



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 07:12 PM EDT

PDB ID : 5D40
Title : Crystal structure of the 5-selective H176Y mutant of Cytochrome TxtE
Authors : Cahn, J.K.B.; Dodani, S.C.; Arnold, F.H.
Deposited on : 2015-08-06
Resolution : 1.51 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

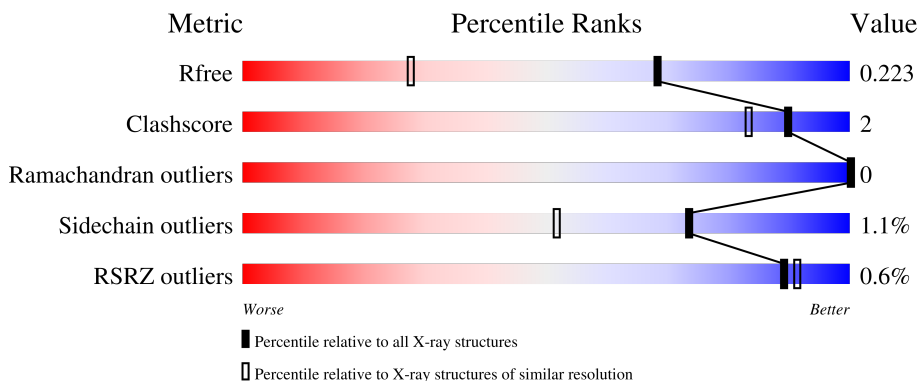
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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}	130704	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	427	
1	B	427	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7672 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 P450-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	403	3181	2027	565	581	8	0	7	0
1	B	403	3165	2013	565	579	8	0	5	0

There are 44 discrepancies between the modelled and reference sequences:

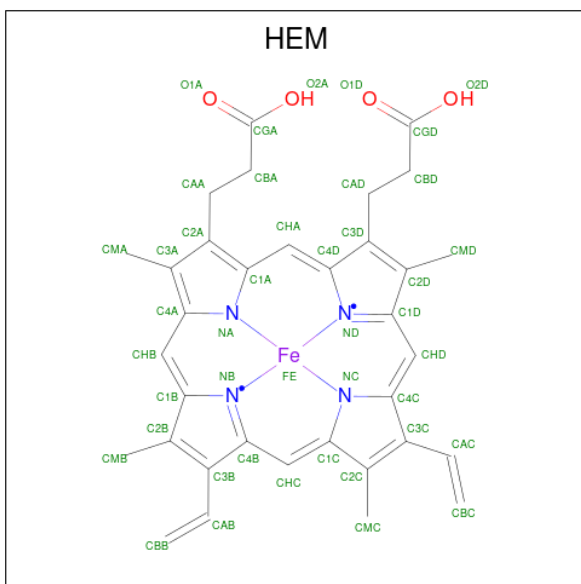
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP C9ZDC6
A	-19	GLY	-	expression tag	UNP C9ZDC6
A	-18	SER	-	expression tag	UNP C9ZDC6
A	-17	SER	-	expression tag	UNP C9ZDC6
A	-16	HIS	-	expression tag	UNP C9ZDC6
A	-15	HIS	-	expression tag	UNP C9ZDC6
A	-14	HIS	-	expression tag	UNP C9ZDC6
A	-13	HIS	-	expression tag	UNP C9ZDC6
A	-12	HIS	-	expression tag	UNP C9ZDC6
A	-11	HIS	-	expression tag	UNP C9ZDC6
A	-10	SER	-	expression tag	UNP C9ZDC6
A	-9	SER	-	expression tag	UNP C9ZDC6
A	-8	GLY	-	expression tag	UNP C9ZDC6
A	-7	LEU	-	expression tag	UNP C9ZDC6
A	-6	VAL	-	expression tag	UNP C9ZDC6
A	-5	PRO	-	expression tag	UNP C9ZDC6
A	-4	ARG	-	expression tag	UNP C9ZDC6
A	-3	GLY	-	expression tag	UNP C9ZDC6
A	-2	SER	-	expression tag	UNP C9ZDC6
A	-1	HIS	-	expression tag	UNP C9ZDC6
A	0	MET	-	expression tag	UNP C9ZDC6
A	176	TYR	HIS	engineered mutation	UNP C9ZDC6
B	-20	MET	-	initiating methionine	UNP C9ZDC6
B	-19	GLY	-	expression tag	UNP C9ZDC6
B	-18	SER	-	expression tag	UNP C9ZDC6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP C9ZDC6
B	-16	HIS	-	expression tag	UNP C9ZDC6
B	-15	HIS	-	expression tag	UNP C9ZDC6
B	-14	HIS	-	expression tag	UNP C9ZDC6
B	-13	HIS	-	expression tag	UNP C9ZDC6
B	-12	HIS	-	expression tag	UNP C9ZDC6
B	-11	HIS	-	expression tag	UNP C9ZDC6
B	-10	SER	-	expression tag	UNP C9ZDC6
B	-9	SER	-	expression tag	UNP C9ZDC6
B	-8	GLY	-	expression tag	UNP C9ZDC6
B	-7	LEU	-	expression tag	UNP C9ZDC6
B	-6	VAL	-	expression tag	UNP C9ZDC6
B	-5	PRO	-	expression tag	UNP C9ZDC6
B	-4	ARG	-	expression tag	UNP C9ZDC6
B	-3	GLY	-	expression tag	UNP C9ZDC6
B	-2	SER	-	expression tag	UNP C9ZDC6
B	-1	HIS	-	expression tag	UNP C9ZDC6
B	0	MET	-	expression tag	UNP C9ZDC6
B	176	TYR	HIS	engineered mutation	UNP C9ZDC6

