



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:03 PM BST

PDB ID : 5OG9
Title : The BM3 mutant WIFI-WC heme domain in complex with testosterone
Authors : Gamble, C.; Munro, A.W.; Leys, D.
Deposited on : 2017-07-12
Resolution : 2.09 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 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 : 2.13.1
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) : 2.13.1

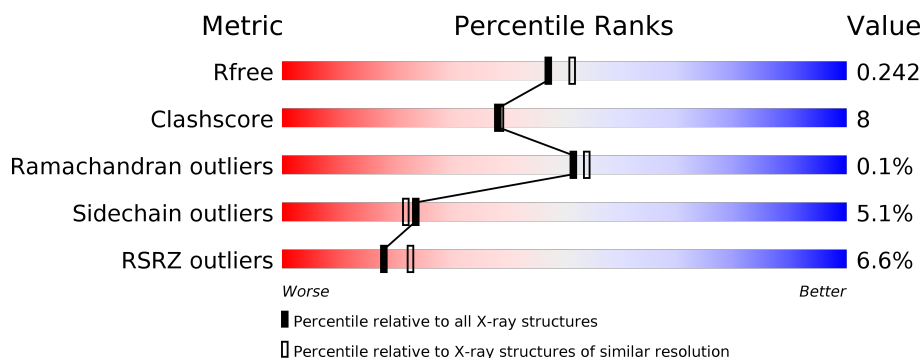
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	473	
1	B	473	

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
4	TES	A	504	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7991 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 Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	3	0
			3668	2350	619	681	18			
1	B	454	Total	C	N	O	S	0	2	0
			3683	2361	623	681	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	TRP	ARG	conflict	UNP F2Q7T0
A	52	TRP	TYR	conflict	UNP F2Q7T0
A	73	ILE	SER	conflict	UNP F2Q7T0
A	83	PHE	ALA	conflict	UNP F2Q7T0
A	88	ILE	PHE	conflict	UNP F2Q7T0
A	182	CYS	LEU	conflict	UNP F2Q7T0
B	48	TRP	ARG	conflict	UNP F2Q7T0
B	52	TRP	TYR	conflict	UNP F2Q7T0
B	73	ILE	SER	conflict	UNP F2Q7T0
B	83	PHE	ALA	conflict	UNP F2Q7T0
B	88	ILE	PHE	conflict	UNP F2Q7T0
B	182	CYS	LEU	conflict	UNP F2Q7T0

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

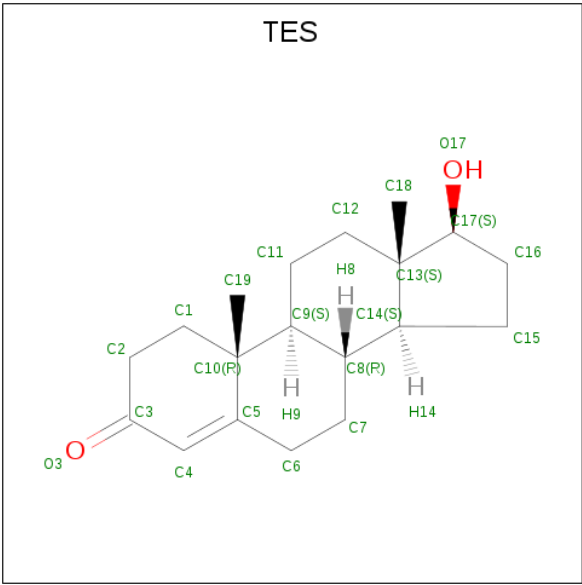


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is TESTOSTERONE (three-letter code: TES) (formula: C₁₉H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	19	2		
4	A	1	Total	C	O	0	0
			21	19	2		
4	B	1	Total	C	O	0	0
			21	19	2		
4	B	1	Total	C	O	0	0
			21	19	2		

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

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

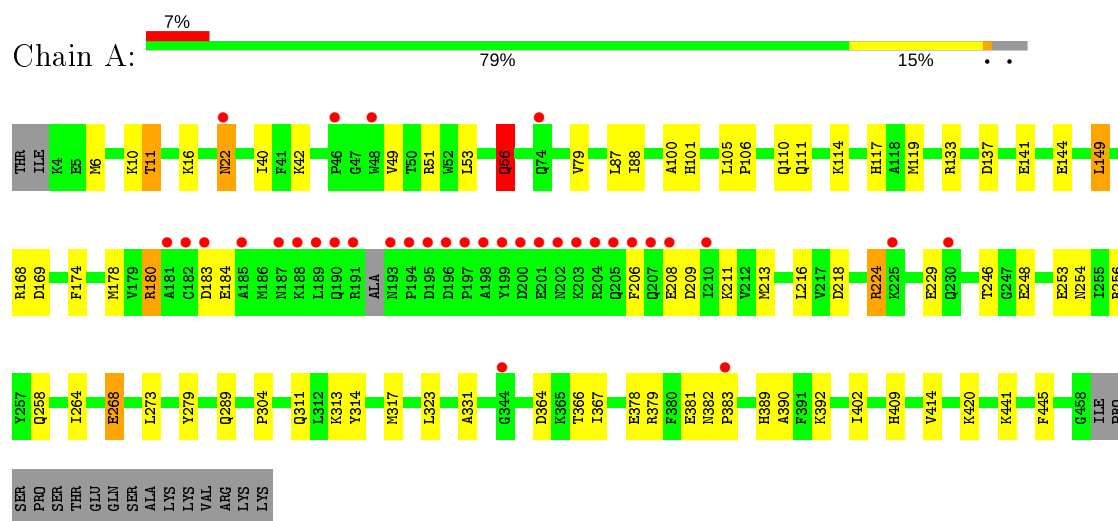
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	221	Total	O	0	0
			221	221		
6	B	247	Total	O	0	0
			247	247		

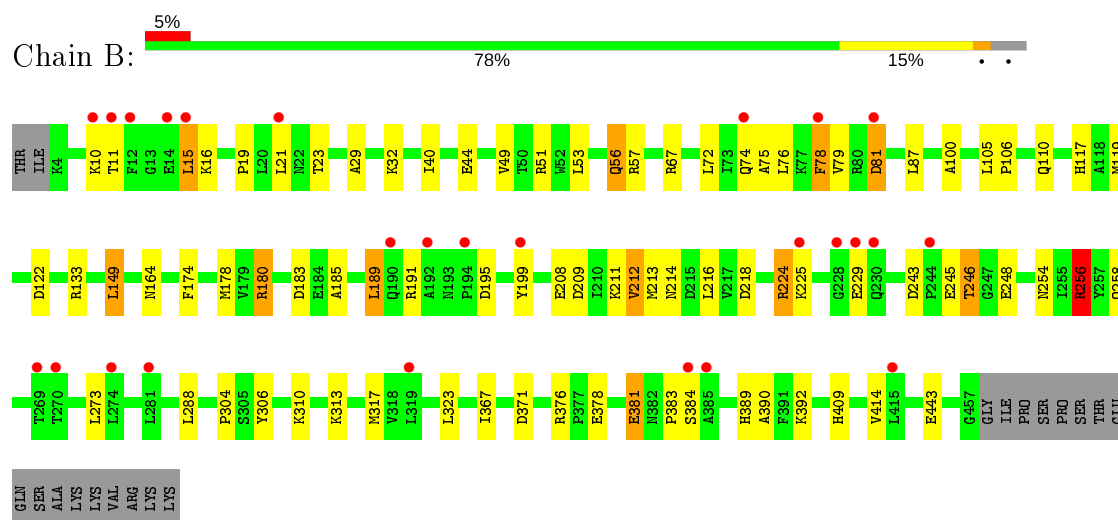
3 Residue-property plots [i](#)

