Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2026 – 01:43 AM EDT

PDB ID	:	6AY4 / pdb_00006ay4
Title	:	Naegleria fowleri CYP51-fluconazole complex
Authors	:	Debnath, A.; Calvet, C.M.; Jennings, G.; Zhou, W.; Aksenov, A.; Luth, M.; Abagyan, R.; Nes, W.D.; McKerrow, J.H.; Podust, L.M.
Deposited on	:	2017-09-07
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 (i) 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 (i)) were used in the production of this report:

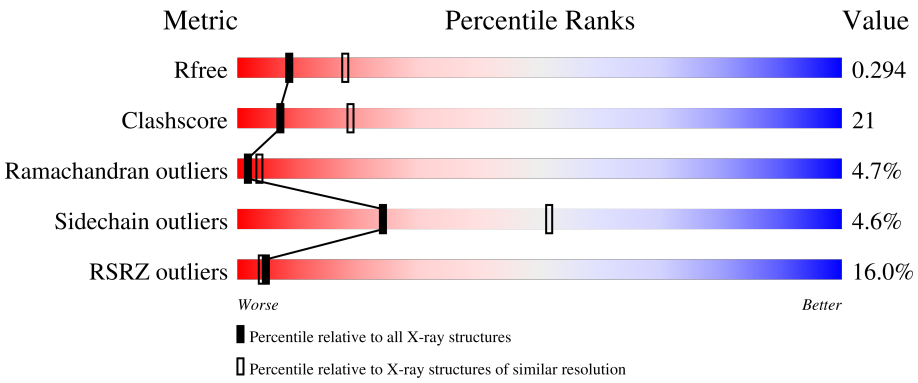
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

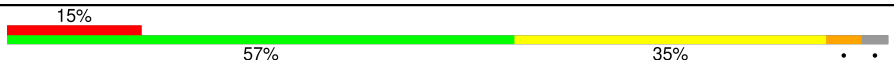
The reported resolution of this entry is 2.70 Å.

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 <=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	466	

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	TPF	A	506	-	-	X	-

2 Entry composition (i)

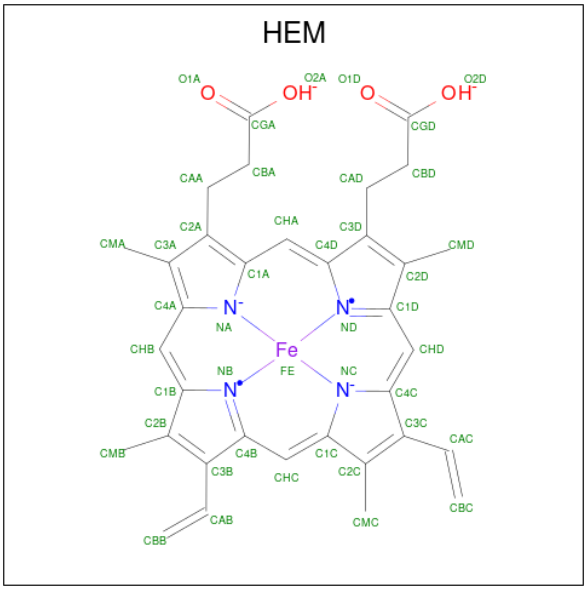
There are 5 unique types of molecules in this entry. The entry contains 3670 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYP51, sterol 14alpha-demethylase.

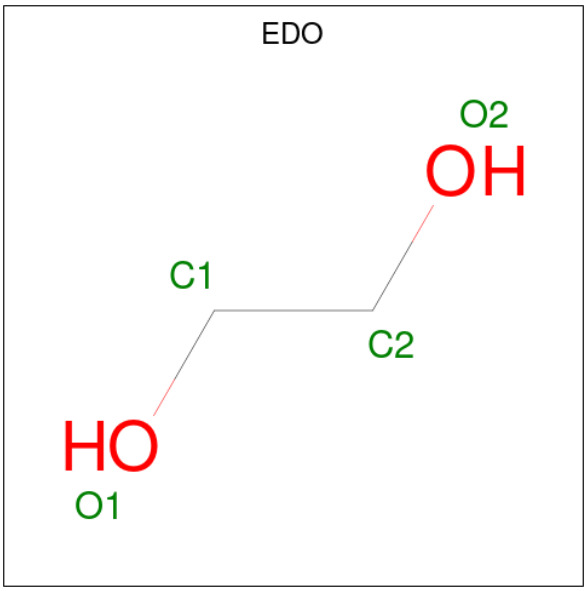
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	3584	2302	605	655	22	0	0	0