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



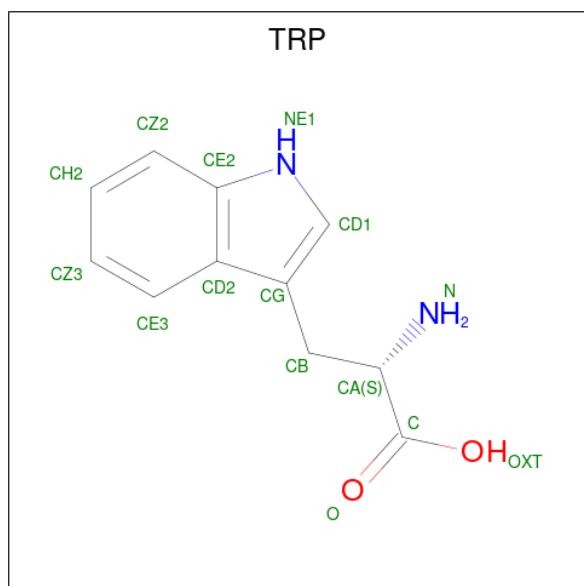
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	43	34	1	4	4	0	0

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

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	15	11	2	2	0	0
3	B	1	15	11	2	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0

- Molecule 6 is water.

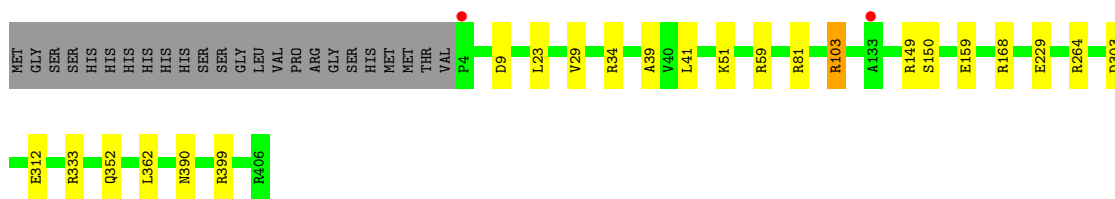
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	607	Total 607	O 607	0	0
6	B	548	Total 548	O 548	0	0

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: P450-like protein

Chain A: 



