



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:16 PM UTC

PDB ID : 2WV2 / pdb_00002wv2
Title : X-ray structure of CYP51 from the human pathogen *Trypanosoma brucei* in complex with fluconazole
Authors : Chen, C.-K.; Leung, S.S.F.; Guilbert, C.; Jacobson, M.; McKerrow, J.H.; Podust, L.M.
Deposited on : 2009-10-12
Resolution : 2.70 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

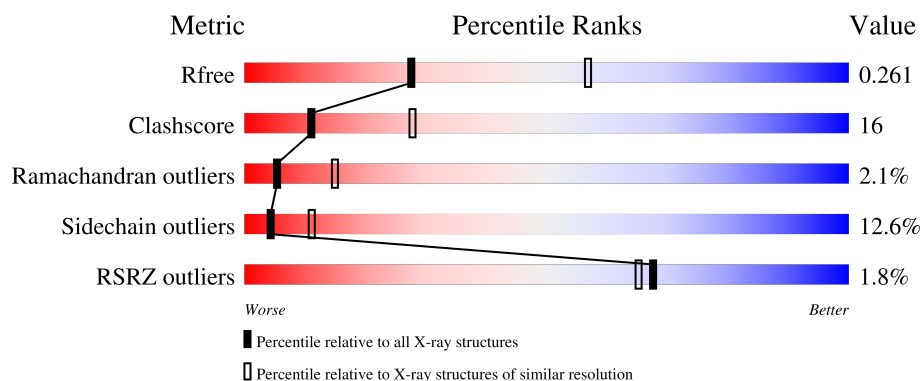
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	475	

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
2	TPF	A	1	-	X	-	-

2 Entry composition [i](#)

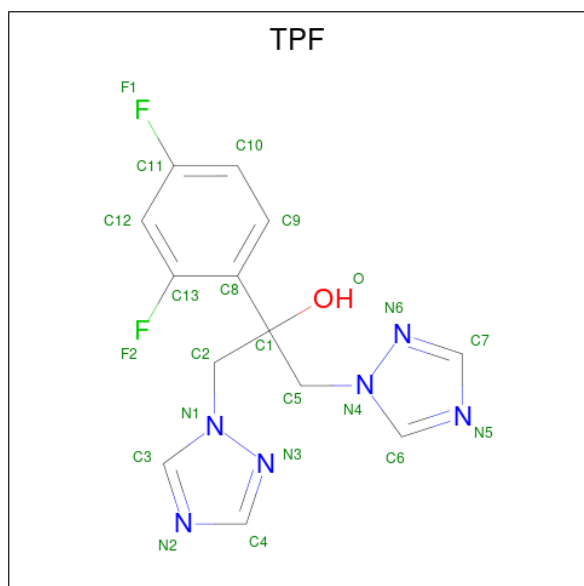
There are 4 unique types of molecules in this entry. The entry contains 3508 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LANOSTEROL 14-ALPHA-DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	443	3428	2192	594	615	27	0	0	0

- Molecule 2 is 2-(2,4-DIFLUOROPHENYL)-1,3-DI(1H-1,2,4-TRIAZOL-1-YL)PROPAN-2-OL (CCD ID: TPF) (formula: C₁₃H₁₂F₂N₆O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	22	13	2	6	1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

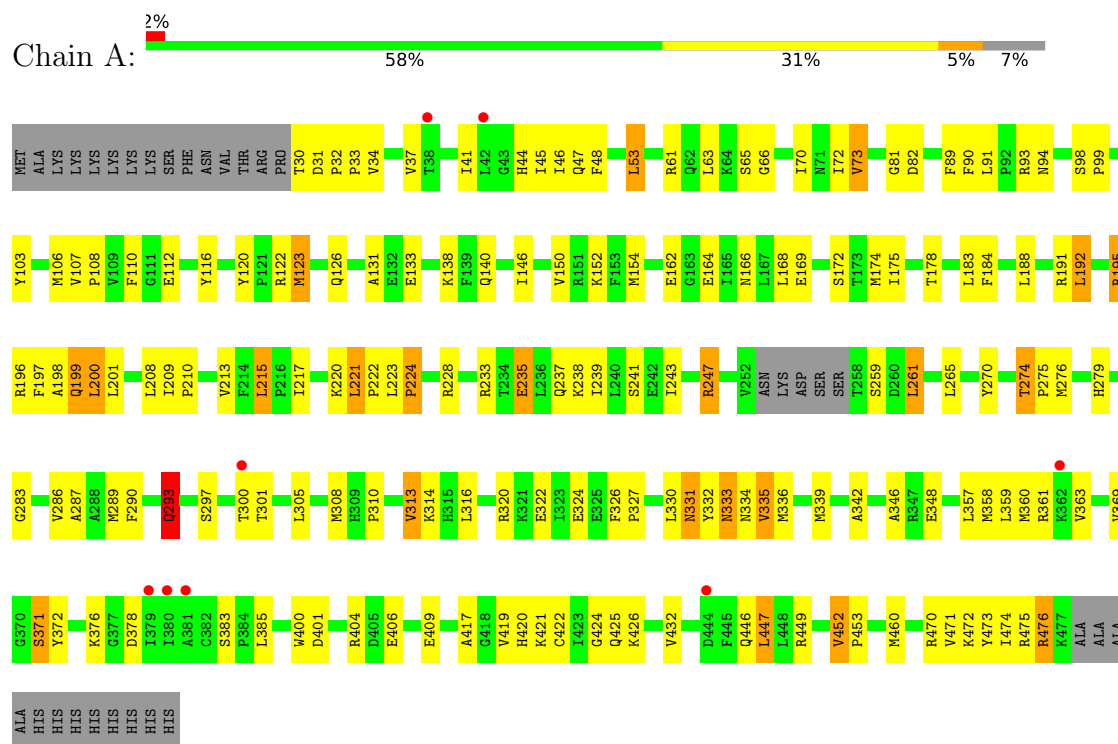
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		