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



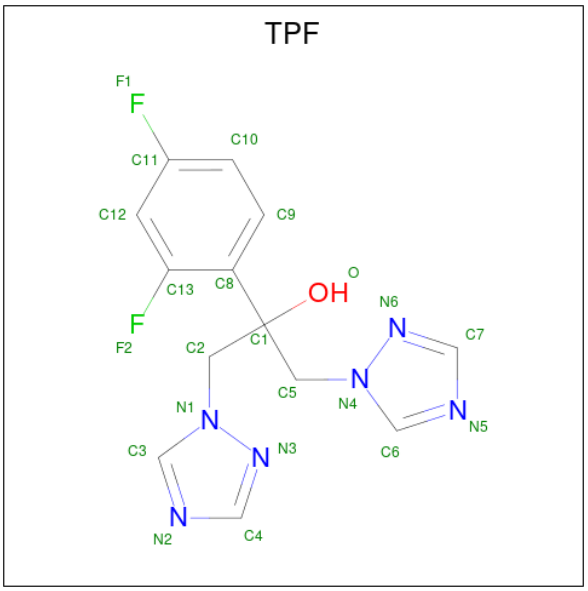
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0
			Total	C	O		
3	A	1	4	2	2	0	0

- Molecule 4 is 2-(2,4-DIFLUOROPHENYL)-1,3-DI(1H-1,2,4-TRIAZOL-1-YL)PROPAN-2-OL (CCD ID: TPF) (formula: $C_{13}H_{12}F_2N_6O$).



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

- Molecule 5 is water.

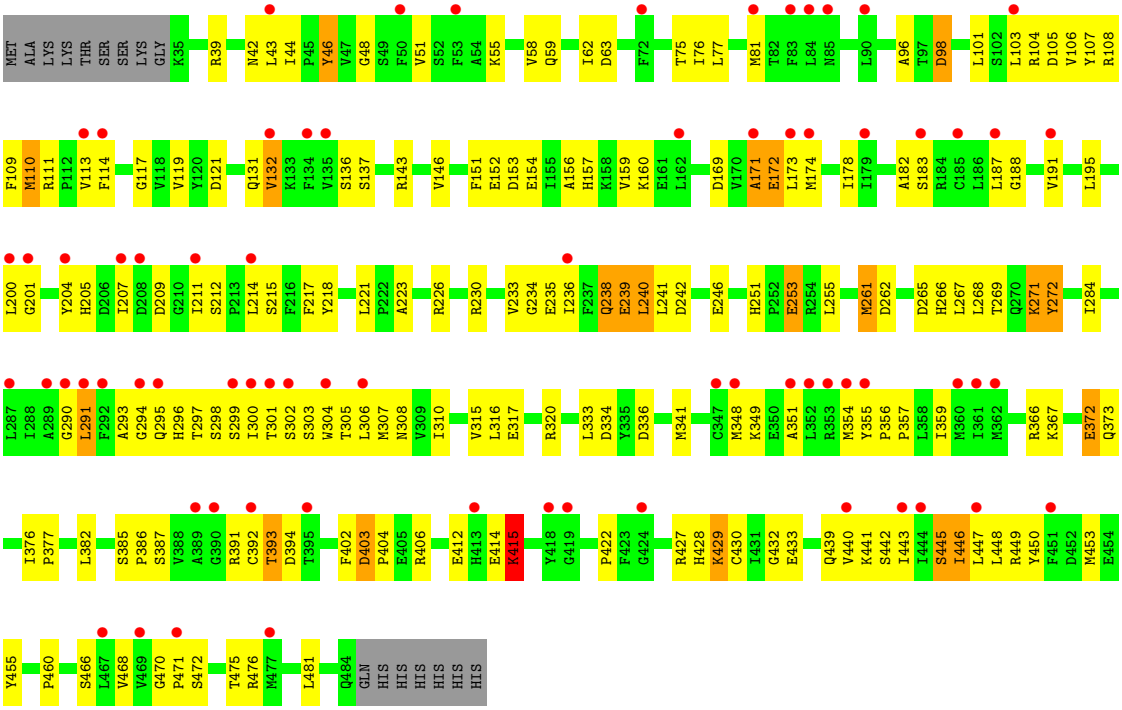
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	5	5	5	0	0

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: CYP51, sterol 14alpha-demethylase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	122.11Å 55.31Å 73.49Å 90.00° 101.52° 90.00°	Depositor
Resolution (Å)	72.01 – 2.70 72.01 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (72.01-2.70) 97.7 (72.01-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.257 , 0.313 0.242 , 0.294	Depositor DCC
R_{free} test set	665 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å^2)	93.2	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 85.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3670	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: TPF, EDO, 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	0.57	0/3662	0.88	8/4945 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	470	GLY	CA-C-N	-6.39	113.20	119.78
1	A	470	GLY	C-N-CA	-6.39	113.20	119.78
1	A	372	GLU	CB-CA-C	-5.85	109.85	116.63
1	A	367	LYS	CA-C-N	-5.43	114.99	120.31
1	A	367	LYS	C-N-CA	-5.43	114.99	120.31
1	A	223	ALA	CA-C-N	5.21	124.66	119.24
1	A	223	ALA	C-N-CA	5.21	124.66	119.24
1	A	367	LYS	N-CA-C	-5.12	104.17	110.31

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3584	0	3599	142	0
2	A	43	0	30	13	0
3	A	16	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	22	0	12	9	0
5	A	5	0	0	1	0
All	All	3670	0	3665	152	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 21.

