



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:12 PM UTC

PDB ID : 7Y98 / pdb_00007y98
Title : Crystal structure of CYP109B4 from *Bacillus Sonorensis* in complex with Testosterone
Authors : Shen, P.P.; Huang, J.-W.; Li, X.; Liu, W.D.; Chen, C.-C.; Guo, R.-T.
Deposited on : 2022-06-24
Resolution : 2.27 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

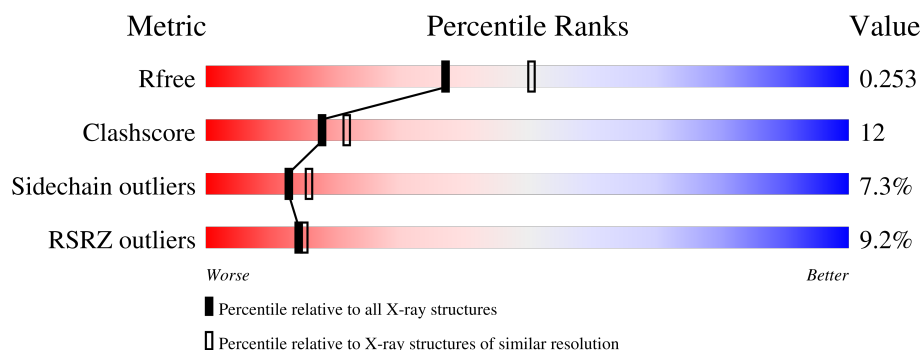
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	406	8% 72% 19% • 7%
1	B	406	9% 69% 20% • 8%

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
3	TES	B	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6389 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.

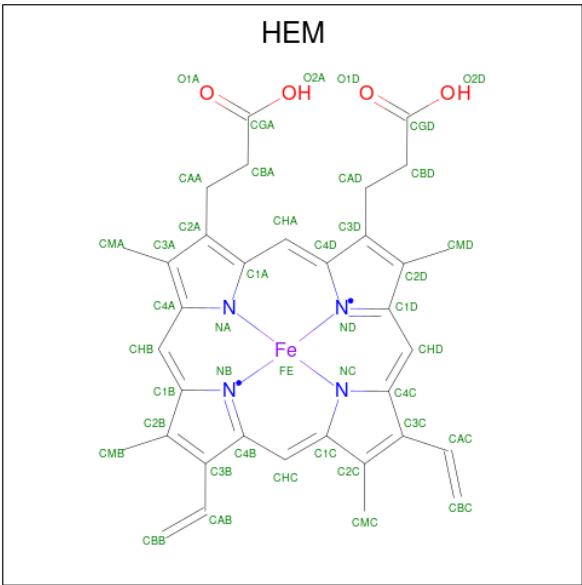
- Molecule 1 is a protein called Cytochrome P450 monooxygenase YjiB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3055	1950	519	573	13			
1	B	374	Total	C	N	O	S	0	0	0
			3031	1935	516	567	13			

There are 8 discrepancies between the modelled and reference sequences:

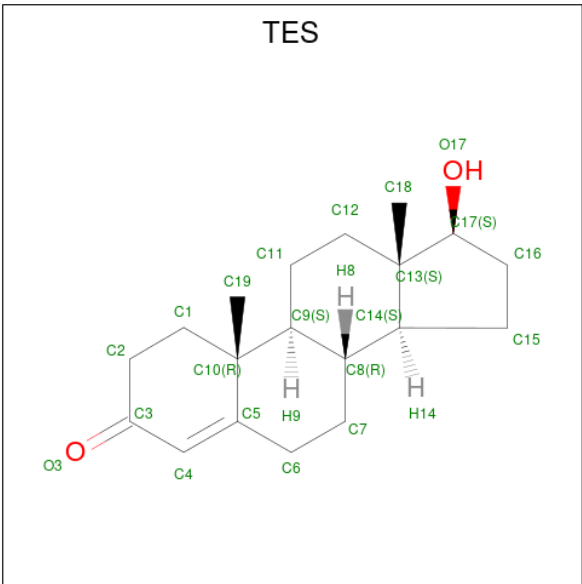
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP M5PFT9
A	40	TYR	CYS	engineered mutation	UNP M5PFT9
A	49	SER	ASN	engineered mutation	UNP M5PFT9
A	264	PHE	LEU	engineered mutation	UNP M5PFT9
B	0	GLY	-	expression tag	UNP M5PFT9
B	40	TYR	CYS	engineered mutation	UNP M5PFT9
B	49	SER	ASN	engineered mutation	UNP M5PFT9
B	264	PHE	LEU	engineered mutation	UNP M5PFT9

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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 TESTOSTERONE (CCD ID: TES) (formula: C₁₉H₂₈O₂) (labeled as "Ligand of Interest" by depositor).



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

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

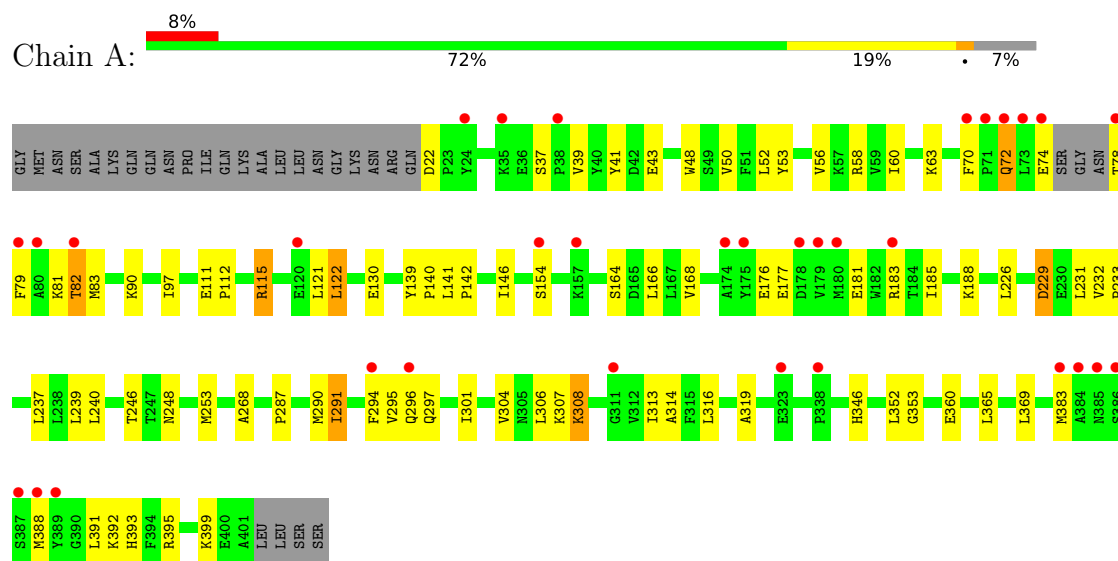
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total	O	0	0
			106	106		
4	B	69	Total	O	0	0
			69	69		