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: LANOSTEROL 14-ALPHA-DEMETHYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.18Å 106.18Å 99.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	92.06 – 2.70 91.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (92.06-2.70) 96.2 (91.95-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.210 , 0.274 0.205 , 0.261	Depositor DCC
R_{free} test set	898 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	100.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3508	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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, TPF

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	0.96	2/3509 (0.1%)	1.17	12/4761 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	LEU	N-CA	-5.50	1.39	1.46
1	A	34	VAL	CA-CB	5.15	1.59	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	SER	N-CA-C	7.00	119.35	110.33
1	A	293	GLN	N-CA-C	6.65	119.36	111.71
1	A	152	LYS	N-CA-C	-6.10	103.97	112.45
1	A	346	ALA	N-CA-C	-5.88	104.78	111.07
1	A	360	MET	N-CA-C	5.47	118.00	109.52
1	A	146	ILE	N-CA-C	-5.39	105.35	110.42
1	A	383	SER	CA-C-N	-5.33	113.24	119.32
1	A	383	SER	C-N-CA	-5.33	113.24	119.32
1	A	120	TYR	N-CA-C	5.10	119.89	113.25
1	A	228	ARG	N-CA-C	-5.09	106.24	112.90
1	A	208	LEU	N-CA-C	5.03	116.94	109.25
1	A	91	LEU	N-CA-C	5.01	120.87	109.81

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	3428	0	3342	104	0
2	A	22	0	12	3	0
3	A	43	0	30	11	0
4	A	15	0	0	1	0
All	All	3508	0	3384	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 16.