All (152) 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:304:TRP:CD2	1:A:471:PRO:HG3	2.02	0.94
1:A:304:TRP:CH2	1:A:471:PRO:HB3	2.04	0.93
1:A:271:LYS:O	1:A:272:TYR:O	1.93	0.87
1:A:255:LEU:O	1:A:261:MET:HE1	1.76	0.85
1:A:304:TRP:CE2	1:A:471:PRO:HG3	2.11	0.85
1:A:304:TRP:CZ2	1:A:471:PRO:HB3	2.16	0.81
1:A:430:CYS:SG	2:A:501:HEM:NC	2.55	0.79
1:A:106:VAL:HG23	1:A:107:TYR:CD2	2.22	0.75
1:A:307:MET:HE1	1:A:475:THR:HG21	1.70	0.73
1:A:117:GLY:HA2	1:A:121:ASP:O	1.91	0.70
1:A:303:SER:O	1:A:307:MET:HG3	1.93	0.69
2:A:501:HEM:NC	4:A:506:TPF:HC7	2.06	0.68
1:A:333:LEU:HD11	1:A:341:MET:HE1	1.74	0.68
1:A:304:TRP:CE2	1:A:471:PRO:CG	2.76	0.68
1:A:430:CYS:SG	2:A:501:HEM:ND	2.70	0.65
1:A:271:LYS:O	1:A:272:TYR:C	2.40	0.65
1:A:238:GLN:O	1:A:239:GLU:C	2.40	0.64
1:A:96:ALA:O	1:A:427:ARG:NH1	2.31	0.64
1:A:304:TRP:CZ2	1:A:471:PRO:CB	2.81	0.64
1:A:376:ILE:HG21	1:A:382:LEU:HD11	1.80	0.63
1:A:334:ASP:OD1	1:A:334:ASP:C	2.42	0.62
1:A:304:TRP:NE1	1:A:471:PRO:HD3	2.14	0.62
1:A:290:GLY:O	1:A:293:ALA:N	2.33	0.61
1:A:239:GLU:O	1:A:242:ASP:N	2.34	0.61
1:A:445:SER:O	1:A:446:ILE:C	2.41	0.61
1:A:271:LYS:C	1:A:272:TYR:O	2.44	0.60
1:A:114:PHE:O	1:A:230:ARG:NH2	2.27	0.60
1:A:403:ASP:O	1:A:403:ASP:CG	2.43	0.60
2:A:501:HEM:C1C	4:A:506:TPF:HC7	2.37	0.59
1:A:294:GLY:HA2	2:A:501:HEM:HMC3	1.85	0.58
1:A:255:LEU:O	1:A:261:MET:CE	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ILE:HG22	1:A:387:SER:OG	2.04	0.57
1:A:460:PRO:HG3	1:A:475:THR:HG22	1.85	0.57
2:A:501:HEM:C4C	4:A:506:TPF:HC7	2.39	0.57
1:A:207:ILE:HD11	1:A:233:VAL:HG21	1.85	0.57
1:A:354:MET:O	1:A:355:TYR:CD1	2.58	0.57
1:A:430:CYS:HB2	2:A:501:HEM:NA	2.20	0.57
1:A:174:MET:HE3	1:A:302:SER:HB3	1.86	0.57
1:A:445:SER:O	1:A:447:LEU:N	2.38	0.56
4:A:506:TPF:F2	4:A:506:TPF:HC22	1.96	0.56
1:A:440:VAL:O	1:A:441:LYS:C	2.49	0.56
1:A:96:ALA:HB3	1:A:101:LEU:HD12	1.88	0.56
1:A:354:MET:O	1:A:391:ARG:NH2	2.33	0.56
1:A:460:PRO:HD3	5:A:601:HOH:O	2.06	0.56
1:A:348:MET:SD	1:A:440:VAL:HB	2.46	0.55
1:A:354:MET:C	1:A:355:TYR:CG	2.85	0.55
1:A:235:GLU:O	1:A:238:GLN:HB3	2.07	0.54
1:A:205:HIS:O	1:A:209:ASP:N	2.41	0.54
2:A:501:HEM:HBD1	2:A:501:HEM:HHA	1.87	0.54
1:A:151:PHE:CZ	1:A:439:GLN:HA	2.44	0.53
4:A:506:TPF:O	4:A:506:TPF:C3	2.57	0.53
1:A:169:ASP:OD1	1:A:475:THR:N	2.37	0.53
1:A:174:MET:SD	1:A:302:SER:HB3	2.49	0.53
1:A:251:HIS:C	1:A:253:GLU:OE1	2.52	0.52
1:A:448:LEU:O	1:A:449:ARG:C	2.52	0.52
1:A:293:ALA:HA	4:A:506:TPF:N6	2.24	0.52
1:A:188:GLY:O	1:A:191:VAL:HG12	2.10	0.52
1:A:104:ARG:O	1:A:108:ARG:HB2	2.09	0.52
1:A:297:THR:HG22	1:A:357:PRO:HG2	1.92	0.51
1:A:265:ASP:O	1:A:266:HIS:C	2.54	0.51
1:A:308:ASN:HB3	1:A:402:PHE:CE2	2.46	0.51
1:A:304:TRP:CD2	1:A:355:TYR:CG	2.99	0.51
1:A:239:GLU:O	1:A:240:LEU:C	2.53	0.50
1:A:291:LEU:O	1:A:295:GLN:HG3	2.11	0.50
1:A:304:TRP:CD1	1:A:471:PRO:HD3	2.47	0.50
4:A:506:TPF:O	4:A:506:TPF:HC3	2.12	0.49
1:A:351:ALA:O	1:A:355:TYR:N	2.45	0.49
1:A:414:GLU:O	1:A:415:LYS:C	2.55	0.49
1:A:171:ALA:O	1:A:173:LEU:N	2.46	0.49
1:A:218:TYR:O	1:A:221:LEU:HG	2.13	0.49
1:A:46:TYR:HH	1:A:218:TYR:HH	1.51	0.48
1:A:110:MET:O	1:A:111:ARG:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ILE:O	1:A:239:GLU:HB3	2.14	0.48
1:A:42:ASN:HB3	1:A:48:GLY:HA2	1.95	0.48
1:A:152:GLU:O	1:A:153:ASP:C	2.55	0.48
2:A:501:HEM:NA	4:A:506:TPF:HC6	2.28	0.48
