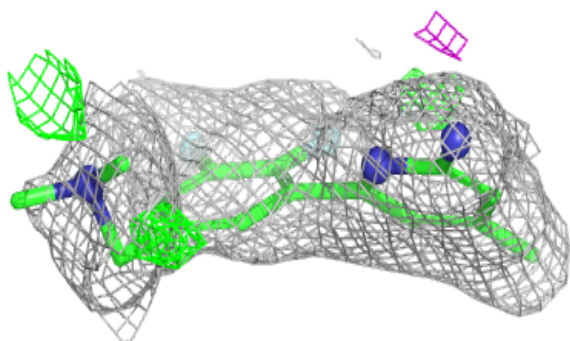
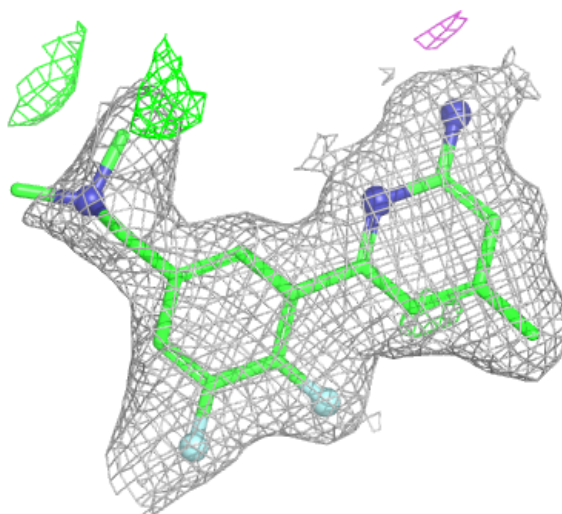
Electron density around HEM D 501:

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and green (positive)



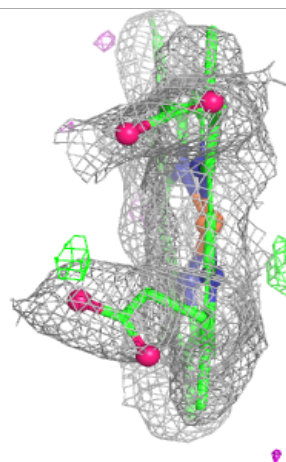
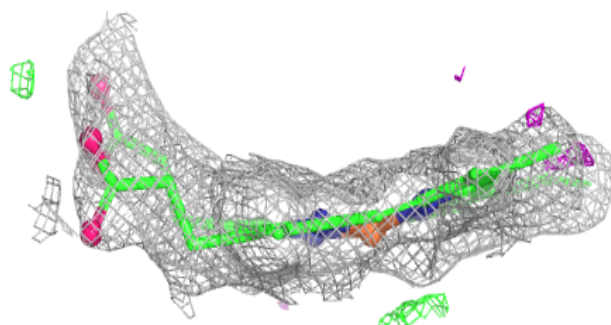
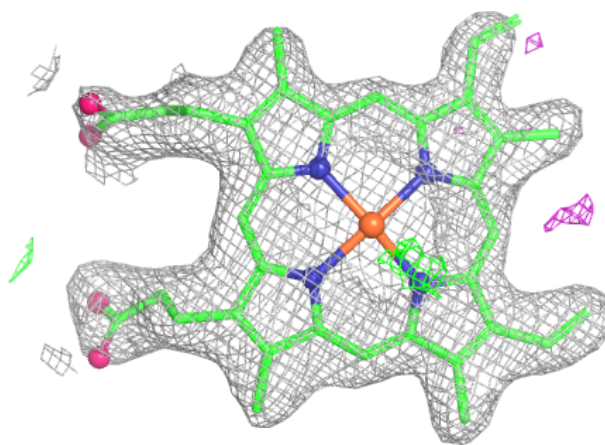
Electron density around A1A0K D 503:

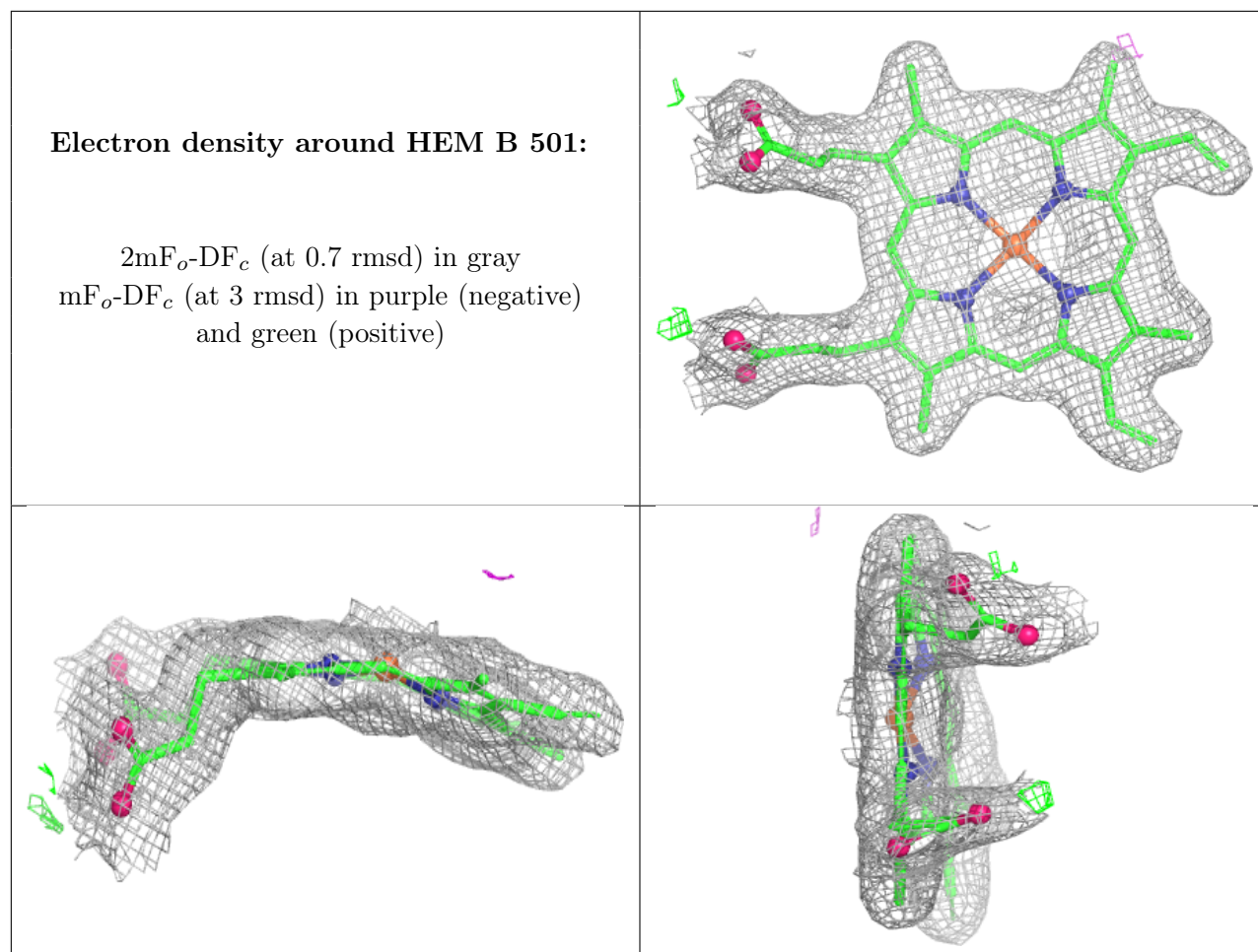
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.