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:335:VAL:HA	1:A:339:MET:HE3	1.50	0.90
3:A:1450:HEM:HMB2	3:A:1450:HEM:HBB2	1.58	0.85
1:A:237:GLN:NE2	1:A:279:HIS:HA	1.93	0.83
1:A:30:THR:O	1:A:372:TYR:HA	1.79	0.82
1:A:335:VAL:CA	1:A:339:MET:HE3	2.18	0.73
3:A:1450:HEM:HBB2	3:A:1450:HEM:CMB	2.19	0.72
1:A:320:ARG:O	1:A:324:GLU:HG2	1.89	0.72
1:A:327:PRO:HD2	1:A:334:ASN:HD21	1.54	0.72
1:A:270:TYR:HD1	1:A:274:THR:HG23	1.54	0.71
1:A:33:PRO:HB2	1:A:63:LEU:HD13	1.73	0.70
1:A:293:GLN:NE2	1:A:293:GLN:HA	2.07	0.69
1:A:192:LEU:HD21	1:A:197:PHE:CD1	2.27	0.69
1:A:327:PRO:HD2	1:A:334:ASN:ND2	2.08	0.69
1:A:221:LEU:CB	1:A:222:PRO:HD3	2.24	0.68
1:A:150:VAL:O	1:A:154:MET:HG3	1.93	0.68
1:A:331:ASN:ND2	1:A:334:ASN:OD1	2.27	0.66
1:A:172:SER:HA	1:A:297:SER:OG	1.94	0.66
1:A:166:ASN:HD22	1:A:169:GLU:H	1.40	0.66
1:A:348:GLU:HA	1:A:348:GLU:OE1	1.96	0.66
1:A:316:LEU:HD11	1:A:320:ARG:NH1	2.15	0.62
1:A:330:LEU:HD23	1:A:334:ASN:HD22	1.65	0.62
3:A:1450:HEM:HBD2	3:A:1450:HEM:HMD1	1.81	0.61
1:A:106:MET:HE1	1:A:290:PHE:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:MET:HE3	1:A:110:PHE:CZ	2.37	0.60
1:A:192:LEU:HD21	1:A:197:PHE:HD1	1.65	0.60
1:A:166:ASN:ND2	1:A:169:GLU:H	1.99	0.60
1:A:357:LEU:HD22	1:A:385:LEU:HD22	1.84	0.60
1:A:237:GLN:HE22	1:A:279:HIS:HA	1.68	0.59
1:A:422:CYS:HA	3:A:1450:HEM:CHA	2.33	0.59
1:A:310:PRO:O	1:A:313:VAL:HG22	2.03	0.59
1:A:401:ASP:O	1:A:404:ARG:HG2	2.03	0.58
1:A:363:VAL:HG12	1:A:376:LYS:HA	1.87	0.57
1:A:239:ILE:O	1:A:243:ILE:HG12	2.04	0.57
1:A:72:ILE:HG22	1:A:73:VAL:HG23	1.86	0.56
1:A:327:PRO:CD	1:A:334:ASN:HD21	2.17	0.56
1:A:184:PHE:HB3	1:A:188:LEU:HB3	1.86	0.56
1:A:221:LEU:CB	1:A:222:PRO:CD	2.83	0.56
2:A:1:TPF:F2	2:A:1:TPF:O	2.08	0.56
1:A:369:VAL:O	1:A:371:SER:O	2.25	0.55
1:A:316:LEU:HD11	1:A:320:ARG:HH11	1.72	0.55
1:A:452:VAL:HG13	1:A:453:PRO:HD2	1.90	0.54
1:A:348:GLU:HG3	1:A:400:TRP:CD1	2.43	0.54
1:A:332:TYR:CE1	1:A:336:MET:HG3	2.43	0.53
1:A:331:ASN:HD22	1:A:331:ASN:C	2.17	0.53
2:A:1:TPF:O	2:A:1:TPF:C3	2.58	0.52
1:A:422:CYS:HA	3:A:1450:HEM:C4D	2.45	0.51
1:A:122:ARG:O	1:A:126:GLN:HG3	2.10	0.51
1:A:420:HIS:ND1	3:A:1450:HEM:O1D	2.41	0.51
1:A:131:ALA:C	1:A:133:GLU:H	2.18	0.51
1:A:61:ARG:HD3	4:A:2001:HOH:O	2.10	0.51
1:A:322:GLU:CD	1:A:339:MET:HA	2.37	0.50
1:A:90:PHE:CG	1:A:417:ALA:HB3	2.47	0.50
3:A:1450:HEM:CHD	3:A:1450:HEM:HBC2	2.41	0.50
1:A:166:ASN:ND2	1:A:168:LEU:H	2.09	0.50
2:A:1:TPF:O	2:A:1:TPF:HC3	2.12	0.49
1:A:195:ARG:O	1:A:196:ARG:C	2.55	0.49
1:A:168:LEU:O	1:A:172:SER:HB2	2.13	0.49
1:A:237:GLN:HE21	1:A:279:HIS:HA	1.77	0.49
1:A:200:LEU:HD11	1:A:235:GLU:HG2	1.95	0.48
1:A:243:ILE:O	1:A:247:ARG:HB2	2.13	0.48
1:A:417:ALA:HA	1:A:421:LYS:HD2	1.95	0.47
1:A:289:MET:HE3	1:A:289:MET:HA	1.96	0.47
1:A:286:VAL:O	1:A:287:ALA:C	2.55	0.47
1:A:198:ALA:O	1:A:199:GLN:C	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LEU:CD2	1:A:334:ASN:HD22	2.27	0.47
3:A:1450:HEM:HBC2	3:A:1450:HEM:HH2	1.97	0.46
1:A:210:PRO:O	1:A:213:VAL:HG23	2.15	0.46
1:A:371:SER:O	1:A:372:TYR:HB2	2.15	0.46
1:A:48:PHE:CD2	1:A:48:PHE:C	2.93	0.46
1:A:32:PRO:HA	1:A:372:TYR:CD1	2.51	0.46
1:A:32:PRO:HA	1:A:372:TYR:CE1	2.50	0.46
1:A:223:LEU:N	1:A:224:PRO:HD3	2.31	0.46
1:A:73:VAL:HG11	1:A:215:LEU:HD11	1.97	0.45
1:A:308:MET:SD	1:A:447:LEU:HD13	2.56	0.45
1:A:473:TYR:C	1:A:473:TYR:CD1	2.95	0.45
1:A:265:LEU:O	1:A:276:MET:HE3	2.16	0.45
1:A:327:PRO:CG	1:A:334:ASN:HD21	2.30	0.45
1:A:476:ARG:H	1:A:476:ARG:HG2	1.68	0.44
1:A:70:ILE:HD11	1:A:72:ILE:HD11	1.99	0.43
3:A:1450:HEM:HMB2	3:A:1450:HEM:CBB	2.39	0.43
1:A:191:ARG:O	1:A:196:ARG:HD2	2.17	0.43
1:A:424:GLY:HA3	3:A:1450:HEM:C3C	2.54	0.43
1:A:37:VAL:HG22	1:A:44:HIS:HE1	1.82	0.43
1:A:103:TYR:HD2	1:A:116:TYR:CD2	2.36	0.43
1:A:300:THR:OG1	1:A:432:VAL:HG22	2.19	0.43
1:A:89:PHE:CZ	1:A:361:ARG:HG2	2.53	0.43
1:A:107:VAL:N	1:A:108:PRO:CD	2.82	0.43
1:A:233:ARG:HH21	1:A:279:HIS:CE1	2.36	0.43
1:A:131:ALA:C	1:A:133:GLU:N	2.76	0.43
1:A:270:TYR:HD1	1:A:274:THR:CG2	2.28	0.43
1:A:94:ASN:ND2	1:A:123:MET:HE1	2.33	0.43
1:A:73:VAL:HG12	1:A:73:VAL:O	2.19	0.43
1:A:331:ASN:O	1:A:332:TYR:C	2.61	0.43
1:A:322:GLU:OE1	1:A:339:MET:HA	2.19	0.42
1:A:335:VAL:HB	1:A:339:MET:CE	2.50	0.42
1:A:166:ASN:ND2	1:A:168:LEU:N	2.67	0.42
1:A:183:LEU:HD13	1:A:261:LEU:HD12	2.02	0.42
1:A:174:MET:O	1:A:178:THR:HG23	2.20	0.41
1:A:72:ILE:CG2	1:A:73:VAL:HG23	2.50	0.41
1:A:326:PHE:CE2	1:A:339:MET:HE2	2.56	0.41
1:A:98:SER:HA	1:A:99:PRO:HD3	1.86	0.41
1:A:301:THR:O	1:A:305:LEU:HG	2.20	0.41
1:A:333:ASN:HD22	1:A:333:ASN:N	2.18	0.41
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.83	0.41
1:A:82:ASP:OD1	1:A:82:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLU:HB3	1:A:470:ARG:HE	1.85	0.41
1:A:175:ILE:HD13	1:A:175:ILE:HA	1.90	0.41
1:A:66:GLY:O	1:A:81:GLY:N	2.54	0.41
1:A:335:VAL:HA	1:A:339:MET:CE	2.37	0.41
1:A:339:MET:HB3	1:A:342:ALA:HB3	2.03	0.41
1:A:283:GLY:HA2	1:A:286:VAL:HG22	2.03	0.40
1:A:138:LYS:C	1:A:140:GLN:H	2.30	0.40
1:A:422:CYS:HB2	3:A:1450:HEM:C1A	2.56	0.40