1:A:131:GLN:O	1:A:132:VAL:C	2.57	0.48
1:A:428:HIS:O	1:A:429:LYS:C	2.57	0.48
1:A:293:ALA:HB1	2:A:501:HEM:C4C	2.48	0.48
1:A:103:LEU:O	1:A:106:VAL:HG22	2.13	0.47
1:A:171:ALA:O	1:A:172:GLU:C	2.57	0.47
1:A:406:ARG:HB2	1:A:412:GLU:OE1	2.14	0.47
4:A:506:TPF:F2	4:A:506:TPF:C2	2.52	0.47
1:A:98:ASP:OD1	1:A:98:ASP:N	2.45	0.47
1:A:183:SER:O	1:A:187:LEU:HB2	2.15	0.47
1:A:159:VAL:O	1:A:160:LYS:C	2.57	0.47
1:A:106:VAL:HG23	1:A:107:TYR:CE2	2.49	0.47
1:A:267:LEU:O	1:A:269:THR:N	2.48	0.47
1:A:307:MET:HE1	1:A:475:THR:CG2	2.43	0.46
1:A:207:ILE:HA	1:A:226:ARG:HG3	1.97	0.46
1:A:403:ASP:O	1:A:404:PRO:C	2.56	0.46
1:A:455:TYR:CD1	1:A:476:ARG:O	2.69	0.46
1:A:432:GLY:O	1:A:433:GLU:C	2.59	0.45
1:A:39:ARG:NH1	1:A:75:THR:OG1	2.40	0.45
1:A:305:THR:O	1:A:306:LEU:C	2.59	0.45
1:A:392:CYS:SG	1:A:393:THR:N	2.89	0.45
1:A:183:SER:CB	1:A:195:LEU:HD11	2.46	0.45
1:A:333:LEU:HD11	1:A:341:MET:CE	2.42	0.44
1:A:386:PRO:O	1:A:387:SER:C	2.59	0.44
1:A:156:ALA:O	1:A:157:HIS:C	2.60	0.44
1:A:152:GLU:O	1:A:154:GLU:N	2.50	0.44
1:A:442:SER:O	1:A:446:ILE:HD12	2.18	0.44
1:A:207:ILE:CD1	1:A:233:VAL:HG21	2.47	0.44
1:A:440:VAL:O	1:A:443:ILE:N	2.51	0.44
1:A:255:LEU:O	1:A:261:MET:SD	2.76	0.44
1:A:105:ASP:OD1	1:A:366:ARG:NH2	2.51	0.43
1:A:214:LEU:O	1:A:217:PHE:N	2.46	0.43
1:A:304:TRP:NE1	1:A:471:PRO:CD	2.82	0.43
1:A:233:VAL:O	1:A:234:GLY:C	2.62	0.43
1:A:334:ASP:OD1	1:A:336:ASP:N	2.51	0.43
1:A:238:GLN:O	1:A:241:LEU:N	2.52	0.43
1:A:298:SER:O	1:A:301:THR:N	2.52	0.43
1:A:306:LEU:HD11	1:A:453:MET:HE1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLY:HA3	1:A:75:THR:O	2.18	0.43
1:A:238:GLN:HB2	1:A:284:ILE:HD11	2.01	0.43
1:A:117:GLY:N	1:A:121:ASP:OD2	2.42	0.42
1:A:178:ILE:CD1	1:A:299:SER:HA	2.49	0.42
1:A:201:GLY:O	1:A:204:TYR:HB2	2.18	0.42
1:A:290:GLY:O	1:A:291:LEU:C	2.62	0.42
1:A:46:TYR:OH	1:A:218:TYR:OH	2.26	0.42
1:A:296:HIS:O	1:A:297:THR:C	2.62	0.42
1:A:359:ILE:O	1:A:385:SER:OG	2.33	0.42
1:A:174:MET:HE3	1:A:302:SER:C	2.44	0.42
1:A:315:VAL:O	1:A:316:LEU:C	2.62	0.42
1:A:174:MET:CE	1:A:302:SER:HB3	2.49	0.42
1:A:183:SER:HB2	1:A:195:LEU:HD11	2.01	0.42
1:A:450:TYR:O	1:A:481:LEU:HD12	2.20	0.42
1:A:200:LEU:HD11	1:A:204:TYR:CE1	2.55	0.41
1:A:267:LEU:C	1:A:269:THR:H	2.28	0.41
1:A:304:TRP:NE1	1:A:355:TYR:HB3	2.35	0.41
1:A:253:GLU:OE1	1:A:253:GLU:N	2.53	0.41
1:A:349:LYS:HA	1:A:349:LYS:HD3	1.93	0.41
1:A:43:LEU:HB3	1:A:44:ILE:HD12	2.01	0.41
1:A:308:ASN:HB3	1:A:402:PHE:CD2	2.56	0.41
1:A:62:ILE:O	1:A:63:ASP:C	2.64	0.41
1:A:58:VAL:O	1:A:59:GLN:C	2.63	0.41
1:A:316:LEU:HD11	1:A:320:ARG:HE	1.86	0.41
1:A:355:TYR:O	1:A:356:PRO:C	2.63	0.41
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	2.03	0.41
1:A:460:PRO:HG3	1:A:475:THR:CG2	2.48	0.41
1:A:211:ILE:HG22	1:A:211:ILE:O	2.21	0.41
1:A:372:GLU:HB3	1:A:373:GLN:H	1.52	0.41
1:A:422:PRO:O	2:A:501:HEM:HMA1	2.20	0.41
1:A:182:ALA:O	1:A:183:SER:C	2.64	0.40
1:A:354:MET:HB3	1:A:355:TYR:CE2	2.56	0.40
1:A:455:TYR:CE1	1:A:476:ARG:O	2.74	0.40
1:A:300:ILE:HD12	1:A:468:VAL:HG12	2.03	0.40
1:A:376:ILE:HA	1:A:377:PRO:HD3	1.96	0.40
1:A:137:SER:O	1:A:266:HIS:NE2	2.55	0.40
1:A:143:ARG:O	1:A:146:VAL:N	2.51	0.40
1:A:262:ASP:OD1	1:A:262:ASP:C	2.64	0.40
1:A:430:CYS:SG	2:A:501:HEM:NB	2.95	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	448/466 (96%)	366 (82%)	61 (14%)	21 (5%)	2 3