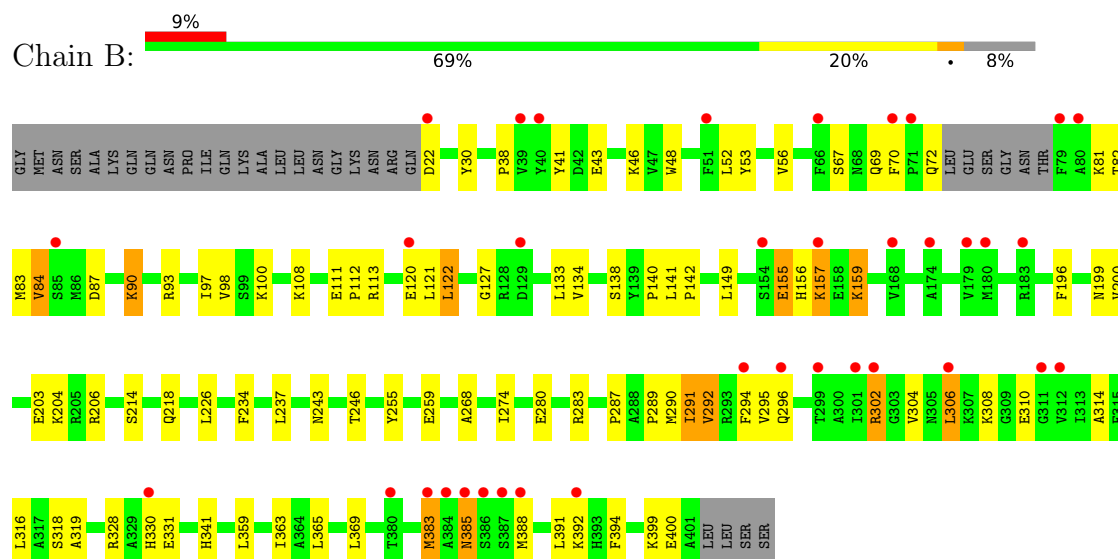
3 Residue-property plots [i](#)

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: Cytochrome P450 monooxygenase YjiB



• Molecule 1: Cytochrome P450 monooxygenase YjiB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.72Å 95.70Å 78.99Å 90.00° 104.30° 90.00°	Depositor
Resolution (Å)	24.65 – 2.27 24.65 – 2.27	Depositor EDS
% Data completeness (in resolution range)	93.8 (24.65-2.27) 93.7 (24.65-2.27)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 2.26Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.237 , 0.276 (Not available) , 0.253	Depositor DCC
R_{free} test set	2012 reflections (4.16%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6389	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.46 % 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 9.8906e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, TES

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	0.81	0/3127	1.06	0/4230
1	B	0.48	0/3103	0.70	0/4197
All	All	0.66	0/6230	0.90	0/8427

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

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	3055	0	3014	51	0
1	B	3031	0	2990	95	0
2	A	43	0	30	5	0
2	B	43	0	30	5	0
3	A	21	0	28	0	0
3	B	21	0	28	12	0
4	A	106	0	0	4	0
4	B	69	0	0	6	0
All	All	6389	0	6120	150	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 12.