- Molecule 1: P450-like protein

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.72Å 99.21Å 105.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.21 – 1.51 38.47 – 1.51	Depositor EDS
% Data completeness (in resolution range)	97.4 (72.21-1.51) 97.4 (38.47-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.51Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.149 , 0.215 0.162 , 0.223	Depositor DCC
R_{free} test set	6063 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	9.9	Xtrriage
Anisotropy	0.586	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7672	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5002e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, CL, 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	0.93	0/3285	0.96	6/4487 (0.1%)
1	B	0.95	2/3260 (0.1%)	1.04	11/4454 (0.2%)
All	All	0.94	2/6545 (0.0%)	1.00	17/8941 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	31	TRP	CE3-CZ3	-5.58	1.28	1.38
1	B	323	SER	CB-OG	5.15	1.49	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333[A]	ARG	NE-CZ-NH2	-13.27	113.67	120.30
1	B	333[B]	ARG	NE-CZ-NH2	-13.27	113.67	120.30
1	B	333[A]	ARG	NE-CZ-NH1	12.76	126.68	120.30
1	B	333[B]	ARG	NE-CZ-NH1	12.76	126.68	120.30
1	B	81	ARG	NE-CZ-NH1	-8.61	116.00	120.30
1	B	81	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	B	149	ARG	NE-CZ-NH2	-7.45	116.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	ASP	CB-CG-OD1	6.83	124.45	118.30
1	A	149	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	27	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	333	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	303	ASP	CB-CG-OD1	5.88	123.60	118.30
1	B	115	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	9	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	168	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	34	ARG	CG-CD-NE	-5.38	100.50	111.80
1	A	333	ARG	NE-CZ-NH1	5.22	122.91	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	59	ARG	Sidechain
1	B	59	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3181	0	3181	10	0
1	B	3165	0	3153	9	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
3	A	15	0	9	0	0
3	B	15	0	9	0	0
4	A	12	0	16	0	0
4	B	42	0	56	1	0
5	B	1	0	0	0	0
6	A	607	0	0	6	7
6	B	548	0	0	6	6
All	All	7672	0	6484	23	7

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 2.

All (23) 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:A:51:LYS:NZ	1:A:352:GLN:OE1	1.89	1.04
1:B:108:ARG:NH2	6:B:602:HOH:O	2.23	0.69
1:B:210:LYS:HD3	6:B:1091:HOH:O	1.92	0.68
1:B:406:ARG:HD3	6:B:984:HOH:O	1.98	0.63
1:A:390:ASN:HD21	1:A:399:ARG:HD3	1.63	0.62
1:B:19:VAL:HG23	6:B:725:HOH:O	1.98	0.62
1:A:229:GLU:HG3	6:A:625:HOH:O	2.05	0.56
1:B:315:GLN:OE1	6:B:601:HOH:O	2.19	0.52
2:A:501:HEM:HHD	2:A:501:HEM:HBC2	1.93	0.50
1:B:233:GLU:HG2	1:B:237:HIS:CD2	2.47	0.49
1:A:23:LEU:HB3	1:A:41[A]:LEU:CD1	2.46	0.46
1:A:150[A]:SER:HB3	6:A:839:HOH:O	2.15	0.46
1:B:129:ILE:HD11	1:B:142:LEU:HD21	1.99	0.45
1:A:312:GLU:HG2	6:A:1018:HOH:O	2.17	0.43
1:B:174:THR:HB	1:B:183:PRO:HG2	2.01	0.43
1:B:234:GLN:O	1:B:238:GLN:HG3	2.19	0.43
1:A:264[A]:ARG:HD2	6:A:622:HOH:O	2.19	0.42
4:B:505:GOL:H12	6:B:726:HOH:O	2.20	0.42
1:A:29:VAL:HA	1:A:39:ALA:O	2.19	0.41
2:A:501:HEM:HHD	2:A:501:HEM:CBC	2.51	0.41
1:A:81:ARG:NE	6:A:607:HOH:O	2.53	0.41
1:A:103:ARG:NH2	6:A:623:HOH:O	2.54	0.40
2:B:501:HEM:CMB	2:B:501:HEM:HBB2	2.52	0.40

All (7) 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)
6:A:1075:HOH:O	6:A:1183:HOH:O[2_544]	2.08	0.12
6:A:1173:HOH:O	6:B:1082:HOH:O[3_555]	2.08	0.12
6:A:957:HOH:O	6:B:1104:HOH:O[4_536]	2.09	0.11
6:A:901:HOH:O	6:B:888:HOH:O[4_436]	2.10	0.10
6:A:1111:HOH:O	6:B:1148:HOH:O[3_555]	2.10	0.10
6:A:986:HOH:O	6:B:983:HOH:O[2_544]	2.14	0.06
6:A:1163:HOH:O	6:B:602:HOH:O[3_555]	2.14	0.06

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	409/427 (96%)	406 (99%)	3 (1%)	0	100	100
1	B	406/427 (95%)	403 (99%)	3 (1%)	0	100	100
All	All	815/854 (95%)	809 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	339/352 (96%)	335 (99%)	4 (1%)	71	47
1	B	336/352 (96%)	333 (99%)	3 (1%)	78	60
All	All	675/704 (96%)	668 (99%)	7 (1%)	73	56