There are no symmetry-related clashes.

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	439/475 (92%)	392 (89%)	38 (9%)	9 (2%)	5 15

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	A	220	LYS
1	A	65	SER
1	A	476	ARG
1	A	73	VAL
1	A	195	ARG
1	A	221	LEU
1	A	224	PRO
1	A	275	PRO

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	356/413 (86%)	311 (87%)	45 (13%)	4 11

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	45	ILE
1	A	46	ILE
1	A	47	GLN
1	A	53	LEU
1	A	93	ARG
1	A	112	GLU
1	A	123	MET
1	A	162	GLU
1	A	192	LEU
1	A	199	GLN
1	A	200	LEU
1	A	201	LEU
1	A	209	ILE
1	A	215	LEU
1	A	217	ILE
1	A	235	GLU
1	A	238	LYS
1	A	241	SER
1	A	247	ARG
1	A	261	LEU
1	A	274	THR
1	A	293	GLN
1	A	313	VAL
1	A	314	LYS
1	A	331	ASN
1	A	333	ASN
1	A	335	VAL
1	A	358	MET
1	A	371	SER

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Mol	Chain	Res	Type
1	A	378	ASP
1	A	406	GLU
1	A	409	GLU
1	A	419	VAL
1	A	425	GLN
1	A	426	LYS
1	A	446	GLN
1	A	447	LEU
1	A	449	ARG
1	A	452	VAL
1	A	460	MET
1	A	471	VAL
1	A	472	LYS
1	A	474	ILE
1	A	475	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	94	ASN
1	A	157	ASN
1	A	166	ASN
1	A	237	GLN
1	A	293	GLN
1	A	331	ASN
1	A	333	ASN
1	A	334	ASN
1	A	425	GLN
1	A	431	GLN

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](#)

2 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$
3	HEM	A	1450	2,1	50,50,50	1.67	11 (22%)	67,82,82	1.95	22 (32%)
2	TPF	A	1	3	24,24,24	2.84	13 (54%)	34,34,34	4.37	24 (70%)