All (150) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:TRP:CE2	1:B:306:LEU:HD11	1.87	1.08
1:B:302:ARG:NE	1:B:302:ARG:HA	1.74	1.01
1:B:48:TRP:CE2	1:B:306:LEU:CD1	2.45	1.00
1:B:48:TRP:NE1	1:B:306:LEU:HD12	1.80	0.97
1:B:48:TRP:NE1	1:B:306:LEU:CD1	2.30	0.95
1:B:83:MET:HE1	1:B:98:VAL:HG21	1.49	0.94
1:B:292:VAL:HG12	3:B:502:TES:H183	1.54	0.90
1:B:291:ILE:CD1	3:B:502:TES:C19	2.55	0.83
1:B:48:TRP:CD2	1:B:306:LEU:HD11	2.14	0.83
1:A:253:MET:HE3	1:A:365:LEU:HD22	1.63	0.81
1:B:302:ARG:HH21	1:B:302:ARG:HG3	1.46	0.78
2:B:501:HEM:HHC	2:B:501:HEM:HBB2	1.66	0.76
1:A:111:GLU:HB3	1:A:112:PRO:HD3	1.67	0.76
1:B:292:VAL:CG1	3:B:502:TES:H183	2.16	0.75
1:B:383:MET:HA	1:B:392:LYS:HG3	1.68	0.75
1:B:38:PRO:HB3	1:B:52:LEU:HD13	1.67	0.75
1:B:70:PHE:HD2	1:B:294:PHE:HE2	1.33	0.74
1:A:141:LEU:HB3	1:A:142:PRO:HD3	1.69	0.73
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.71	0.72
1:B:100:LYS:NZ	4:B:601:HOH:O	2.21	0.72
1:B:302:ARG:NE	1:B:302:ARG:CA	2.52	0.71
1:A:346:HIS:ND1	4:A:601:HOH:O	2.23	0.71
1:B:48:TRP:CH2	1:B:304:VAL:HG11	2.27	0.69
1:B:283:ARG:CG	1:B:341:HIS:HB3	2.22	0.69
1:A:70:PHE:CE1	1:A:294:PHE:HE2	2.11	0.68
1:B:291:ILE:HD12	3:B:502:TES:H193	1.76	0.67
1:B:302:ARG:HG3	1:B:302:ARG:NH2	2.10	0.66
1:A:82:THR:HB	1:A:237:LEU:HD22	1.77	0.66
1:B:291:ILE:HD12	3:B:502:TES:C19	2.26	0.64
1:B:283:ARG:HG3	1:B:341:HIS:HB3	1.79	0.64
1:B:38:PRO:CB	1:B:52:LEU:HD13	2.27	0.63
1:B:292:VAL:HG12	3:B:502:TES:C18	2.28	0.63
1:B:48:TRP:CD1	1:B:306:LEU:CD1	2.82	0.63
1:A:383:MET:HE2	1:A:392:LYS:HA	1.81	0.62
1:B:82:THR:HB	1:B:237:LEU:HD22	1.81	0.62
1:B:83:MET:CE	1:B:234:PHE:CE1	2.84	0.60
1:B:291:ILE:HD11	3:B:502:TES:H192	1.84	0.60
1:B:291:ILE:HD11	3:B:502:TES:C19	2.30	0.60
1:B:38:PRO:HB3	1:B:52:LEU:CD1	2.32	0.59
1:B:48:TRP:CH2	1:B:304:VAL:CG1	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:LYS:HD2	4:B:621:HOH:O	2.01	0.59
1:B:292:VAL:HG12	3:B:502:TES:H121	1.85	0.59
1:A:90:LYS:HG3	4:A:686:HOH:O	2.03	0.59
1:B:48:TRP:CD1	1:B:306:LEU:HD12	2.38	0.58
1:B:259:GLU:CD	4:B:602:HOH:O	2.47	0.58
1:B:84:VAL:HG23	2:B:501:HEM:HAD2	1.86	0.57
1:B:268:ALA:HB2	1:B:369:LEU:HD22	1.86	0.57
1:B:296:GLN:HG3	1:B:296:GLN:O	1.99	0.57
1:A:97:ILE:HG21	1:A:226:LEU:HG	1.85	0.57
1:B:302:ARG:C	1:B:302:ARG:CZ	2.77	0.57
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.86	0.57
1:A:392:LYS:HD2	1:A:393:HIS:CD2	2.41	0.55
1:A:83:MET:HE1	1:A:352:LEU:HD22	1.89	0.55
1:A:253:MET:CE	1:A:365:LEU:HD22	2.34	0.55
1:A:232:VAL:HB	1:A:233:PRO:HD3	1.90	0.53
1:A:50:VAL:HG23	1:A:314:ALA:HA	1.91	0.53
1:B:83:MET:HE3	1:B:234:PHE:CE1	2.43	0.53
1:B:302:ARG:HA	1:B:302:ARG:HE	1.67	0.53
1:B:56:VAL:HG13	1:B:314:ALA:HB1	1.91	0.53
1:B:199:ASN:O	1:B:203:GLU:HG3	2.09	0.52
1:B:359:LEU:O	1:B:363:ILE:HG13	2.09	0.52
1:A:383:MET:HG2	1:A:391:LEU:C	2.35	0.52
1:B:48:TRP:CD1	1:B:306:LEU:HD11	2.43	0.52
1:A:130:GLU:OE2	1:A:395:ARG:NE	2.38	0.51
1:B:295:VAL:HG23	1:B:310:GLU:O	2.10	0.51
1:A:142:PRO:HA	1:A:360:GLU:OE2	2.11	0.51
1:A:287:PRO:HG2	2:A:501:HEM:HMB2	1.93	0.51
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.92	0.51
1:B:48:TRP:NE1	1:B:306:LEU:HD11	2.09	0.51
1:A:301:ILE:HD12	1:A:306:LEU:HD11	1.93	0.50
1:A:72:GLN:HE21	1:A:72:GLN:N	2.09	0.50
1:B:283:ARG:HG2	1:B:341:HIS:HB3	1.92	0.50
1:B:121:LEU:HD21	1:B:140:PRO:HG2	1.94	0.50
1:B:385:ASN:HD21	1:B:388:MET:HB2	1.77	0.49
1:B:134:VAL:HA	1:B:138:SER:OG	2.13	0.49
1:B:291:ILE:CD1	3:B:502:TES:H191	2.40	0.49
1:B:214:SER:O	1:B:218:GLN:HG3	2.13	0.49
1:B:246:THR:HA	2:B:501:HEM:HBB1	1.94	0.49
1:A:39:VAL:HG21	1:A:301:ILE:HG22	1.94	0.48
1:B:48:TRP:CG	1:B:306:LEU:HD11	2.48	0.48
1:A:166:LEU:HD21	1:A:185:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ASN:HB2	4:B:609:HOH:O	2.12	0.48
1:A:115:ARG:HH21	1:A:115:ARG:CG	2.27	0.48
1:A:253:MET:CE	1:A:365:LEU:HB2	2.44	0.48
1:B:113:ARG:HH12	1:B:149:LEU:HD23	1.79	0.48
1:B:141:LEU:HB3	1:B:142:PRO:HD3	1.95	0.48
1:A:139:TYR:N	1:A:140:PRO:HD2	2.28	0.48
1:B:97:ILE:HG21	1:B:226:LEU:HD22	1.94	0.48
1:B:274:ILE:HG12	1:B:365:LEU:HD12	1.96	0.47
1:B:155:GLU:H	1:B:155:GLU:HG3	1.45	0.47
1:A:295:VAL:HG12	1:A:308:LYS:HA	1.97	0.47
1:B:53:TYR:HA	1:B:319:ALA:HB1	1.97	0.47
1:A:70:PHE:CD1	1:A:294:PHE:HE2	2.31	0.47
1:A:248:ASN:HD21	1:A:388:MET:HE3	1.79	0.47
1:B:69:GLN:HG3	1:B:87:ASP:OD2	2.15	0.47
1:B:287:PRO:HG2	2:B:501:HEM:HMB3	1.96	0.47
1:B:330:HIS:CG	1:B:330:HIS:O	2.68	0.47
1:B:41:TYR:HB2	1:B:48:TRP:CZ3	2.51	0.46
1:A:56:VAL:HG13	1:A:314:ALA:HB1	1.97	0.46
1:B:41:TYR:HB2	1:B:48:TRP:CH2	2.51	0.46
1:B:111:GLU:HB3	1:B:112:PRO:HD3	1.99	0.45
1:B:127:GLY:N	1:B:400:GLU:OE2	2.38	0.45
1:B:41:TYR:CE2	1:B:43:GLU:HA	2.52	0.45
1:B:48:TRP:CZ3	1:B:304:VAL:HG11	2.52	0.45
1:A:253:MET:HE3	1:A:365:LEU:CD2	2.42	0.45
1:B:156:HIS:ND1	1:B:196:PHE:HE1	2.14	0.45
1:B:383:MET:HA	1:B:392:LYS:CG	2.44	0.45
1:A:122:LEU:HD23	1:A:122:LEU:HA	1.75	0.44
1:B:385:ASN:ND2	1:B:388:MET:HB2	2.32	0.44
1:A:246:THR:HA	2:A:501:HEM:HBB1	1.99	0.44
1:A:22:ASP:N	1:A:22:ASP:OD1	2.50	0.44
1:B:83:MET:CE	1:B:234:PHE:CD1	3.01	0.44
1:A:146:ILE:HG21	1:A:239:LEU:HD23	2.00	0.43
1:A:291:ILE:HD13	1:A:316:LEU:HD11	2.01	0.43
1:A:41:TYR:CE2	1:A:43:GLU:HA	2.53	0.43
1:B:30:TYR:HB3	1:B:318:SER:HB2	2.01	0.43
1:B:83:MET:HE3	1:B:234:PHE:HE1	1.82	0.43
1:B:328:ARG:HB3	1:B:331:GLU:HG3	2.01	0.42
1:B:90:LYS:HE2	1:B:90:LYS:HB2	1.70	0.42
1:B:289:PRO:HD2	4:B:610:HOH:O	2.18	0.42
1:A:353:GLY:HA3	2:A:501:HEM:C3C	2.54	0.42
1:A:399:LYS:HB3	1:A:399:LYS:HE2	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:632:HOH:O	1:B:108:LYS:HE3	2.18	0.42
1:A:268:ALA:HB2	1:A:369:LEU:HD22	2.02	0.42
1:B:157:LYS:HE3	1:B:157:LYS:HB3	1.56	0.42
1:A:115:ARG:CG	1:A:115:ARG:NH2	2.81	0.42
1:B:255:TYR:O	1:B:259:GLU:HB2	2.20	0.42
1:A:231:LEU:HD12	1:A:231:LEU:HA	1.89	0.42
1:B:22:ASP:OD1	1:B:22:ASP:N	2.53	0.42
1:B:122:LEU:HA	1:B:122:LEU:HD23	1.79	0.42
1:B:388:MET:HE2	3:B:502:TES:H61	2.02	0.42
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.90	0.41
1:A:41:TYR:HB2	1:A:48:TRP:CZ3	2.55	0.41
1:A:50:VAL:CG2	1:A:314:ALA:HA	2.50	0.41
1:B:200:VAL:O	1:B:204:LYS:HG2	2.20	0.41
1:B:292:VAL:HG12	3:B:502:TES:C12	2.49	0.41
1:B:70:PHE:HD2	1:B:294:PHE:CE2	2.24	0.41
1:A:388:MET:HG2	4:A:620:HOH:O	2.21	0.41
1:B:291:ILE:HG12	1:B:316:LEU:HD11	2.02	0.41
1:A:53:TYR:HA	1:A:319:ALA:HB1	2.03	0.41
1:A:115:ARG:HH21	1:A:115:ARG:HG2	1.85	0.41
1:B:159:LYS:HB3	1:B:159:LYS:HE3	1.94	0.41
1:B:280:GLU:OE2	1:B:283:ARG:NH1	2.38	0.41
1:A:229:ASP:OD1	1:A:229:ASP:N	2.51	0.41
1:B:302:ARG:NH2	1:B:302:ARG:CG	2.77	0.41
1:A:185:ILE:N	1:A:185:ILE:HD13	2.36	0.40
1:B:259:GLU:OE2	4:B:602:HOH:O	2.22	0.40
1:B:133:LEU:HB3	1:B:394:PHE:HB3	2.03	0.40
1:A:79:PHE:CE2	1:A:240:LEU:HD23	2.56	0.40
1:A:290:MET:HG3	1:A:313:ILE:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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	335/359 (93%)	308 (92%)	27 (8%)	11	13
1	B	332/359 (92%)	310 (93%)	22 (7%)	15	19
All	All	667/718 (93%)	618 (93%)	49 (7%)	13	16