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	103	ARG
1	A	159	GLU
1	A	362	LEU
1	B	34	ARG
1	B	210	LYS
1	B	267	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	A	390	ASN
1	B	293	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	GOL	B	504	-	5,5,5	0.28	0	5,5,5	0.52	0
4	GOL	B	508	-	5,5,5	1.19	1 (20%)	5,5,5	1.09	0
4	GOL	A	504	-	5,5,5	1.50	1 (20%)	5,5,5	1.00	0
4	GOL	B	503	-	5,5,5	1.10	0	5,5,5	0.31	0
4	GOL	B	507	-	5,5,5	0.73	0	5,5,5	0.50	0
3	TRP	B	502	-	14,16,16	1.21	2 (14%)	16,22,22	1.12	2 (12%)
3	TRP	A	502	-	14,16,16	1.21	1 (7%)	16,22,22	0.99	1 (6%)
4	GOL	B	505	-	5,5,5	1.75	1 (20%)	5,5,5	1.68	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	506	-	5,5,5	0.34	0	5,5,5	0.63	0
4	GOL	A	503	-	5,5,5	1.92	1 (20%)	5,5,5	2.02	1 (20%)
4	GOL	B	509	-	5,5,5	0.65	0	5,5,5	0.22	0
2	HEM	B	501	6,1	41,50,50	1.35	5 (12%)	45,82,82	1.66	9 (20%)
2	HEM	A	501	1	41,50,50	1.36	6 (14%)	45,82,82	1.93	14 (31%)

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	GOL	B	504	-	-	0/4/4/4	-
4	GOL	B	508	-	-	0/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	B	503	-	-	0/4/4/4	-
4	GOL	B	507	-	-	1/4/4/4	-
3	TRP	B	502	-	-	0/7/8/8	0/2/2/2
3	TRP	A	502	-	-	0/7/8/8	0/2/2/2
4	GOL	B	505	-	-	0/4/4/4	-
4	GOL	B	506	-	-	0/4/4/4	-
4	GOL	A	503	-	-	0/4/4/4	-
4	GOL	B	509	-	-	2/4/4/4	-
2	HEM	B	501	6,1	-	0/12/54/54	-
2	HEM	A	501	1	-	1/12/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3C-C2C	-4.69	1.33	1.40
3	A	502	TRP	CZ2-CE2	-3.53	1.35	1.41
4	A	503	GOL	O3-C3	3.42	1.56	1.42
2	B	501	HEM	C4D-C3D	3.38	1.50	1.45
4	B	505	GOL	O1-C1	3.20	1.55	1.42
2	A	501	HEM	C4B-NB	-3.05	1.32	1.38
4	A	504	GOL	O2-C2	2.55	1.51	1.43
2	B	501	HEM	C4D-ND	-2.44	1.36	1.40
2	A	501	HEM	O1D-CGD	2.40	1.30	1.22
2	B	501	HEM	CHB-C1B	2.37	1.41	1.35
2	A	501	HEM	C3C-C2C	-2.35	1.37	1.40
3	B	502	TRP	OXT-C	-2.26	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NB	2.23	2.07	1.96
3	B	502	TRP	CZ2-CE2	-2.19	1.38	1.41
2	B	501	HEM	FE-NB	2.06	2.07	1.96
4	B	508	GOL	O2-C2	2.06	1.49	1.43
2	A	501	HEM	C4D-C3D	2.01	1.48	1.45
2	A	501	HEM	CHC-C4B	-2.01	1.35	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C1B-NB-C4B	5.26	110.50	105.07
2	A	501	HEM	C4B-CHC-C1C	4.97	129.12	122.56
2	B	501	HEM	C1B-NB-C4B	4.51	109.73	105.07
2	B	501	HEM	CHC-C4B-NB	4.12	128.91	124.43
4	A	503	GOL	O3-C3-C2	3.79	128.37	110.20
2	A	501	HEM	CHC-C4B-NB	3.51	128.24	124.43
4	B	505	GOL	O1-C1-C2	3.33	126.18	110.20
2	A	501	HEM	CMA-C3A-C4A	-3.05	123.78	128.46
2	B	501	HEM	CHB-C1B-NB	2.92	127.99	124.38
2	B	501	HEM	O2A-CGA-CBA	2.85	123.17	114.03
2	A	501	HEM	C3D-C4D-ND	2.78	113.26	110.17
2	A	501	HEM	C4D-ND-C1D	-2.68	102.30	105.07
2	B	501	HEM	C3C-C4C-NC	-2.56	106.12	110.94
2	B	501	HEM	CHA-C4D-C3D	-2.45	120.73	125.33
2	A	501	HEM	O2A-CGA-CBA	2.43	121.85	114.03
2	B	501	HEM	C2D-C1D-ND	2.39	112.74	109.88
2	A	501	HEM	CMD-C2D-C1D	2.37	128.65	125.04
2	A	501	HEM	CMA-C3A-C2A	2.33	129.34	124.94
2	B	501	HEM	CMA-C3A-C4A	-2.33	124.89	128.46
3	B	502	TRP	OXT-C-CA	2.28	121.15	113.38
2	A	501	HEM	C2C-C3C-C4C	2.26	108.47	106.90
3	B	502	TRP	CH2-CZ2-CE2	-2.23	116.87	120.08
2	A	501	HEM	C3B-C2B-C1B	-2.21	104.84	106.49
2	A	501	HEM	C2D-C1D-ND	2.16	112.46	109.88
2	A	501	HEM	CHB-C1B-NB	2.09	126.97	124.38
3	A	502	TRP	CH2-CZ2-CE2	-2.08	117.09	120.08
2	A	501	HEM	CAD-C3D-C4D	2.04	128.22	124.66
2	B	501	HEM	CHA-C4D-ND	2.01	126.87	124.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