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
3	HEM	A	1450	2,1	-	2/14/54/54	-
2	TPF	A	1	3	-	8/16/16/16	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	TPF	C8-C13	6.59	1.48	1.39
3	A	1450	HEM	C3D-C2D	5.55	1.48	1.36
2	A	1	TPF	C5-C1	4.60	1.60	1.54
2	A	1	TPF	N4-N6	4.50	1.44	1.36
2	A	1	TPF	N1-N3	4.06	1.43	1.36
2	A	1	TPF	C7-N6	3.69	1.38	1.32
3	A	1450	HEM	C3C-C2C	-3.66	1.29	1.37
2	A	1	TPF	C1-C8	-3.27	1.49	1.53
2	A	1	TPF	C10-C9	3.13	1.43	1.38
2	A	1	TPF	C6-N4	3.01	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1450	HEM	CHC-C4B	-3.00	1.32	1.39
2	A	1	TPF	C4-N3	2.84	1.37	1.32
3	A	1450	HEM	C1C-NC	-2.79	1.34	1.39
2	A	1	TPF	C7-N5	2.71	1.41	1.35
3	A	1450	HEM	CHC-C1C	-2.60	1.33	1.38
3	A	1450	HEM	O1D-CGD	2.56	1.30	1.22
2	A	1	TPF	C10-C11	2.54	1.42	1.37
2	A	1	TPF	C6-N5	2.53	1.38	1.32
3	A	1450	HEM	FE-NA	2.43	2.03	1.95
3	A	1450	HEM	C4D-ND	-2.42	1.36	1.40
3	A	1450	HEM	C4B-NB	-2.37	1.34	1.38
2	A	1	TPF	C4-N2	2.34	1.40	1.35
3	A	1450	HEM	C1A-NA	-2.28	1.35	1.39
3	A	1450	HEM	CHA-C1A	-2.09	1.34	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	TPF	C1-C8-C13	-13.64	110.76	122.83
2	A	1	TPF	C2-N1-N3	-6.96	111.13	121.25
2	A	1	TPF	C9-C10-C11	6.77	125.33	118.38
2	A	1	TPF	C1-C5-N4	-6.00	104.22	112.34
2	A	1	TPF	F2-C13-C8	-5.70	112.75	119.01
2	A	1	TPF	C10-C9-C8	-5.57	111.73	122.02
2	A	1	TPF	C5-N4-N6	-5.39	113.42	121.25
2	A	1	TPF	C3-N1-N3	5.35	116.76	109.39
2	A	1	TPF	C5-C1-C8	-5.10	97.95	110.83
3	A	1450	HEM	C4A-CHB-C1B	-5.03	114.43	126.25
3	A	1450	HEM	CHC-C4B-NB	4.62	129.40	124.42
2	A	1	TPF	C1-C2-N1	-4.58	106.14	112.34
2	A	1	TPF	N1-C3-N2	-4.35	101.42	110.42
2	A	1	TPF	C9-C8-C13	4.31	122.34	116.28
3	A	1450	HEM	C4D-ND-C1D	4.23	110.22	105.21
3	A	1450	HEM	C4C-CHD-C1D	-3.96	117.61	126.02
2	A	1	TPF	C9-C8-C1	3.88	126.08	120.94
3	A	1450	HEM	CBC-CAC-C3C	-3.73	108.89	127.53
2	A	1	TPF	C3-N2-C4	3.58	112.54	102.85
3	A	1450	HEM	CHC-C1C-NC	3.44	128.19	124.45
2	A	1	TPF	C6-N4-N6	3.33	113.99	109.39
2	A	1	TPF	O-C1-C2	-3.28	100.58	108.18
2	A	1	TPF	O-C1-C5	3.26	115.74	108.18
2	A	1	TPF	N4-C6-N5	-3.23	103.75	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1450	HEM	C4C-C3C-C2C	3.19	109.58	106.81
2	A	1	TPF	C13-C12-C11	-3.07	113.41	116.67
3	A	1450	HEM	CMC-C2C-C1C	2.87	129.78	124.73
2	A	1	TPF	C2-C1-C8	2.79	117.87	110.83
3	A	1450	HEM	CHA-C4D-ND	2.75	127.76	124.37
3	A	1450	HEM	CHD-C4C-C3C	2.63	129.64	125.21
3	A	1450	HEM	C1A-CHA-C4D	2.61	132.38	126.25
3	A	1450	HEM	CBA-CAA-C2A	-2.57	105.42	112.53
2	A	1	TPF	C6-N5-C7	2.51	109.64	102.85
3	A	1450	HEM	C1C-CHC-C4B	2.48	131.29	126.02
3	A	1450	HEM	O2A-CGA-CBA	2.45	121.73	114.00
3	A	1450	HEM	CHC-C4B-C3B	-2.43	120.23	125.07
2	A	1	TPF	C5-C1-C2	2.38	113.97	109.06
3	A	1450	HEM	CAC-C3C-C2C	-2.33	120.85	128.43
3	A	1450	HEM	CAD-C3D-C4D	2.33	128.76	124.70
2	A	1	TPF	F2-C13-C12	2.32	123.28	118.64
3	A	1450	HEM	CBB-CAB-C3B	-2.27	116.21	127.53
3	A	1450	HEM	O1A-CGA-CBA	-2.26	115.94	123.09
3	A	1450	HEM	C4B-C3B-C2B	2.16	109.27	107.28
3	A	1450	HEM	CHC-C1C-C2C	-2.10	121.11	125.49
2	A	1	TPF	N3-C4-N2	-2.08	108.97	114.90
3	A	1450	HEM	CMA-C3A-C4A	-2.05	122.30	125.42