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: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.39 Å 89.50 Å 172.55 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.64 – 2.09 29.62 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.64-2.09) 98.9 (29.62-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.08 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.193 , 0.239 0.199 , 0.242	Depositor DCC
R_{free} test set	3155 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7991	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, TES, 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	0.76	2/3755 (0.1%)	0.89	9/5077 (0.2%)
1	B	0.74	0/3772	0.87	8/5102 (0.2%)
All	All	0.75	2/7527 (0.0%)	0.88	17/10179 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	GLU	CB-CG	6.43	1.64	1.52
1	A	144	GLU	CG-CD	5.55	1.60	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ARG	NE-CZ-NH2	-11.64	114.48	120.30
1	B	224	ARG	NE-CZ-NH2	-11.34	114.63	120.30
1	A	224	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	B	224	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	A	56	GLN	CA-CB-CG	6.30	127.26	113.40
1	B	67	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	144	GLU	OE1-CD-OE2	-6.23	115.82	123.30
1	A	137	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	256	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	133	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	122	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	133	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	256	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	379	ARG	CB-CA-C	-5.23	99.93	110.40
1	A	169	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	B	224	ARG	CG-CD-NE	-5.08	101.14	111.80
1	A	141	GLU	CG-CD-OE1	-5.06	108.19	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3668	0	3620	52	0
1	B	3683	0	3647	59	0
2	A	43	0	30	3	0
2	B	43	0	30	0	0
3	A	1	0	0	0	0
4	A	42	0	56	2	0
4	B	42	0	56	4	0
5	A	1	0	0	1	0
6	A	221	0	0	12	0
6	B	247	0	0	3	0
All	All	7991	0	7439	113	0

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 8.

All (113) 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:119:MET:HE1	6:A:649:HOH:O	1.58	1.01
1:B:119:MET:HE1	6:B:644:HOH:O	1.67	0.93
1:B:243:ASP:HB3	1:B:246:THR:HG22	1.59	0.83
1:B:76:LEU:O	1:B:79:VAL:HG22	1.82	0.80
1:A:254:ASN:HD21	1:A:258:GLN:HE21	1.31	0.78
1:A:311:GLN:HG2	6:A:793:HOH:O	1.84	0.77
1:B:178:MET:HB2	1:B:213:MET:HE3	1.66	0.77
1:B:254:ASN:HD21	1:B:258:GLN:HE21	1.30	0.76
1:B:191:ARG:HD2	1:B:199:TYR:CZ	2.21	0.75
1:B:117:HIS:HD2	1:B:409:HIS:HE1	1.34	0.75
1:B:164:ASN:HA	6:B:686:HOH:O	1.88	0.72
1:A:168:ARG:NH1	6:A:601:HOH:O	2.09	0.71
1:A:105:LEU:HD12	1:A:402:ILE:HD11	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189[A]:LEU:HD21	4:B:502:TES:O3	1.91	0.70
1:B:384:SER:O	6:B:601:HOH:O	2.11	0.69
1:B:313:LYS:HG2	1:B:317:MET:HE2	1.75	0.69
1:B:246:THR:HG23	1:B:248:GLU:H	1.59	0.67
1:B:117:HIS:HD2	1:B:409:HIS:CE1	2.12	0.67
1:B:110:GLN:HG3	1:B:306:TYR:OH	1.95	0.67
1:B:378:GLU:O	1:B:381:GLU:HB2	1.94	0.66
1:A:178:MET:SD	1:A:264:ILE:HD12	2.36	0.65
1:A:313:LYS:HG2	1:A:317:MET:HE2	1.79	0.65
1:B:21:LEU:HD13	4:B:502:TES:H22	1.79	0.64
1:A:378:GLU:O	1:A:381:GLU:HB2	1.99	0.62
1:B:78[B]:PHE:CD1	1:B:185:ALA:HB1	2.34	0.62
1:A:178:MET:HB2	1:A:213:MET:HE3	1.81	0.62
1:A:42:LYS:NZ	6:A:602:HOH:O	2.33	0.62
1:B:371:ASP:OD2	1:B:376:ARG:NH1	2.33	0.61
1:B:313:LYS:HG2	1:B:317:MET:CE	2.32	0.60
1:A:22:ASN:HD21	1:B:195:ASP:HB2	1.66	0.59
1:A:313:LYS:HG2	1:A:317:MET:CE	2.32	0.59
1:B:78[B]:PHE:CG	1:B:185:ALA:HB1	2.37	0.59
1:B:246:THR:HG23	1:B:248:GLU:HG3	1.87	0.56
1:B:389:HIS:HA	1:B:392:LYS:HE2	1.87	0.56
1:A:88:ILE:O	1:A:88:ILE:CG2	2.53	0.56
1:A:218:ASP:OD1	1:A:256:ARG:NH1	2.38	0.56
1:B:178:MET:HB2	1:B:213:MET:CE	2.36	0.55
1:B:218:ASP:OD1	1:B:256:ARG:NH1	2.39	0.55
1:A:389:HIS:ND1	1:A:392:LYS:HE3	2.22	0.54
1:A:389:HIS:HA	1:A:392:LYS:HE2	1.89	0.54
1:B:117:HIS:CD2	1:B:409:HIS:HE1	2.20	0.53
1:A:117:HIS:HE1	1:A:304:PRO:O	1.92	0.53
1:B:110:GLN:HE22	1:B:310:LYS:NZ	2.07	0.53
1:B:246:THR:CG2	1:B:248:GLU:H	2.21	0.53
1:A:149:LEU:HD21	1:A:414:VAL:HG21	1.91	0.52
1:A:117:HIS:HD2	1:A:409:HIS:NE2	2.08	0.52
1:B:214:ASN:HB3	1:B:256:ARG:HH21	1.75	0.52
1:A:254:ASN:ND2	1:A:258:GLN:HE21	2.05	0.52
1:A:178:MET:HB2	1:A:213:MET:CE	2.40	0.52
1:A:268[B]:GLU:HB2	6:A:721:HOH:O	2.09	0.52
1:B:389:HIS:ND1	1:B:392:LYS:HE3	2.25	0.51
1:A:314:TYR:HA	1:A:317:MET:HE3	1.92	0.51
1:B:254:ASN:ND2	1:B:258:GLN:HE21	2.04	0.50
1:B:81:ASP:C	1:B:81:ASP:OD1	2.50	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:PHE:CD1	1:A:216:LEU:HD22	2.47	0.50
1:B:149:LEU:HD21	1:B:414:VAL:HG21	1.92	0.50
1:B:87:LEU:HD13	1:B:100:ALA:HB3	1.94	0.48
1:B:117:HIS:HE1	1:B:304:PRO:O	1.97	0.48
1:A:88:ILE:O	1:A:88:ILE:HG22	2.12	0.48
1:B:44:GLU:HG3	1:B:49:VAL:HG22	1.96	0.48
1:B:191:ARG:HD2	1:B:199:TYR:CE1	2.49	0.48
1:A:56:GLN:CG	1:A:367:ILE:HD11	2.44	0.47
1:A:119:MET:CE	6:A:610:HOH:O	2.62	0.47
1:B:11:THR:HG23	1:B:16:LYS:HA	1.96	0.47
1:B:367:ILE:HG21	1:B:390:ALA:HB1	1.96	0.47
1:B:79:VAL:HG21	4:B:503:TES:C2	2.45	0.46
1:B:56:GLN:HG2	1:B:367:ILE:HD11	1.97	0.46
1:B:56:GLN:HG3	1:B:57:ARG:N	2.28	0.46
1:B:174:PHE:CD1	1:B:216:LEU:HD22	2.50	0.46
1:A:119:MET:HE2	6:A:610:HOH:O	2.15	0.46
1:A:367:ILE:HG21	1:A:390:ALA:HB1	1.98	0.45
1:A:42:LYS:HE2	1:A:49:VAL:HG21	1.97	0.45
1:B:78[B]:PHE:C	1:B:78[B]:PHE:CD1	2.90	0.45
1:A:79:VAL:HG11	4:A:504:TES:H11	1.98	0.45
1:B:78[A]:PHE:HD1	1:B:78[A]:PHE:HA	1.72	0.44
1:A:11:THR:HG22	1:A:16:LYS:HA	1.98	0.44
1:B:15:LEU:HB3	1:B:19:PRO:HD3	1.98	0.44
1:B:105:LEU:N	1:B:106:PRO:CD	2.81	0.44
1:A:56:GLN:HG3	1:A:367:ILE:HD11	2.00	0.44
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.99	0.44
1:A:88:ILE:HG13	2:A:501:HEM:CAD	2.48	0.43
1:B:273:LEU:HD13	1:B:323:LEU:HG	2.00	0.43
1:A:101:HIS:HD2	6:A:674:HOH:O	2.00	0.43
1:A:105:LEU:CD1	1:A:402:ILE:HD11	2.46	0.43
1:A:331:ALA:HB3	4:A:503:TES:H181	2.00	0.43
1:A:364:ASP:OD1	1:A:366:THR:HB	2.18	0.43
1:A:382:ASN:HA	1:A:383:PRO:HD3	1.91	0.43
1:B:78[B]:PHE:CD1	1:B:185:ALA:CB	3.01	0.43
1:B:178:MET:HG3	1:B:213:MET:HE1	2.00	0.42
1:A:289:GLN:NE2	6:A:617:HOH:O	2.52	0.42
1:A:311:GLN:CG	6:A:793:HOH:O	2.51	0.42
1:B:208:GLU:O	1:B:212:VAL:HG13	2.19	0.42
1:B:29:ALA:O	1:B:32:LYS:HG2	2.19	0.42
1:B:119:MET:HB2	1:B:119:MET:HE3	1.84	0.42
1:A:105:LEU:N	1:A:106:PRO:CD	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.50	0.42
1:B:288:LEU:C	1:B:288:LEU:HD23	2.40	0.42
1:A:253:GLU:HG3	6:A:712:HOH:O	2.19	0.42
1:B:40:ILE:HD12	1:B:53:LEU:CD2	2.50	0.42
1:A:178:MET:HE1	6:A:656:HOH:O	2.20	0.42
1:A:273:LEU:HD13	1:A:323:LEU:HG	2.02	0.42
1:A:420:LYS:HD3	5:A:505:CL:CL	2.57	0.41
1:A:279:TYR:HA	1:A:445:PHE:CZ	2.56	0.41
1:A:40:ILE:HD12	1:A:53:LEU:CD2	2.51	0.41
1:B:75:ALA:O	1:B:189[B]:LEU:HD21	2.22	0.40
1:A:180:ARG:HB3	1:A:209:ASP:OD2	2.21	0.40
1:A:184:GLU:HG2	1:A:206:PHE:HB2	2.04	0.40
1:B:243:ASP:CG	1:B:245:GLU:HG2	2.42	0.40
1:A:110:GLN:HE21	1:A:114:LYS:NZ	2.20	0.40
1:A:87:LEU:HD13	1:A:100:ALA:HB3	2.03	0.40
1:B:180:ARG:HB3	1:B:209:ASP:OD2	2.22	0.40
1:B:178:MET:CB	1:B:213:MET:HE3	2.44	0.40
4:B:503:TES:H193	4:B:503:TES:H111	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	453/473 (96%)	440 (97%)	12 (3%)	1 (0%)	47	49
1	B	454/473 (96%)	442 (97%)	12 (3%)	0	100	100
All	All	907/946 (96%)	882 (97%)	24 (3%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/415 (95%)	378 (96%)	18 (4%)	27	27
1	B	399/415 (96%)	374 (94%)	25 (6%)	18	15
All	All	795/830 (96%)	752 (95%)	43 (5%)	24	20