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	SER
1	A	58	ARG
1	A	60	ILE
1	A	63	LYS
1	A	72	GLN
1	A	74	GLU
1	A	78	THR
1	A	81	LYS
1	A	82	THR
1	A	115	ARG
1	A	121	LEU
1	A	122	LEU
1	A	154	SER
1	A	164	SER
1	A	168	VAL
1	A	176	GLU
1	A	177	GLU
1	A	181	GLU
1	A	183	ARG
1	A	188	LYS
1	A	229	ASP
1	A	291	ILE
1	A	296	GLN
1	A	297	GLN
1	A	304	VAL
1	A	307	LYS
1	A	308	LYS
1	B	46	LYS
1	B	67	SER
1	B	72	GLN
1	B	81	LYS

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Mol	Chain	Res	Type
1	B	84	VAL
1	B	90	LYS
1	B	93	ARG
1	B	120	GLU
1	B	122	LEU
1	B	155	GLU
1	B	157	LYS
1	B	159	LYS
1	B	206	ARG
1	B	290	MET
1	B	291	ILE
1	B	292	VAL
1	B	302	ARG
1	B	306	LEU
1	B	308	LYS
1	B	383	MET
1	B	385	ASN
1	B	391	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	199	ASN
1	A	243	ASN
1	A	337	HIS
1	B	69	GLN
1	B	207	ASN
1	B	236	ASN
1	B	243	ASN
1	B	276	GLN
1	B	385	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	A	501	1	50,50,50	1.36	7 (14%)	67,82,82	1.10	2 (2%)
3	TES	B	502	-	24,24,24	0.47	0	39,39,39	1.23	6 (15%)
2	HEM	B	501	1	50,50,50	1.41	6 (12%)	67,82,82	1.13	4 (5%)
3	TES	A	502	-	24,24,24	0.39	0	39,39,39	1.00	3 (7%)

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	A	501	1	-	1/14/54/54	-
3	TES	B	502	-	-	-	0/4/4/4
2	HEM	B	501	1	-	1/14/54/54	-
3	TES	A	502	-	-	-	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	FE-NB	4.13	2.07	1.94
2	B	501	HEM	FE-ND	3.60	2.06	1.94
2	A	501	HEM	FE-NB	3.39	2.05	1.94
2	A	501	HEM	CAC-C3C	3.05	1.55	1.47
2	B	501	HEM	CAC-C3C	2.99	1.55	1.47
2	A	501	HEM	FE-NA	2.84	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-ND	2.72	2.03	1.94
2	B	501	HEM	CAB-C3B	2.65	1.54	1.47
2	A	501	HEM	CAB-C3B	2.58	1.54	1.47
2	B	501	HEM	CMC-C2C	2.27	1.55	1.50
2	A	501	HEM	CMC-C2C	2.22	1.55	1.50
2	B	501	HEM	FE-NA	2.12	2.02	1.95
2	A	501	HEM	CMA-C3A	2.01	1.54	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	TES	C12-C11-C9	3.21	118.58	113.14
2	B	501	HEM	C3B-C4B-NB	-2.94	107.35	109.47
3	A	502	TES	C9-C10-C5	2.66	113.54	109.65
2	B	501	HEM	C1B-NB-C4B	2.65	108.34	105.21
3	B	502	TES	C11-C12-C13	2.64	117.20	112.74
3	B	502	TES	C11-C9-C10	2.64	116.34	113.08
3	A	502	TES	C1-C10-C9	-2.51	105.41	108.74
2	A	501	HEM	C3B-C4B-NB	-2.33	107.79	109.47
3	B	502	TES	C13-C14-C8	-2.33	111.10	114.41
3	B	502	TES	C15-C14-C8	2.28	122.74	119.10
2	A	501	HEM	C1B-NB-C4B	2.22	107.84	105.21
2	B	501	HEM	C4D-ND-C1D	2.21	107.82	105.21
3	B	502	TES	C14-C8-C9	-2.18	106.23	109.09
3	A	502	TES	C16-C17-C13	-2.16	102.82	104.52
2	B	501	HEM	C3B-C2B-C1B	2.00	107.92	106.41