There are no chirality outliers.

All (10) torsion outliers are listed below:

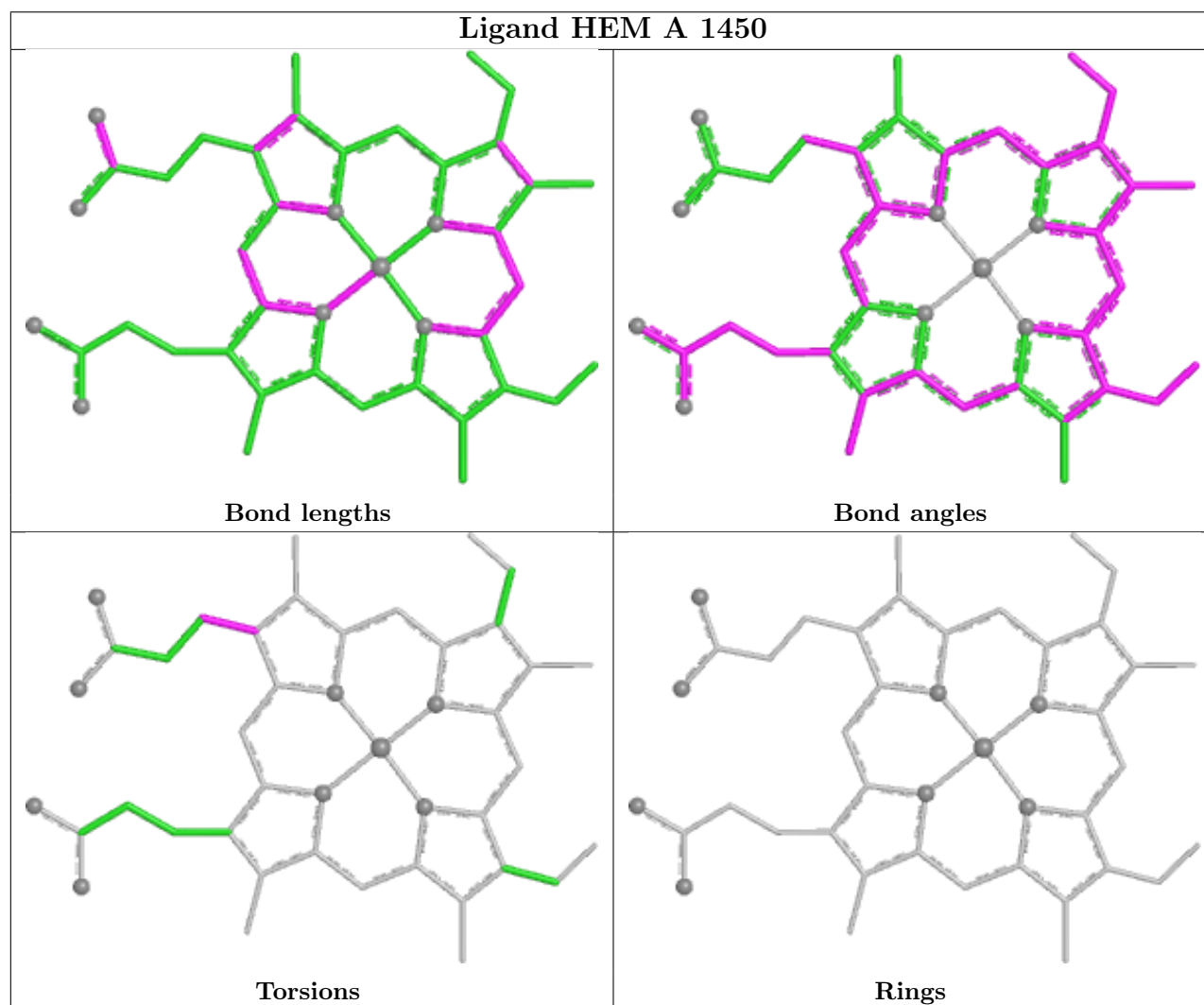
Mol	Chain	Res	Type	Atoms
2	A	1	TPF	O-C1-C8-C13
2	A	1	TPF	C2-C1-C8-C9
2	A	1	TPF	C2-C1-C8-C13
2	A	1	TPF	C5-C1-C8-C9
2	A	1	TPF	C1-C2-N1-C3
2	A	1	TPF	C1-C2-N1-N3
3	A	1450	HEM	C4D-C3D-CAD-CBD
2	A	1	TPF	O-C1-C8-C9
3	A	1450	HEM	C2D-C3D-CAD-CBD
2	A	1	TPF	C5-C1-C8-C13