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	SER
1	A	272	TYR
1	A	445	SER
1	A	119	VAL
1	A	171	ALA
1	A	268	LEU
1	A	291	LEU
1	A	446	ILE
1	A	46	TYR
1	A	77	LEU
1	A	109	PHE
1	A	172	GLU
1	A	238	GLN
1	A	239	GLU
1	A	317	GLU
1	A	429	LYS
1	A	55	LYS
1	A	310	ILE
1	A	132	VAL
1	A	415	LYS
1	A	113	VAL

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	390/418 (93%)	372 (95%)	18 (5%)	24 51

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	VAL
1	A	76	ILE
1	A	81	MET
1	A	98	ASP
1	A	110	MET
1	A	136	SER
1	A	212	SER
1	A	240	LEU
1	A	246	GLU
1	A	253	GLU
1	A	261	MET
1	A	271	LYS
1	A	393	THR
1	A	394	ASP
1	A	403	ASP
1	A	415	LYS
1	A	466	SER
1	A	472	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	205	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	EDO	A	503	-	3,3,3	0.49	0	2,2,2	0.44	0
3	EDO	A	504	-	3,3,3	0.48	0	2,2,2	0.17	0
3	EDO	A	502	-	3,3,3	0.47	0	2,2,2	0.32	0
2	HEM	A	501	4,1	50,50,50	2.91	26 (52%)	67,82,82	2.63	25 (37%)
4	TPF	A	506	2	24,24,24	1.82	4 (16%)	34,34,34	2.69	17 (50%)
3	EDO	A	505	-	3,3,3	0.38	0	2,2,2	0.46	0

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	EDO	A	503	-	-	1/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
2	HEM	A	501	4,1	-	4/14/54/54	-
4	TPF	A	506	2	-	4/16/16/16	0/3/3/3
3	EDO	A	505	-	-	0/1/1/1	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	506	TPF	C8-C13	6.13	1.47	1.39
2	A	501	HEM	C3B-C2B	5.68	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-C2C	5.08	1.47	1.37
2	A	501	HEM	C3D-C2D	4.97	1.47	1.36
2	A	501	HEM	FE-NB	4.94	2.10	1.94
2	A	501	HEM	CHC-C1C	4.73	1.47	1.38
2	A	501	HEM	CHA-C4D	4.68	1.47	1.38
2	A	501	HEM	FE-ND	4.64	2.09	1.94
2	A	501	HEM	CHD-C4C	4.56	1.47	1.38
2	A	501	HEM	CBB-CAB	4.50	1.52	1.30
2	A	501	HEM	FE-NC	4.40	2.09	1.95
2	A	501	HEM	CHB-C1B	4.37	1.47	1.38
2	A	501	HEM	FE-NA	4.18	2.09	1.95
2	A	501	HEM	CHC-C4B	3.83	1.47	1.39
2	A	501	HEM	CHA-C1A	3.73	1.47	1.39
2	A	501	HEM	CHD-C1D	3.52	1.47	1.39
2	A	501	HEM	CHB-C4A	3.35	1.46	1.39
4	A	506	TPF	C1-C8	-3.09	1.49	1.53
2	A	501	HEM	C4C-NC	-3.03	1.33	1.39
2	A	501	HEM	C1B-NB	-2.89	1.35	1.40
2	A	501	HEM	C4A-NA	-2.88	1.34	1.39
2	A	501	HEM	C2A-C3A	2.80	1.46	1.38
2	A	501	HEM	C1A-NA	-2.76	1.34	1.39
4	A	506	TPF	N1-N3	2.71	1.41	1.36
2	A	501	HEM	C4D-C3D	2.68	1.49	1.45
2	A	501	HEM	C4D-ND	-2.67	1.35	1.40
2	A	501	HEM	C1C-NC	-2.45	1.35	1.39
2	A	501	HEM	C4B-NB	-2.33	1.34	1.38
2	A	501	HEM	C3B-C4B	2.16	1.49	1.44
4	A	506	TPF	C4-N3	2.05	1.35	1.32