There are no chirality outliers.

All (2) torsion outliers are listed below:

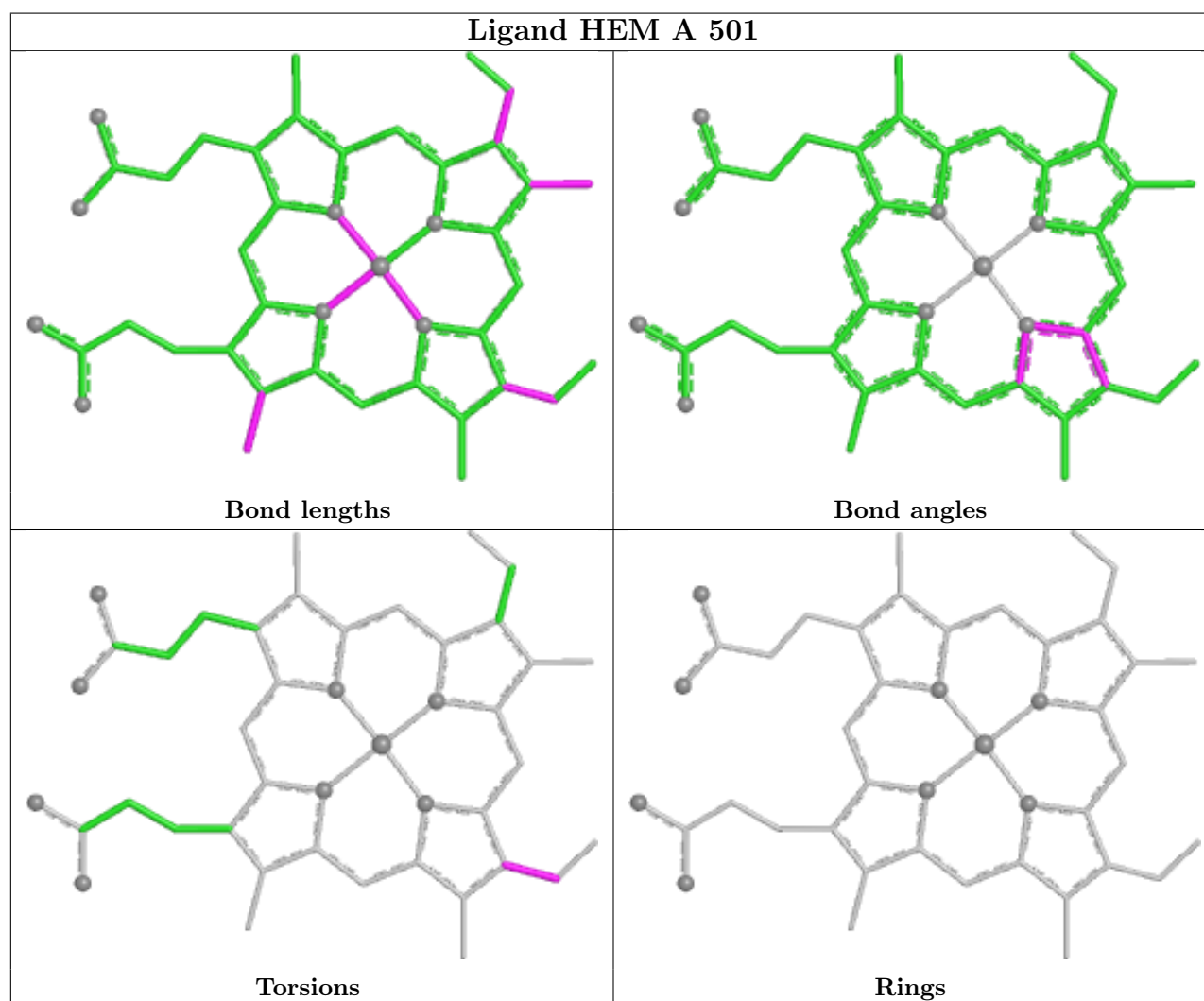
Mol	Chain	Res	Type	Atoms
2	B	501	HEM	C4B-C3B-CAB-CBB
2	A	501	HEM	C4B-C3B-CAB-CBB

There are no ring outliers.

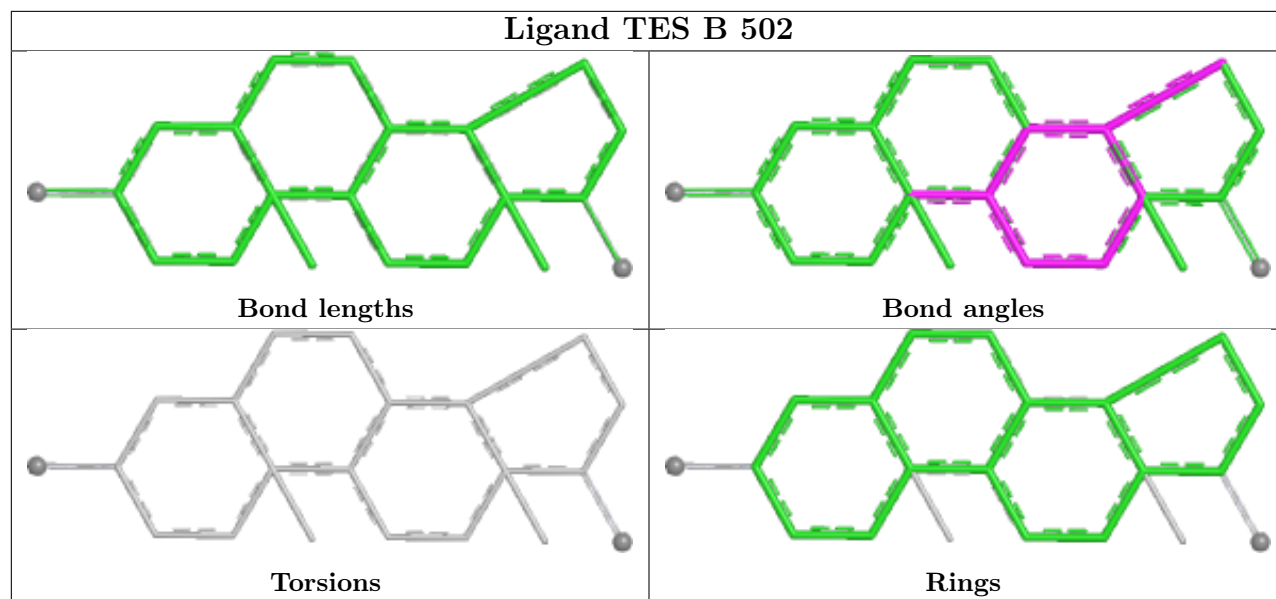
3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	5	0
3	B	502	TES	12	0
2	B	501	HEM	5	0