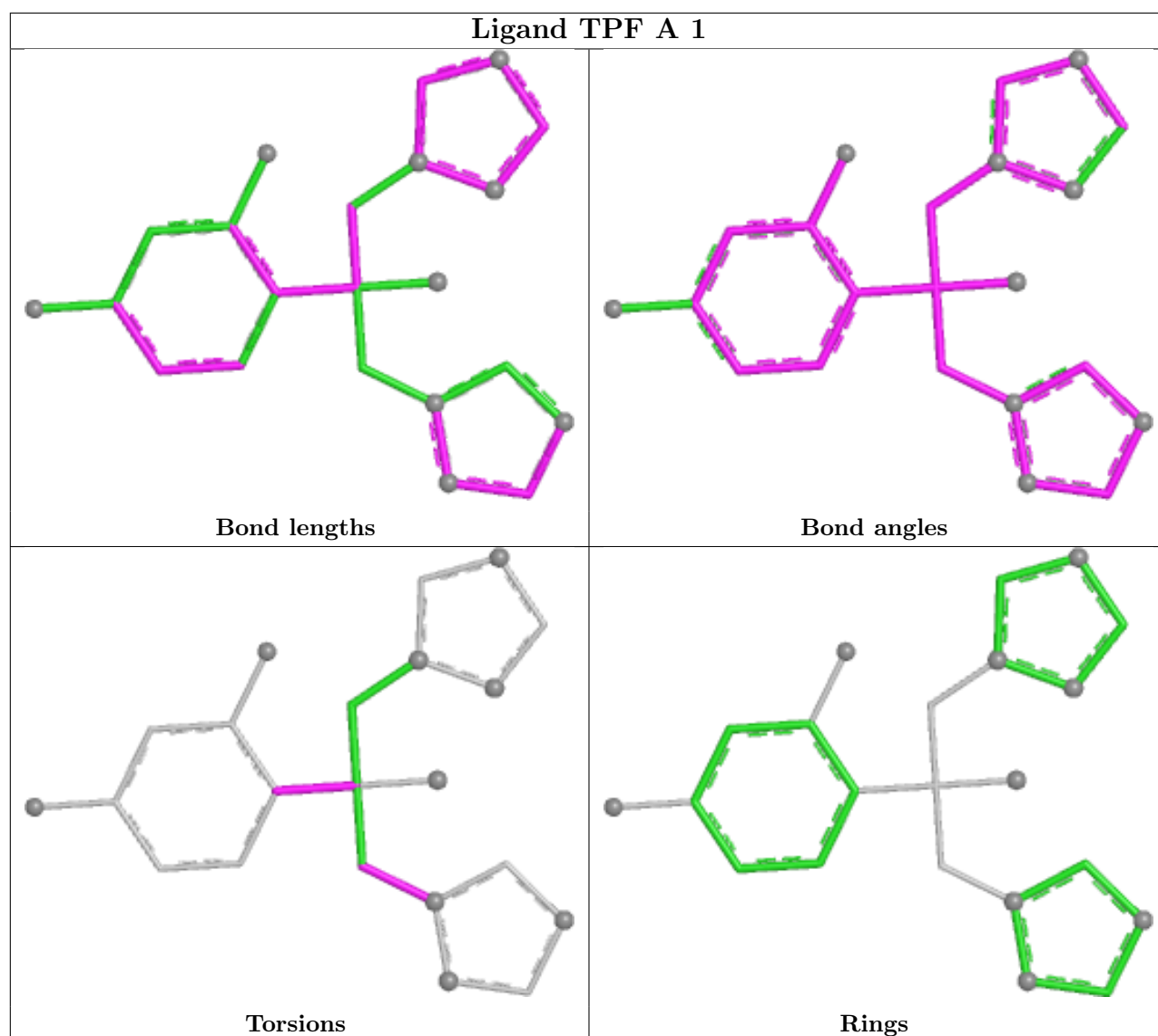
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1450	HEM	11	0
2	A	1	TPF	3	0

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





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	443/475 (93%)	-0.01	8 (1%) 67 65	33, 45, 57, 81	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	THR	3.9
1	A	381	ALA	2.7
1	A	444	ASP	2.6
1	A	300	THR	2.6
1	A	380	ILE	2.5
1	A	362	LYS	2.4
1	A	42	LEU	2.4
1	A	379	ILE	2.1