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	A	10	LYS
1	A	11	THR
1	A	51	ARG
1	A	56	GLN
1	A	111	GLN
1	A	149	LEU
1	A	180	ARG
1	A	183	ASP
1	A	208	GLU
1	A	211	LYS
1	A	224	ARG
1	A	229	GLU
1	A	246	THR
1	A	248	GLU
1	A	268[A]	GLU
1	A	268[B]	GLU
1	A	441	LYS
1	B	10	LYS
1	B	15	LEU
1	B	23	THR
1	B	51	ARG
1	B	56	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	72	LEU
1	B	74	GLN
1	B	78[A]	PHE
1	B	78[B]	PHE
1	B	81	ASP
1	B	149	LEU
1	B	180	ARG
1	B	183	ASP
1	B	189[A]	LEU
1	B	189[B]	LEU
1	B	211	LYS
1	B	212	VAL
1	B	224	ARG
1	B	225	LYS
1	B	229	GLU
1	B	246	THR
1	B	256	ARG
1	B	381	GLU
1	B	383	PRO
1	B	443	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	28	GLN
1	A	101	HIS
1	A	110	GLN
1	A	117	HIS
1	A	164	ASN
1	A	187	ASN
1	A	254	ASN
1	B	28	GLN
1	B	110	GLN
1	B	117	HIS
1	B	164	ASN
1	B	187	ASN
1	B	254	ASN
1	B	360	GLN
1	B	405	GLN
1	B	409	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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$
2	HEM	B	501	1,6	27,50,50	1.11	2 (7%)	17,82,82	1.29	3 (17%)
2	HEM	A	501	1,6	27,50,50	1.43	4 (14%)	17,82,82	1.70	6 (35%)
4	TES	A	504	-	24,24,24	0.80	1 (4%)	39,39,39	2.10	16 (41%)
4	TES	A	503	-	24,24,24	0.67	0	39,39,39	1.58	8 (20%)
4	TES	B	503	-	24,24,24	0.70	0	39,39,39	1.49	8 (20%)
4	TES	B	502	-	24,24,24	0.77	0	39,39,39	1.58	9 (23%)