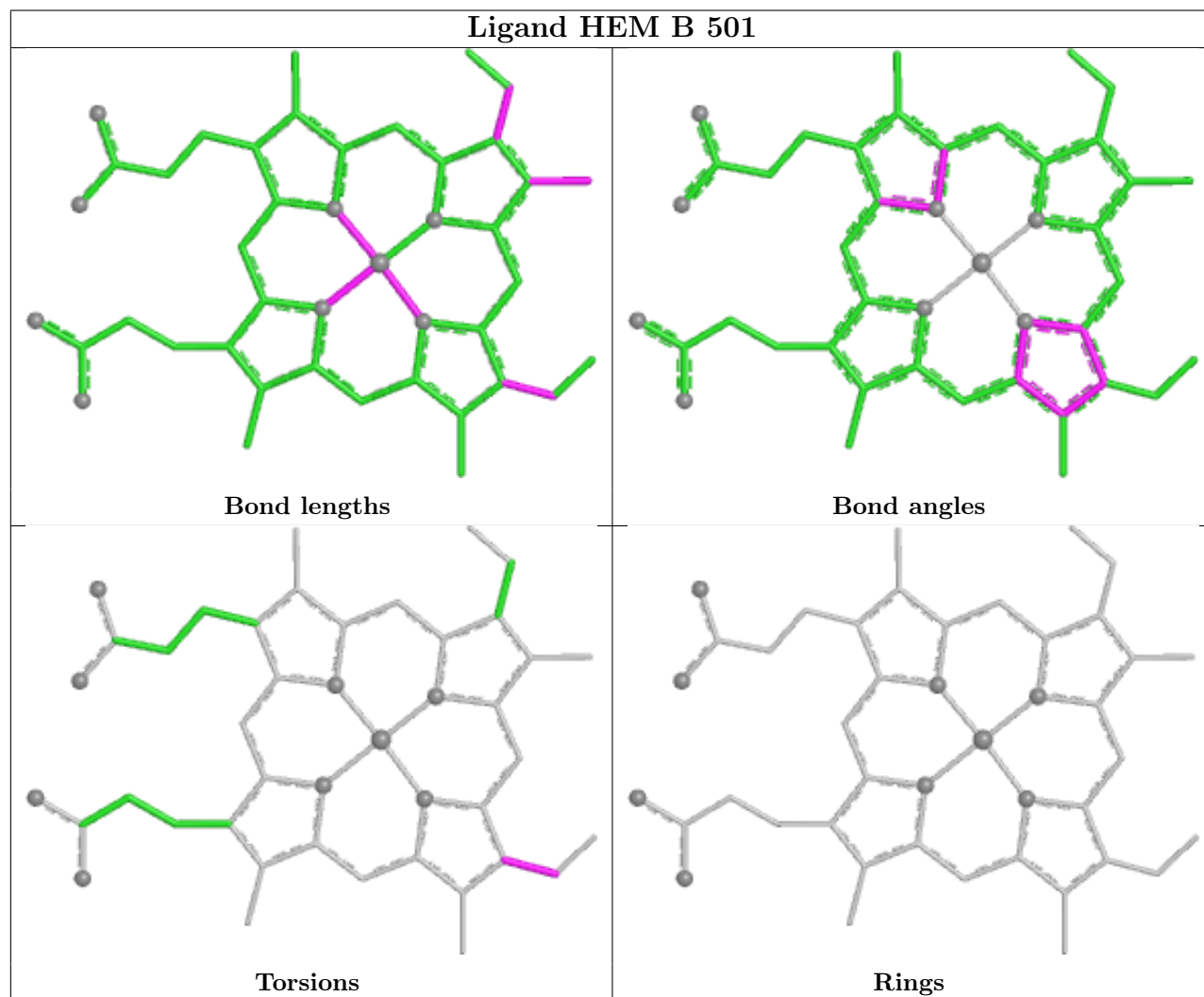
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