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	506	TPF	C1-C8-C13	-9.57	114.36	122.83
2	A	501	HEM	C3B-C4B-NB	8.76	115.76	109.47
2	A	501	HEM	C3C-C2C-C1C	-6.64	100.77	107.05
2	A	501	HEM	C3B-C2B-C1B	-6.19	101.76	106.41
2	A	501	HEM	C2B-C1B-NB	5.72	116.41	109.84
2	A	501	HEM	C4B-C3B-C2B	-5.10	102.59	107.28
2	A	501	HEM	C2D-C1D-ND	4.49	115.09	109.90
2	A	501	HEM	CAD-C3D-C4D	4.32	132.23	124.70
4	A	506	TPF	C12-C13-C8	-4.14	119.37	123.88
4	A	506	TPF	C5-N4-N6	-4.00	115.43	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	C1D-C2D-C3D	-3.85	102.93	106.98
4	A	506	TPF	C9-C8-C1	3.85	126.03	120.94
2	A	501	HEM	CAD-CBD-CGD	-3.77	103.66	113.67
2	A	501	HEM	C2C-C1C-NC	3.61	116.31	109.64
2	A	501	HEM	C2A-C1A-NA	3.60	114.15	110.15
2	A	501	HEM	CHD-C1D-C2D	-3.29	119.83	125.03
2	A	501	HEM	C3D-C4D-ND	3.27	113.76	110.17
2	A	501	HEM	C4A-C3A-C2A	-3.09	103.28	106.82
2	A	501	HEM	C3A-C4A-NA	3.00	114.96	110.14
4	A	506	TPF	C13-C12-C11	2.98	119.85	116.67
2	A	501	HEM	CHC-C1C-C2C	-2.89	119.47	125.49
4	A	506	TPF	C2-N1-N3	-2.87	117.08	121.25
4	A	506	TPF	C1-C5-N4	2.85	116.20	112.34
2	A	501	HEM	CAA-CBA-CGA	-2.65	106.63	113.67
2	A	501	HEM	C1A-C2A-C3A	-2.60	102.84	106.87
2	A	501	HEM	CBB-CAB-C3B	-2.59	114.57	127.53
2	A	501	HEM	CHB-C4A-C3A	-2.59	119.91	127.43
2	A	501	HEM	C4C-C3C-C2C	-2.59	104.57	106.81
4	A	506	TPF	C9-C10-C11	2.55	121.00	118.38
2	A	501	HEM	C4D-C3D-C2D	-2.51	103.23	106.89
4	A	506	TPF	C3-N2-C4	2.51	109.63	102.85
2	A	501	HEM	CHB-C1B-C2B	-2.51	119.82	126.95
4	A	506	TPF	C6-N5-C7	2.50	109.62	102.85
4	A	506	TPF	F2-C13-C12	2.46	123.57	118.64
4	A	506	TPF	C9-C8-C13	2.35	119.59	116.28
4	A	506	TPF	C5-N4-C6	2.33	133.38	128.82
4	A	506	TPF	N6-C7-N5	-2.23	108.52	114.90
4	A	506	TPF	N3-C4-N2	-2.16	108.73	114.90
4	A	506	TPF	N4-C6-N5	-2.12	106.03	110.42
2	A	501	HEM	CAA-C2A-C1A	2.09	129.02	124.94
2	A	501	HEM	CAD-C3D-C2D	-2.02	124.08	127.87
4	A	506	TPF	N1-C3-N2	-2.01	106.27	110.42

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2D-C3D-CAD-CBD
2	A	501	HEM	C4D-C3D-CAD-CBD
4	A	506	TPF	C1-C2-N1-N3
4	A	506	TPF	C1-C2-N1-C3
3	A	503	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	506	TPF	C5-C1-C2-N1
2	A	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O1D
4	A	506	TPF	C8-C1-C2-N1