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
2	HEM	B	501	1,6	-	0/6/54/54	-
4	TES	A	504	-	-	-	0/4/4/4
2	HEM	A	501	1,6	-	0/6/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TES	A	503	-	-	-	0/4/4/4
4	TES	B	503	-	-	-	0/4/4/4
4	TES	B	502	-	-	-	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-C2B	-3.91	1.34	1.40
2	B	501	HEM	C4D-C3D	2.97	1.49	1.42
2	A	501	HEM	C1A-CHA	-2.83	1.33	1.41
2	A	501	HEM	CAD-C3D	2.63	1.56	1.52
2	A	501	HEM	C4B-NB	-2.55	1.30	1.36
4	A	504	TES	C11-C9	2.07	1.57	1.53
2	B	501	HEM	C3B-C2B	-2.01	1.37	1.40

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	TES	C14-C13-C17	5.54	105.13	99.27
4	A	504	TES	C15-C16-C17	4.48	110.46	105.75
4	A	503	TES	C1-C10-C9	3.96	114.26	108.73
4	B	502	TES	C14-C8-C9	-3.86	103.93	109.09
4	A	503	TES	C7-C6-C5	-3.67	105.02	111.93
4	B	502	TES	C7-C8-C9	3.67	115.05	110.49
2	A	501	HEM	CMA-C3A-C4A	-3.54	123.02	128.46
4	A	504	TES	C12-C11-C9	3.39	118.99	113.11
4	A	504	TES	C19-C10-C5	-3.38	102.87	108.34
4	A	504	TES	C6-C7-C8	3.22	117.51	111.69
4	B	503	TES	C9-C10-C5	3.11	114.53	109.65
4	A	504	TES	C14-C8-C9	-3.11	104.93	109.09
4	B	503	TES	C16-C17-C13	3.10	107.00	104.53
4	B	503	TES	C12-C11-C9	3.09	118.46	113.11
4	B	502	TES	C11-C9-C8	-3.05	107.36	111.75
4	A	504	TES	C15-C14-C13	3.03	107.50	103.84
4	A	503	TES	C11-C9-C8	-2.74	107.81	111.75
4	A	504	TES	C2-C3-C4	2.72	120.93	116.74
4	A	503	TES	C2-C1-C10	2.71	118.55	113.45
2	A	501	HEM	CMA-C3A-C2A	2.63	129.90	124.94
4	B	502	TES	C6-C7-C8	2.56	116.32	111.69
4	A	504	TES	C6-C5-C10	2.55	121.48	116.77
4	A	504	TES	C7-C6-C5	2.54	116.70	111.93
4	B	502	TES	C6-C5-C4	-2.46	116.76	120.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	TES	C19-C10-C9	-2.45	108.76	111.68
4	B	502	TES	C6-C5-C10	2.42	121.24	116.77
4	B	503	TES	C19-C10-C5	-2.40	104.46	108.34
2	A	501	HEM	C3B-C4B-NB	-2.34	106.18	109.21
4	A	504	TES	C1-C2-C3	-2.33	106.64	111.62
4	B	503	TES	C6-C5-C4	-2.27	117.07	120.87
4	B	503	TES	C6-C5-C10	2.26	120.94	116.77
2	B	501	HEM	CBA-CAA-C2A	-2.25	108.34	112.49
4	B	503	TES	C14-C8-C9	-2.24	106.09	109.09
4	A	504	TES	C13-C14-C8	-2.24	111.07	114.38
2	A	501	HEM	CMC-C2C-C3C	2.23	128.84	124.68
4	A	504	TES	C7-C8-C9	2.19	113.20	110.49
4	A	504	TES	C18-C13-C17	-2.19	106.07	109.54
4	B	503	TES	C14-C13-C17	2.17	101.56	99.27
4	B	502	TES	C14-C13-C17	2.17	101.56	99.27
4	A	503	TES	C11-C9-C10	2.15	115.92	113.08
4	A	504	TES	C1-C10-C9	2.15	111.72	108.73
2	B	501	HEM	CBD-CAD-C3D	-2.11	108.60	112.48
4	B	502	TES	C7-C8-C14	2.10	115.68	112.08
4	A	504	TES	C10-C5-C4	-2.10	119.28	122.68
2	B	501	HEM	C3C-C4C-NC	-2.10	106.98	110.94
2	A	501	HEM	CAA-CBA-CGA	2.08	116.16	112.67
4	A	503	TES	C2-C3-C4	2.05	119.90	116.74
4	A	503	TES	C14-C8-C9	-2.04	106.36	109.09
4	B	502	TES	C2-C3-C4	2.04	119.88	116.74
2	A	501	HEM	CBD-CAD-C3D	-2.01	108.77	112.48

There are no chirality outliers.

There are no torsion outliers.

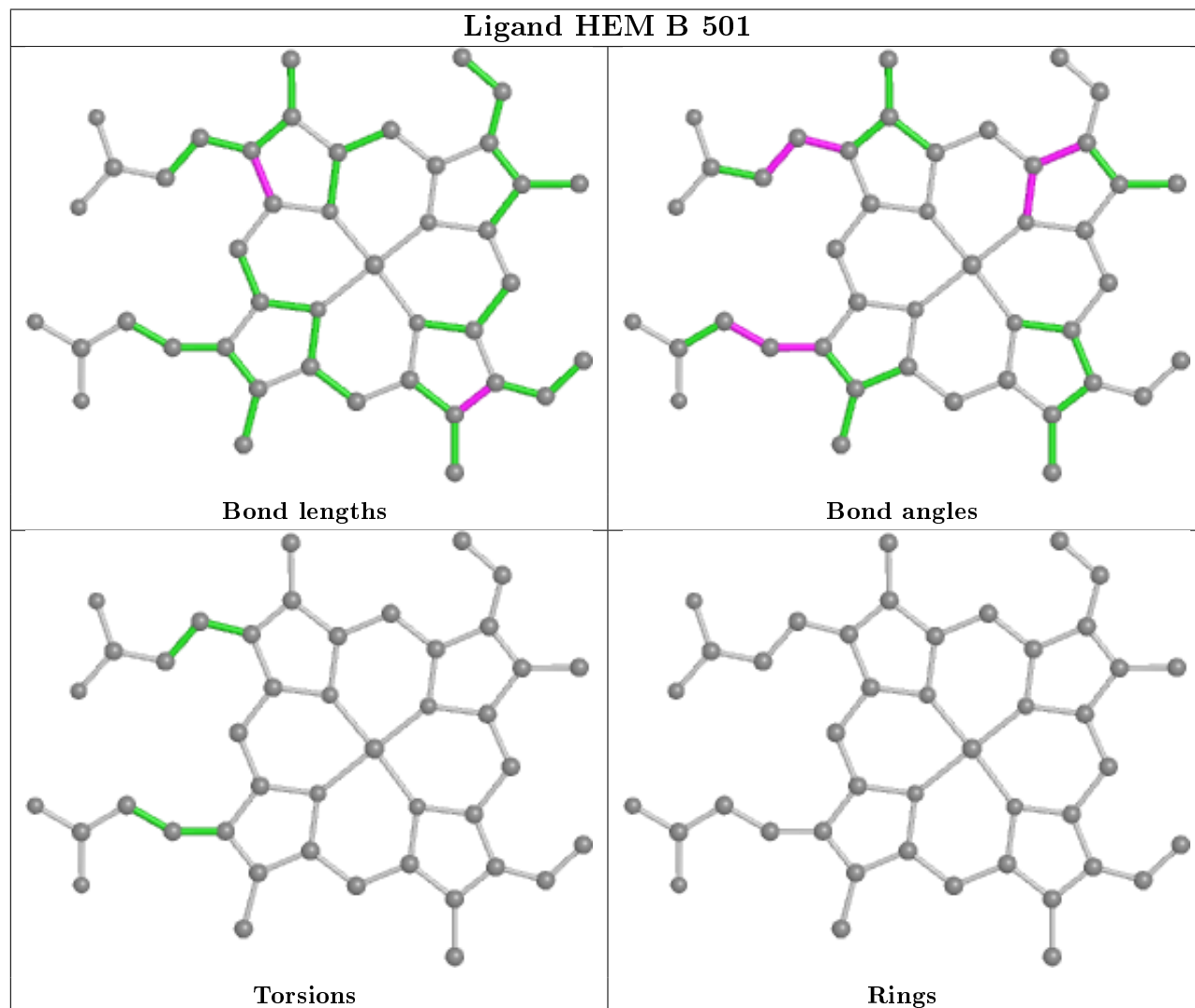
There are no ring outliers.