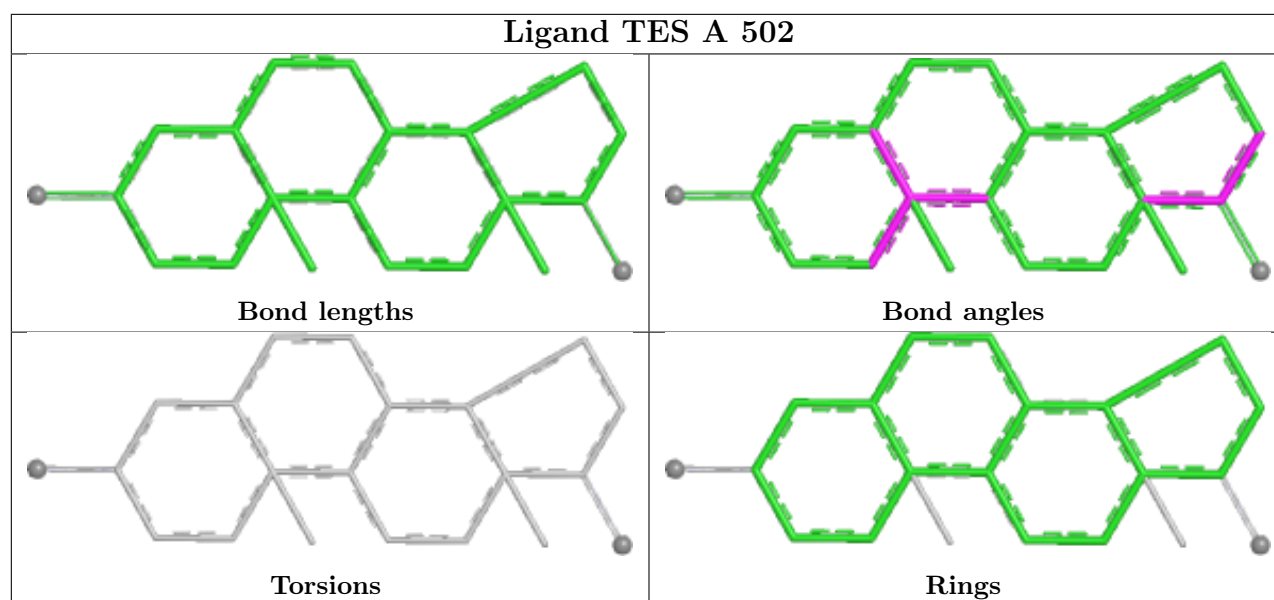


Ligand TES B 502



Ligand HEM B 501





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	377/406 (92%)	0.58	33 (8%) 15 16	34, 48, 86, 125	0
1	B	374/406 (92%)	0.75	36 (9%) 13 14	37, 56, 93, 123	0
All	All	751/812 (92%)	0.66	69 (9%) 14 15	34, 52, 89, 125	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	PHE	6.6
1	A	71	PRO	5.4
1	A	154	SER	4.9
1	B	301	ILE	4.9
1	A	323	GLU	4.7
1	A	388	MET	4.6
1	A	70	PHE	4.2
1	A	78	THR	4.2
1	B	384	ALA	4.1
1	B	388	MET	4.1
1	B	80	ALA	4.0
1	A	383	MET	3.9
1	A	386	SER	3.9
1	A	73	LEU	3.8
1	B	70	PHE	3.8
1	B	386	SER	3.7
1	A	384	ALA	3.4
1	B	385	ASN	3.3
1	B	71	PRO	3.3
1	B	387	SER	3.3
1	A	79	PHE	3.2
1	B	154	SER	3.2
1	A	385	ASN	3.1
1	B	302	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	387	SER	3.0
1	B	383	MET	3.0
1	A	24	TYR	2.9
1	A	80	ALA	2.9
1	A	157	LYS	2.8
1	B	179	VAL	2.7
1	A	179	VAL	2.7
1	A	180	MET	2.7
1	B	51	PHE	2.6
1	B	39	VAL	2.6
1	B	312	VAL	2.6
1	A	120	GLU	2.6
1	B	157	LYS	2.6
1	B	174	ALA	2.5
1	A	294	PHE	2.5
1	B	180	MET	2.4
1	A	183	ARG	2.4
1	B	168	VAL	2.4
1	B	296	GLN	2.4
1	B	311	GLY	2.3
1	B	129	ASP	2.3
1	A	175	TYR	2.3
1	B	380	THR	2.3
1	B	66	PHE	2.3
1	B	299	THR	2.3
1	B	120	GLU	2.3
1	A	38	PRO	2.2
1	A	72	GLN	2.2
1	A	74	GLU	2.2
1	A	35	LYS	2.2
1	A	389	TYR	2.2
1	B	85	SER	2.2
1	B	40	TYR	2.1
1	B	294	PHE	2.1
1	B	392	LYS	2.1
1	A	82	THR	2.1
1	B	183	ARG	2.1
1	B	22	ASP	2.1
1	A	296	GLN	2.1
1	B	330	HIS	2.1
1	A	311	GLY	2.1
1	A	174	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	338	PRO	2.0
1	A	178	ASP	2.0
1	B	306	LEU	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](#)

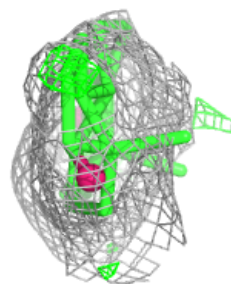
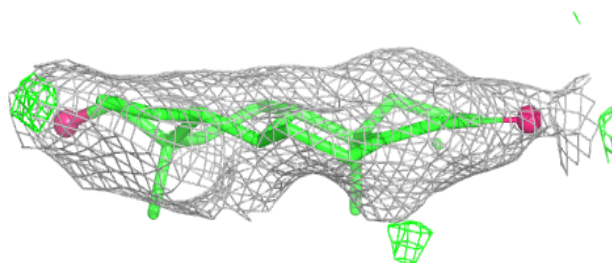
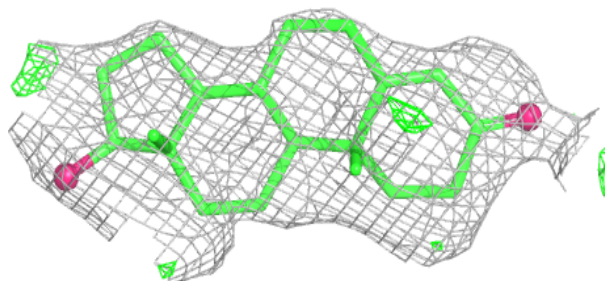
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TES	B	502	21/21	0.77	0.18	74,81,89,96	0
3	TES	A	502	21/21	0.84	0.11	44,57,71,75	0
2	HEM	A	501	43/43	0.96	0.09	30,38,42,48	0
2	HEM	B	501	43/43	0.96	0.09	33,43,51,56	0

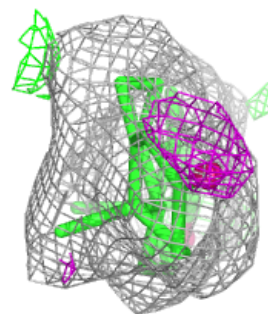
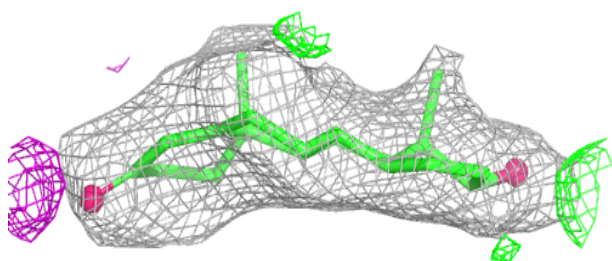
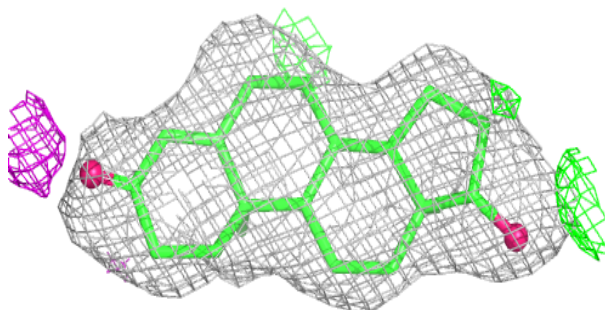
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TES 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)