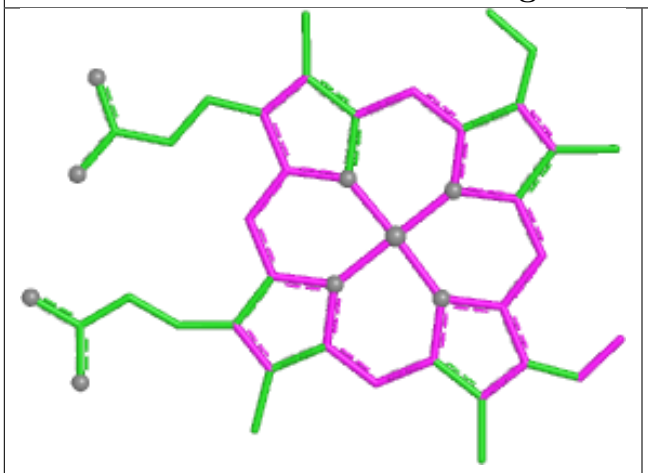
There are no ring outliers.

2 monomers are involved in 18 short contacts:

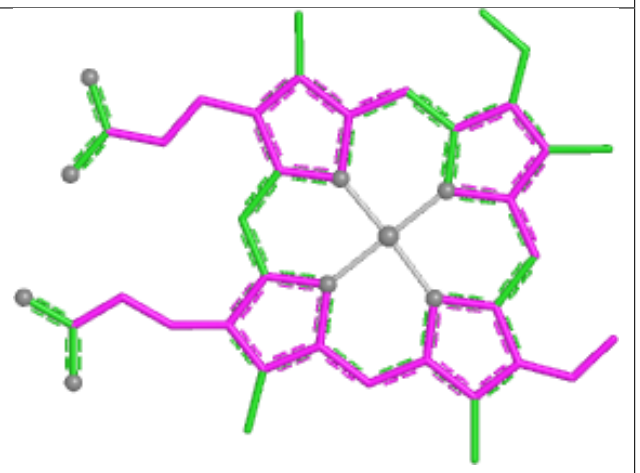
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	13	0
4	A	506	TPF	9	0

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 then 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.