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](#)

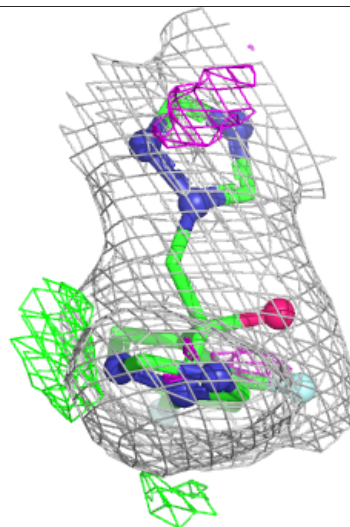
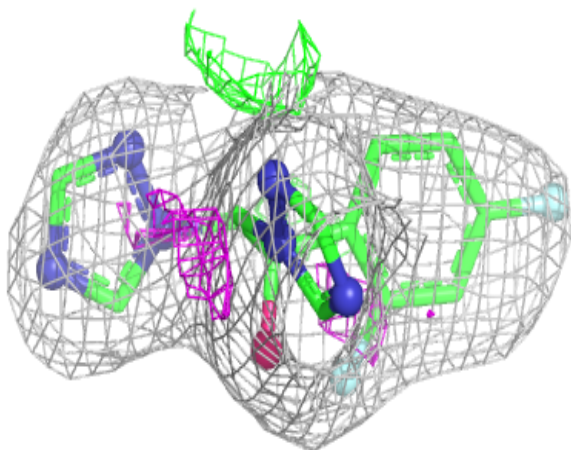
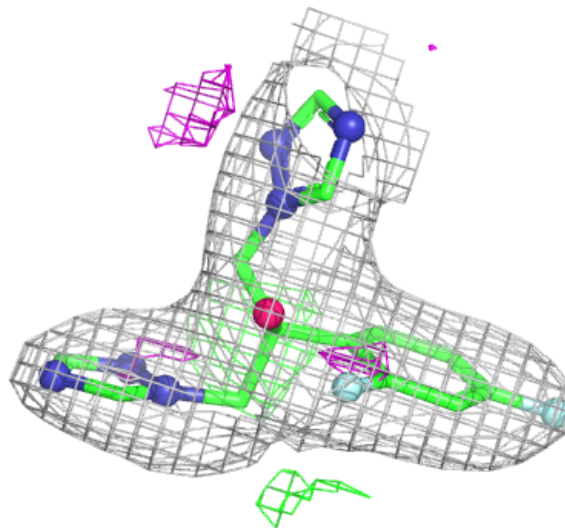
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TPF	A	1	22/22	0.84	0.09	62,67,82,85	0
3	HEM	A	1450	43/43	0.98	0.07	49,55,65,72	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.

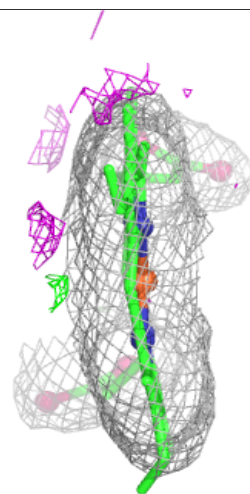
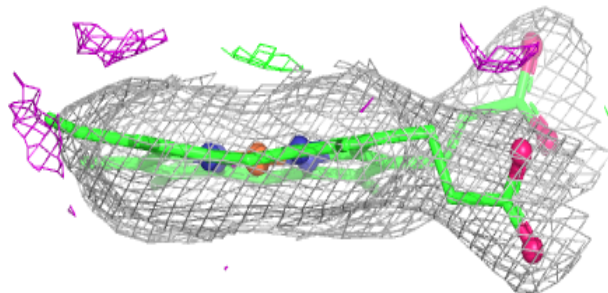
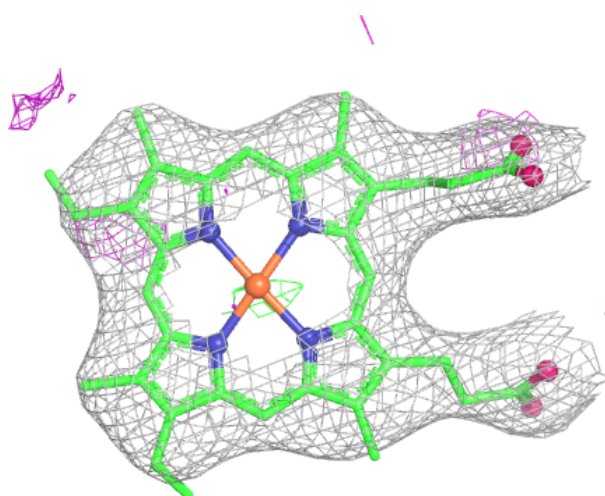
Electron density around TPF A 1:

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 1450:

$2mF_o-DF_c$ (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.