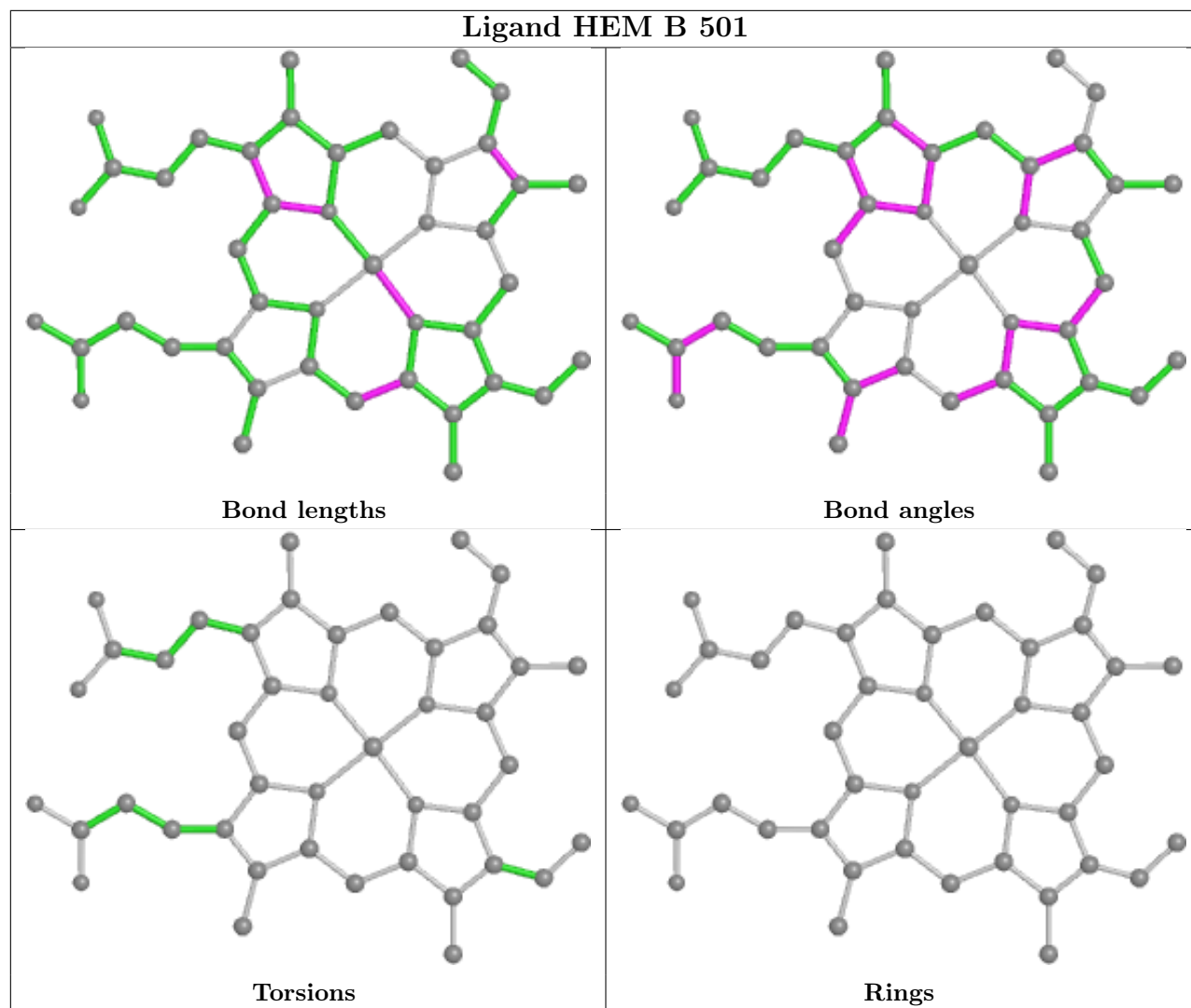
Mol	Chain	Res	Type	Atoms
4	B	507	GOL	C1-C2-C3-O3
4	B	509	GOL	C1-C2-C3-O3
4	B	509	GOL	O2-C2-C3-O3
2	A	501	HEM	CAA-CBA-CGA-O2A