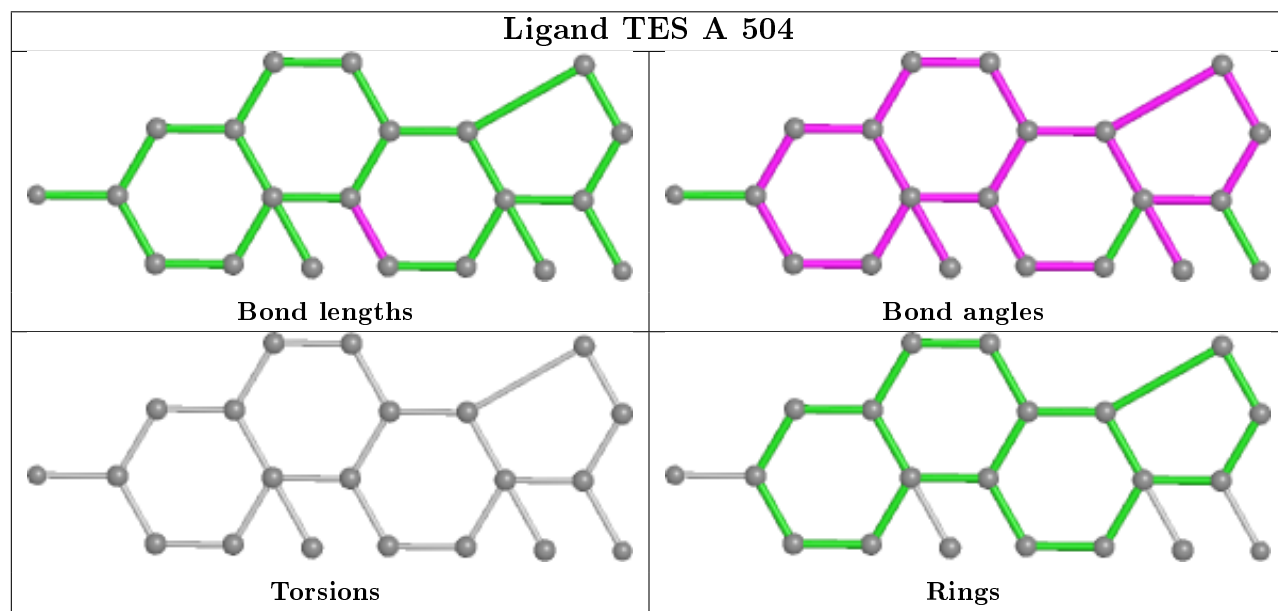
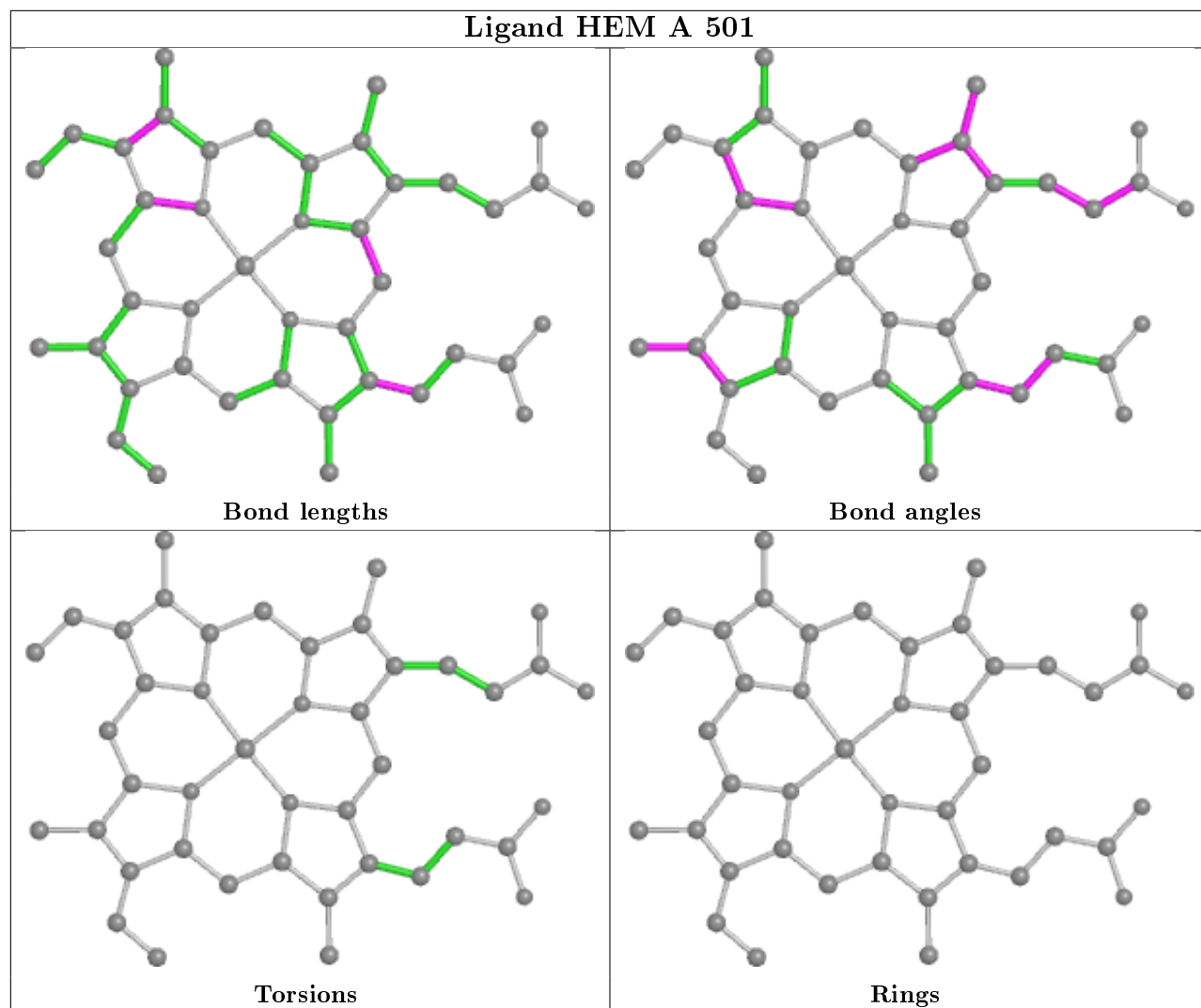
5 monomers are involved in 9 short contacts:

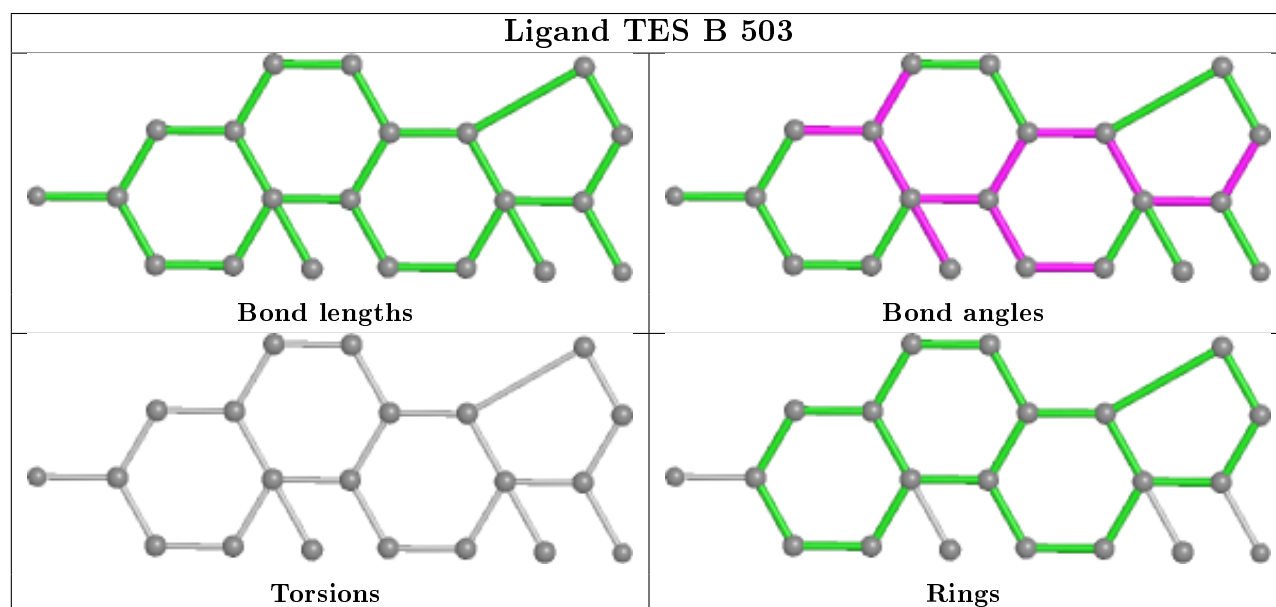
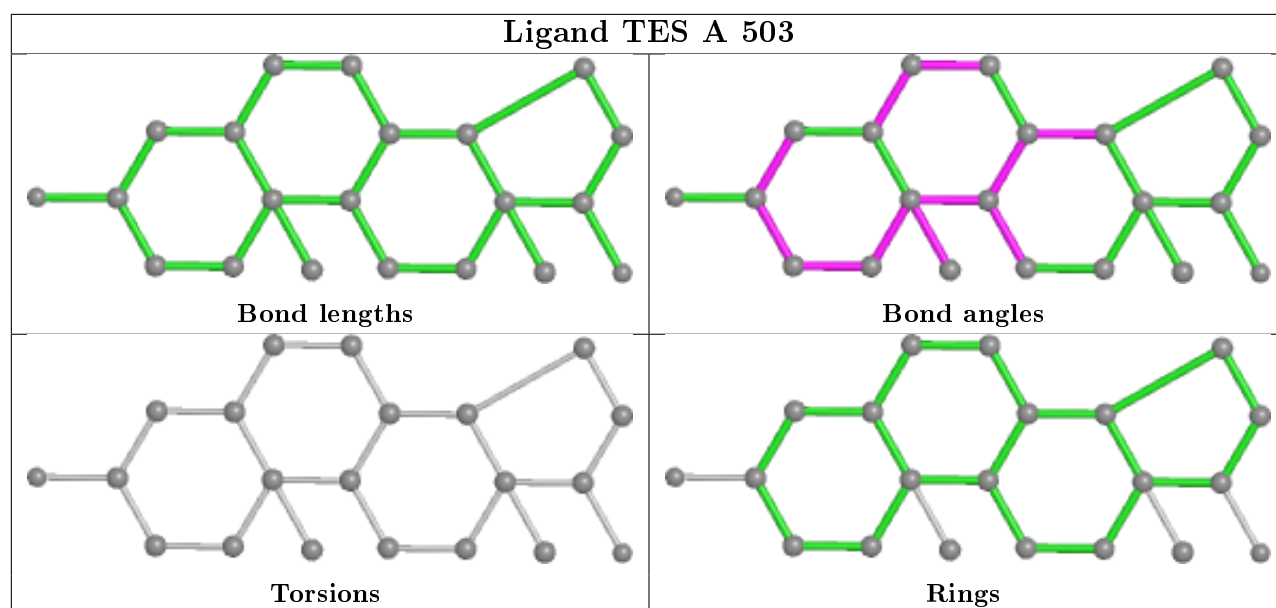
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	3	0
4	A	504	TES	1	0
4	A	503	TES	1	0
4	B	503	TES	2	0
4	B	502	TES	2	0