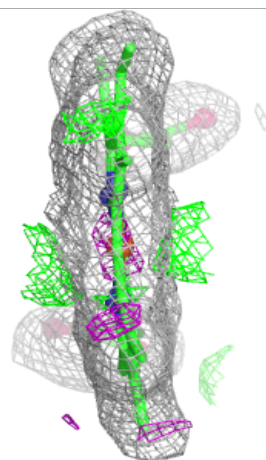
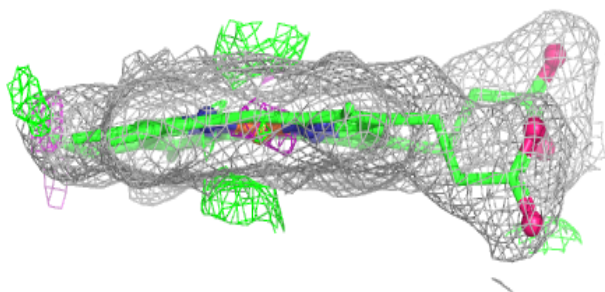
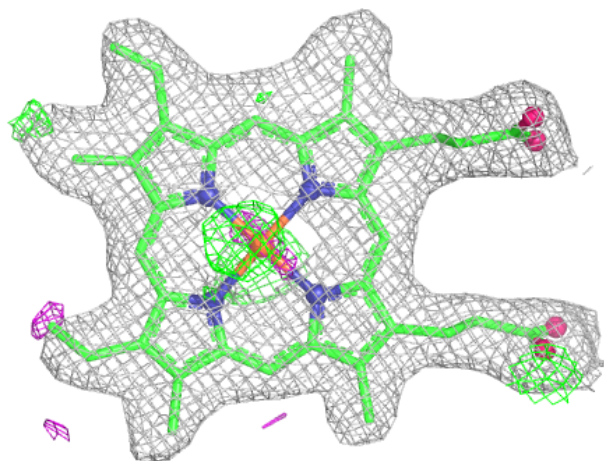
**Electron density around TES A 502:**

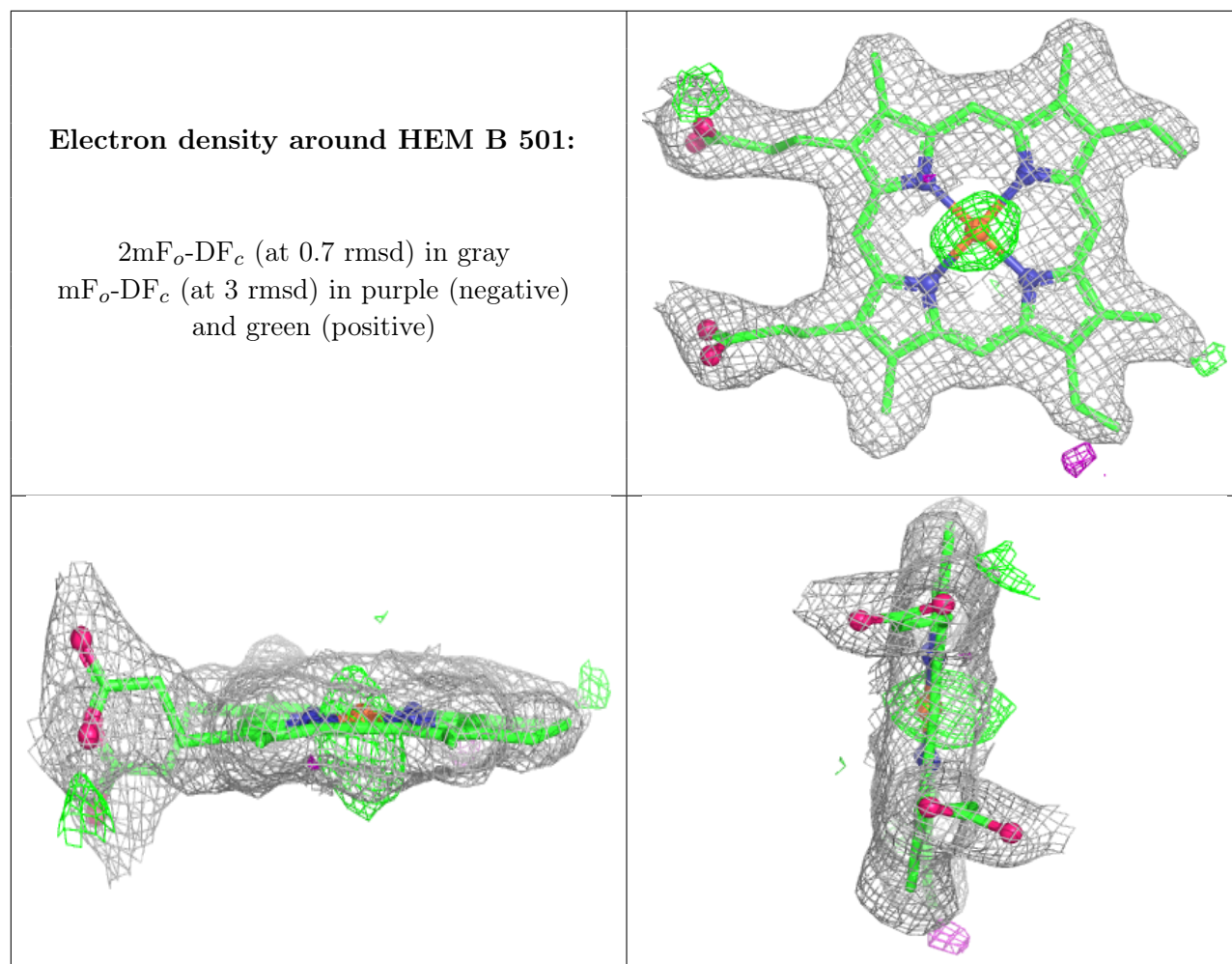
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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 ⓘ

There are no such residues in this entry.