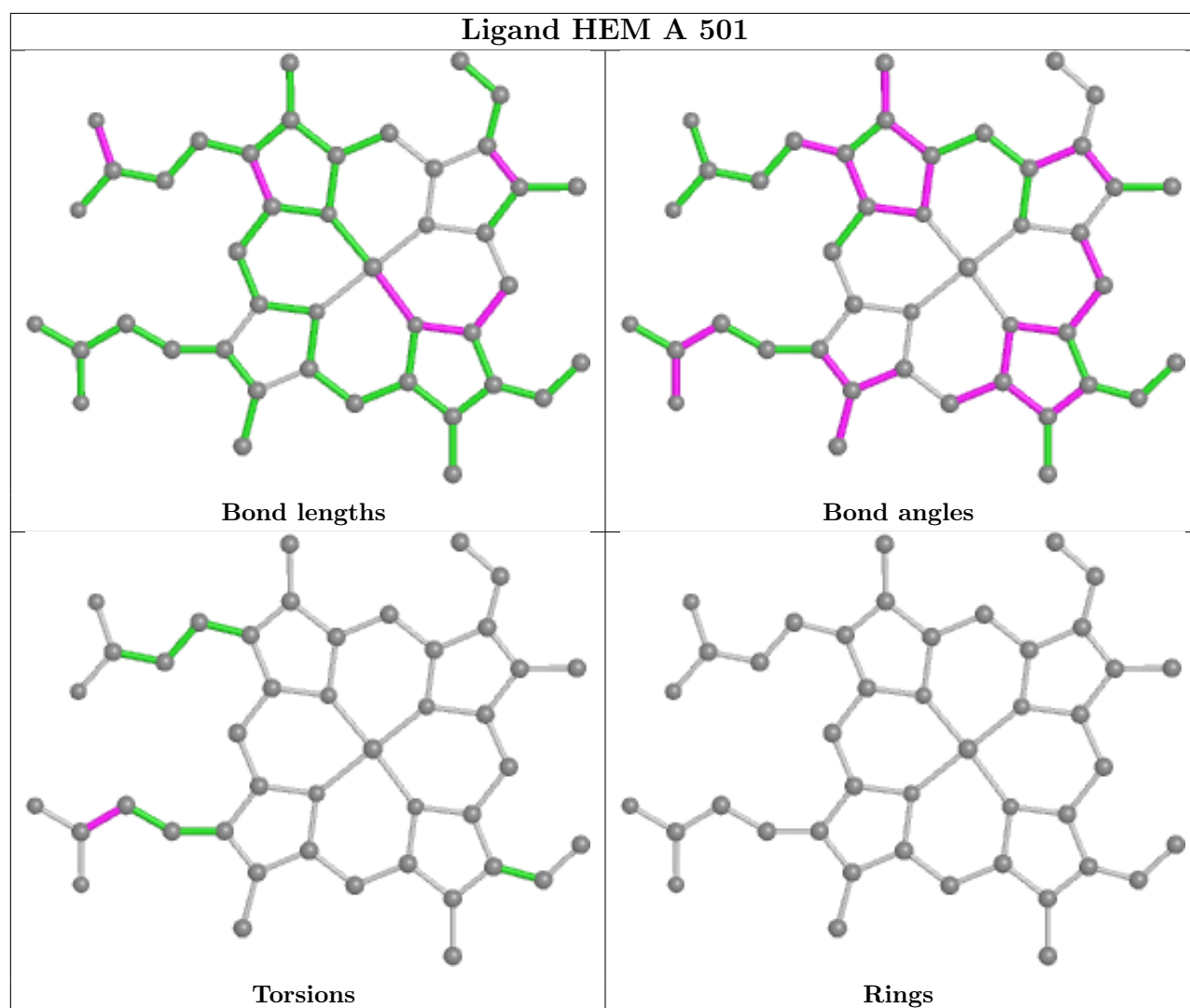
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	505	GOL	1	0
2	B	501	HEM	1	0
2	A	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.