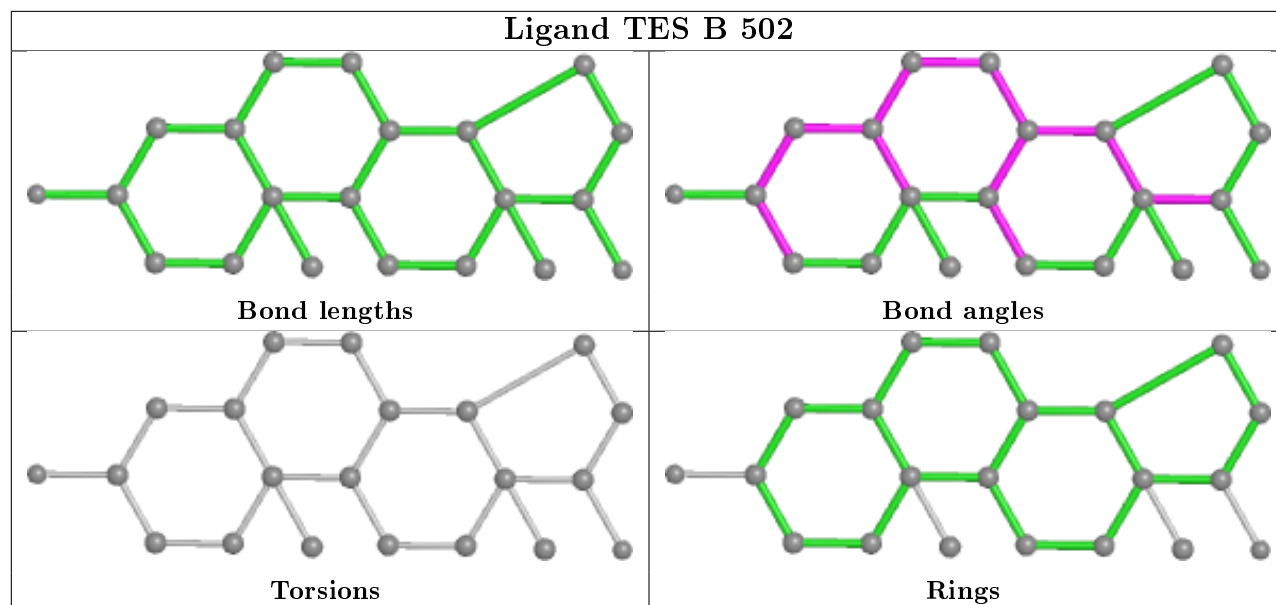
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	454/473 (95%)	0.46	34 (7%) 14 18	21, 41, 91, 141	0
1	B	454/473 (95%)	0.26	26 (5%) 23 29	22, 38, 70, 95	0
All	All	908/946 (95%)	0.36	60 (6%) 18 23	21, 40, 80, 141	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	PHE	9.1
1	A	199	TYR	8.3
1	A	198	ALA	7.9
1	A	197	PRO	7.7
1	A	203	LYS	6.8
1	A	194	PRO	6.1
1	A	189[A]	LEU	6.0
1	A	210	ILE	5.6
1	B	228	GLY	5.4
1	A	187	ASN	5.2
1	A	196	ASP	5.1
1	A	185	ALA	5.0
1	A	190	GLN	4.9
1	A	200	ASP	4.9
1	B	12	PHE	4.7
1	A	182	CYS	4.6
1	A	204	ARG	4.5
1	B	229	GLU	4.3
1	B	230	GLN	4.2
1	A	205	GLN	3.9
1	B	15	LEU	3.9
1	A	201	GLU	3.5
1	B	10	LYS	3.5
1	A	195	ASP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	202	ASN	3.4
1	B	14	GLU	3.3
1	A	191	ARG	3.3
1	A	225	LYS	3.2
1	A	48	TRP	3.2
1	A	193	ASN	3.2
1	B	199	TYR	3.1
1	B	74	GLN	3.1
1	B	415	LEU	2.9
1	A	208	GLU	2.9
1	A	344	GLY	2.7
1	B	78[A]	PHE	2.7
1	A	383	PRO	2.7
1	B	192	ALA	2.7
1	A	46	PRO	2.6
1	B	384	SER	2.6
1	A	22	ASN	2.6
1	A	74	GLN	2.5
1	A	188	LYS	2.5
1	B	385	ALA	2.5
1	A	230	GLN	2.4
1	B	244	PRO	2.4
1	B	274	LEU	2.3
1	A	183	ASP	2.3
1	B	319	LEU	2.3
1	B	11	THR	2.3
1	B	21	LEU	2.2
1	A	207	GLN	2.2
1	B	225	LYS	2.2
1	B	194	PRO	2.1
1	B	281	LEU	2.1
1	B	81	ASP	2.1
1	B	270	THR	2.1
1	B	190	GLN	2.0
1	B	269	THR	2.0
1	A	181	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

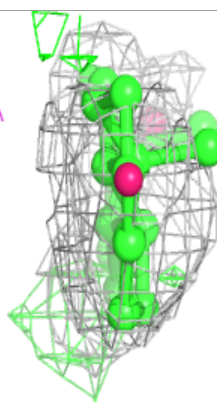
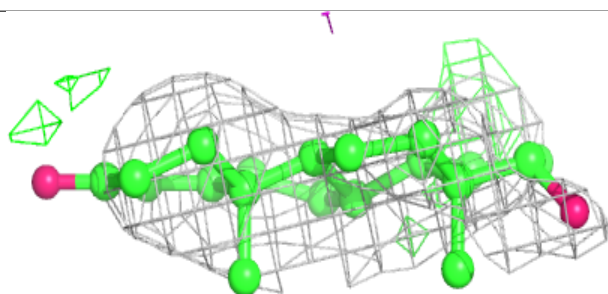
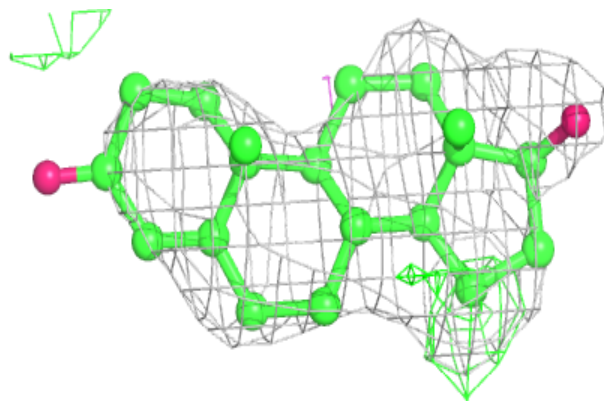
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TES	A	504	21/21	0.70	0.45	81,96,105,122	0
4	TES	B	502	21/21	0.82	0.24	53,69,90,95	0
4	TES	A	503	21/21	0.84	0.26	62,89,98,99	0
4	TES	B	503	21/21	0.85	0.31	68,71,81,94	0
2	HEM	B	501	43/43	0.97	0.16	20,25,29,31	0
2	HEM	A	501	43/43	0.98	0.12	23,26,34,38	0
5	CL	A	505	1/1	0.98	0.13	36,36,36,36	0
3	ZN	A	502	1/1	0.99	0.07	30,30,30,30	0

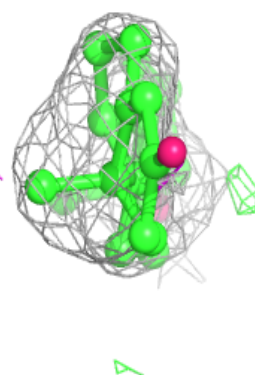
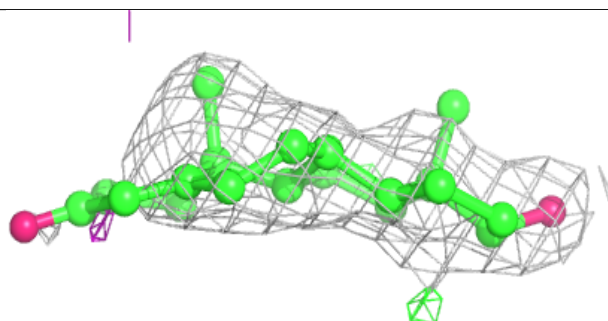
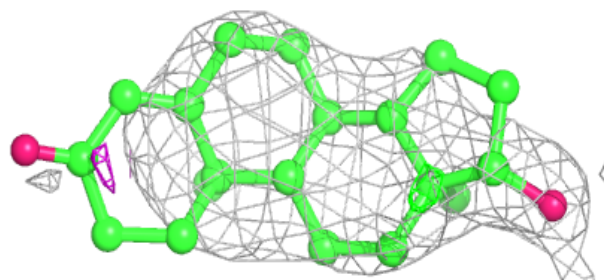
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TES A 504:

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

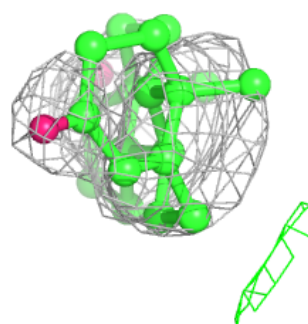
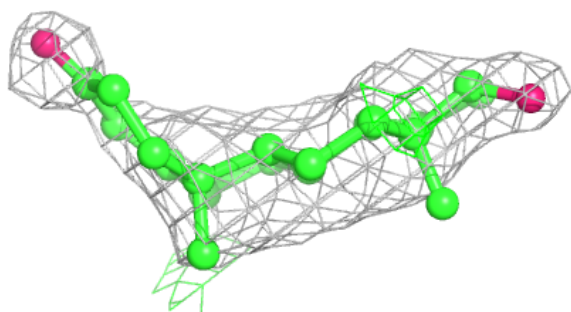
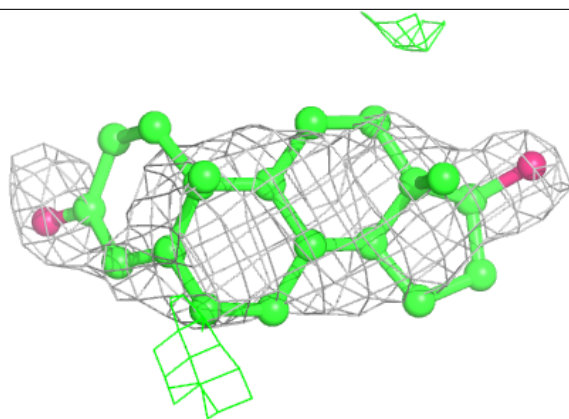
**Electron density around TES B 502:**

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

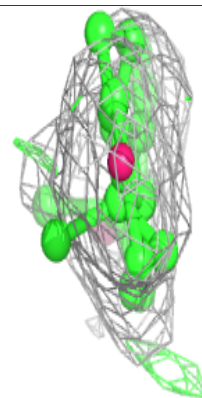
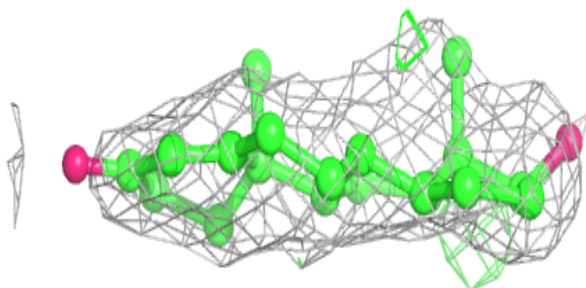
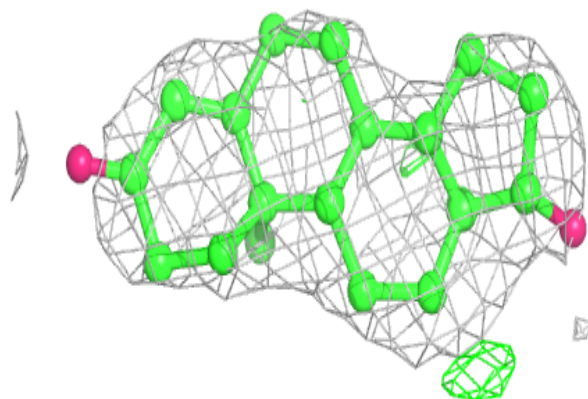


Electron density around TES A 503:

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

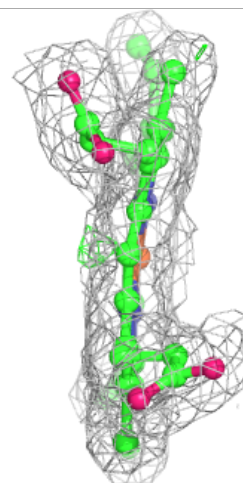
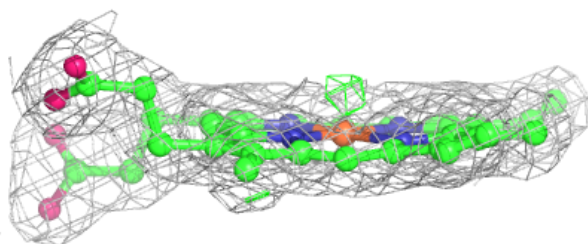
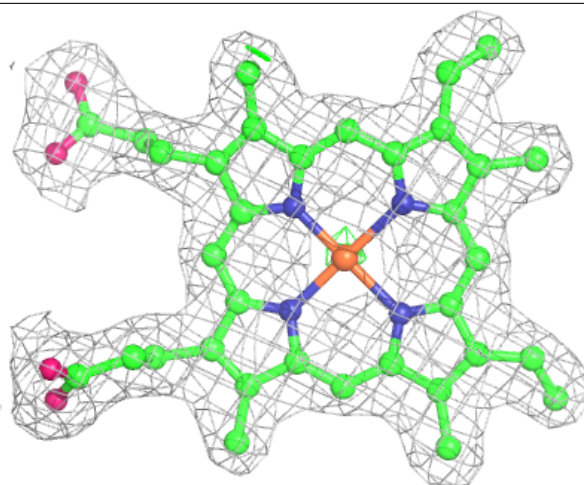
**Electron density around TES B 503:**

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



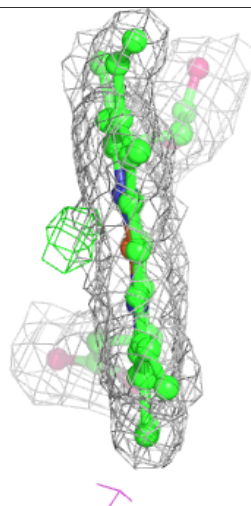
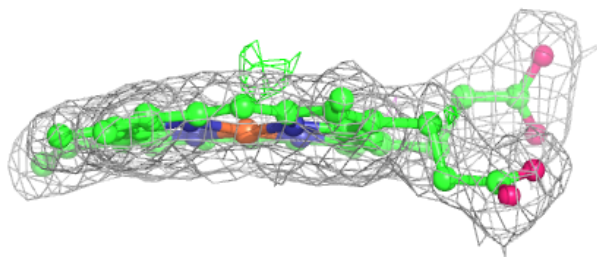
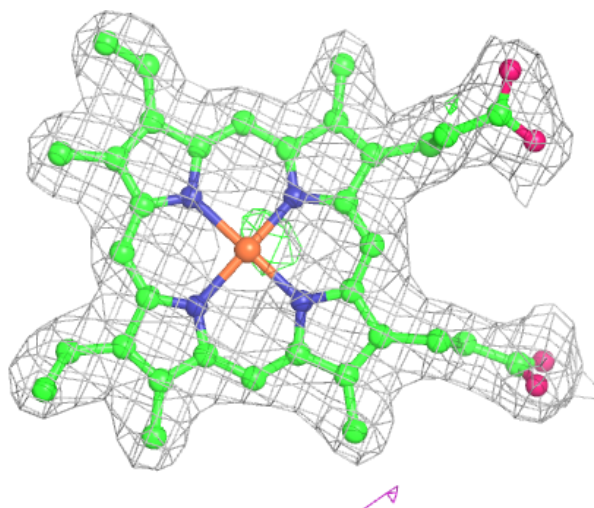
Electron density around HEM B 501:

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



Electron density around HEM 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.