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	403/427 (94%)	-0.22	2 (0%) 91 93	5, 11, 25, 41	12 (2%)
1	B	403/427 (94%)	-0.23	3 (0%) 87 90	5, 11, 24, 38	12 (2%)
All	All	806/854 (94%)	-0.23	5 (0%) 89 91	5, 11, 24, 41	24 (2%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	ALA	3.5
1	A	4	PRO	2.8
1	B	76	ASP	2.4
1	B	212	LEU	2.4
1	B	4	PRO	2.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

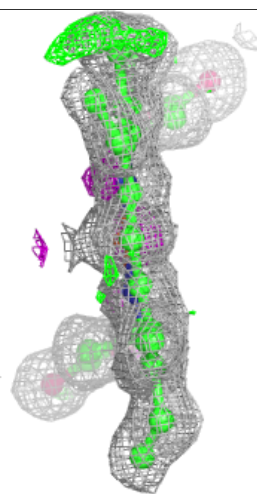
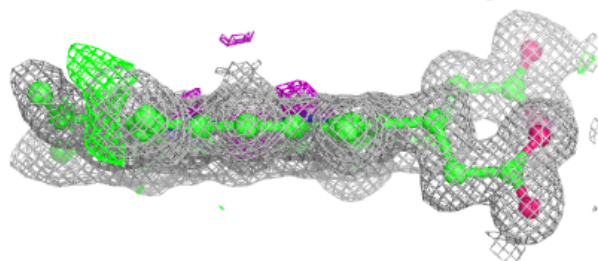
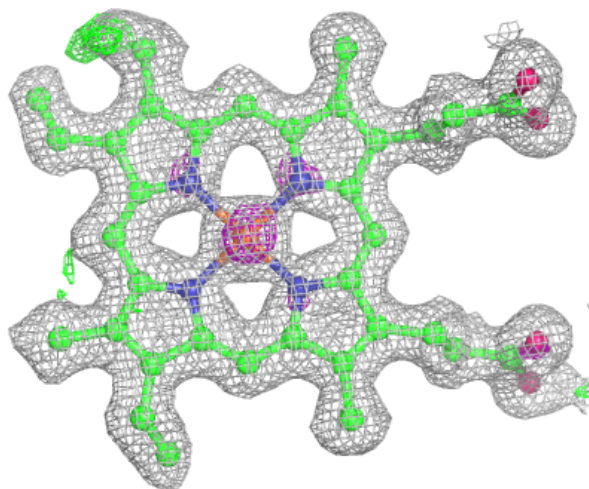
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

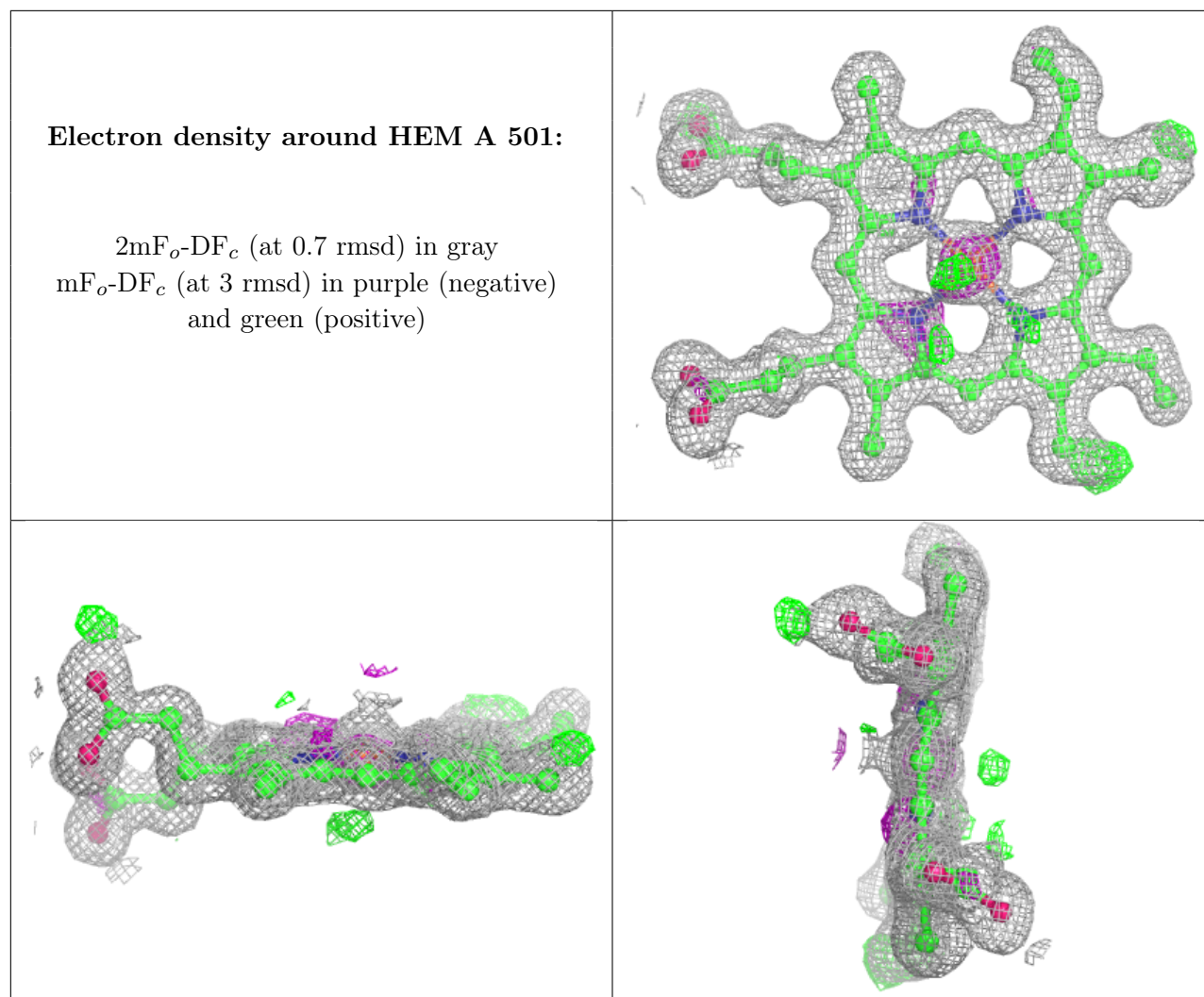
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	509	6/6	0.89	0.10	25,29,36,41	0
4	GOL	A	504	6/6	0.90	0.12	15,18,21,23	0
4	GOL	B	505	6/6	0.92	0.13	10,18,24,28	0
4	GOL	B	508	6/6	0.92	0.10	14,19,23,23	0
4	GOL	A	503	6/6	0.92	0.12	11,18,23,31	0
4	GOL	B	506	6/6	0.93	0.10	25,31,39,39	0
4	GOL	B	507	6/6	0.93	0.08	21,27,36,37	0
3	TRP	A	502	15/15	0.95	0.10	6,7,11,11	0
4	GOL	B	503	6/6	0.96	0.08	11,13,14,25	0
4	GOL	B	504	6/6	0.97	0.07	12,14,15,15	0
2	HEM	B	501	43/43	0.98	0.08	5,6,10,14	0
2	HEM	A	501	43/43	0.98	0.08	4,7,9,15	0
3	TRP	B	502	15/15	0.98	0.08	5,6,7,7	0
5	CL	B	510	1/1	1.00	0.03	13,13,13,13	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 HEM B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.