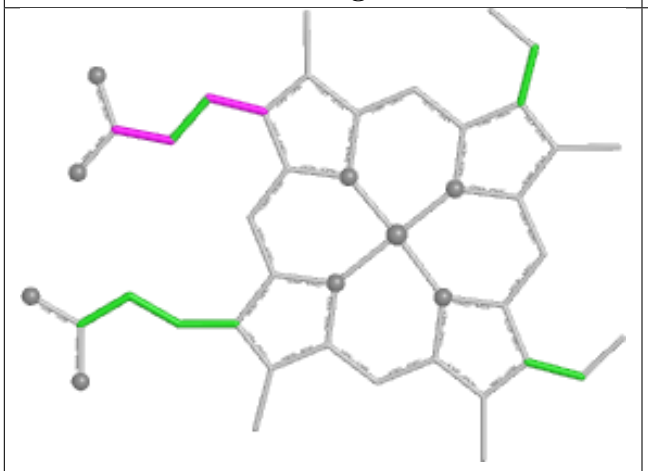
Ligand HEM A 501



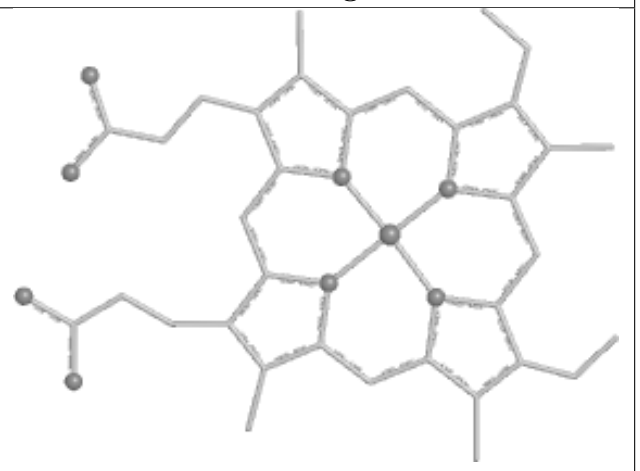
Bond lengths



Bond angles

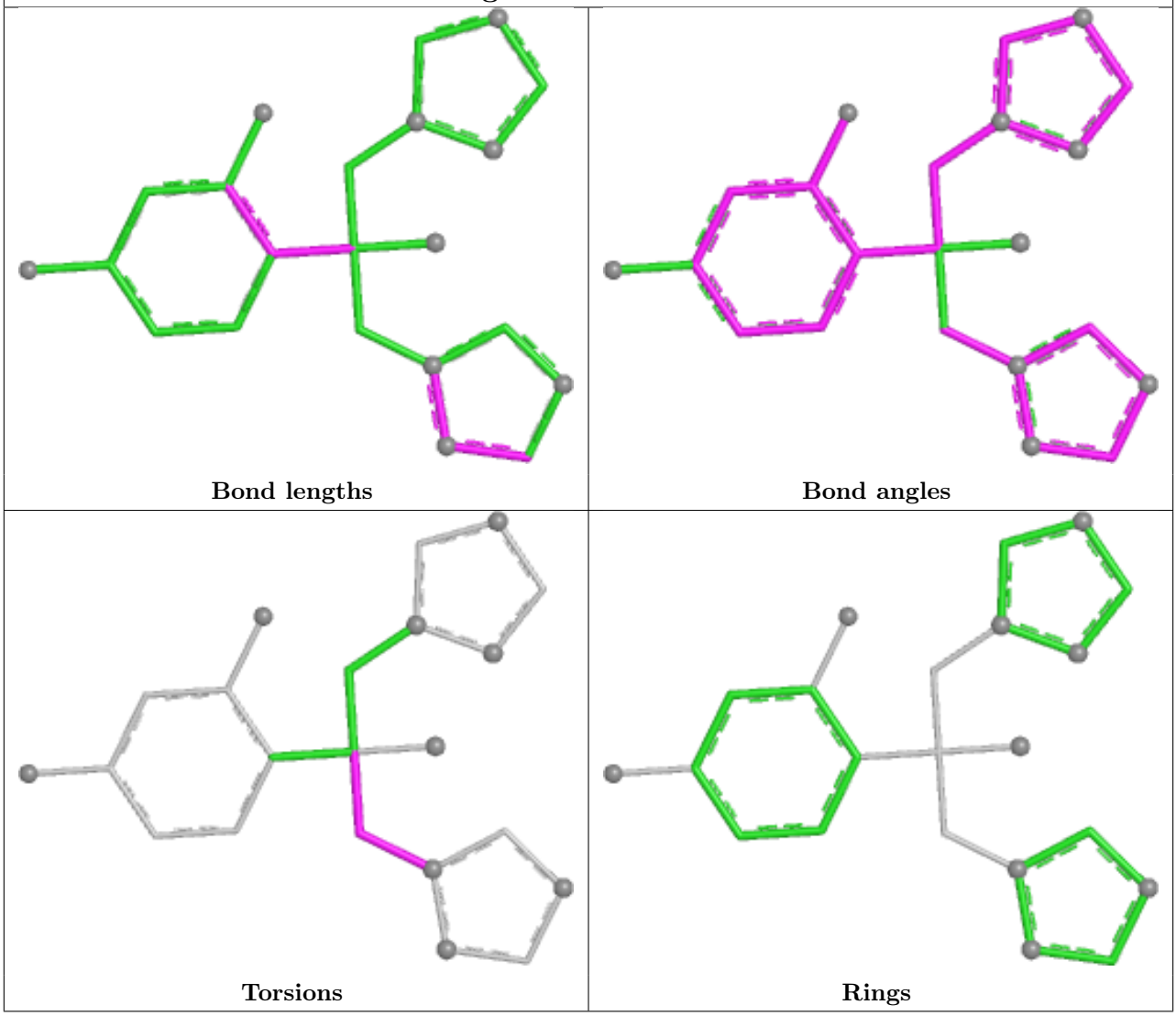


Torsions



Rings

Ligand TPF A 506



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	450/466 (96%)	1.10	72 (16%) 5 4	57, 97, 128, 162	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	TYR	6.4
1	A	471	PRO	6.1
1	A	183	SER	5.1
1	A	304	TRP	4.9
1	A	361	ILE	4.1
1	A	287	LEU	4.1
1	A	354	MET	3.9
1	A	204	TYR	3.7
1	A	302	SER	3.6
1	A	390	GLY	3.6
1	A	187	LEU	3.5
1	A	291	LEU	3.4
1	A	200	LEU	3.3
1	A	289	ALA	3.3
1	A	114	PHE	3.3
1	A	295	GLN	3.0
1	A	208	ASP	2.9
1	A	443	ILE	2.9
1	A	173	LEU	2.9
1	A	113	VAL	2.9
1	A	418	TYR	2.8
1	A	440	VAL	2.8
1	A	424	GLY	2.8
1	A	360	MET	2.8
1	A	50	PHE	2.8
1	A	362	MET	2.7
1	A	306	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	392	CYS	2.7
1	A	469	VAL	2.7
1	A	352	LEU	2.6
1	A	191	VAL	2.6
1	A	211	ILE	2.6
1	A	135	VAL	2.6
1	A	451	PHE	2.6
1	A	348	MET	2.5
1	A	467	LEU	2.5
1	A	162	LEU	2.5
1	A	214	LEU	2.5
1	A	301	THR	2.5
1	A	294	GLY	2.5
1	A	395	THR	2.5
1	A	72	PHE	2.5
1	A	43	LEU	2.4
1	A	236	ILE	2.4
1	A	185	CYS	2.4
1	A	299	SER	2.3
1	A	90	LEU	2.3
1	A	447	LEU	2.3
1	A	353	ARG	2.3
1	A	85	ASN	2.3
1	A	201	GLY	2.3
1	A	207	ILE	2.2
1	A	347	CYS	2.2
1	A	351	ALA	2.2
1	A	444	ILE	2.2
1	A	134	PHE	2.2
1	A	179	ILE	2.2
1	A	419	GLY	2.2
1	A	477	MET	2.2
1	A	53	PHE	2.2
1	A	83	PHE	2.2
1	A	300	ILE	2.2
1	A	103	LEU	2.2
1	A	389	ALA	2.1
1	A	290	GLY	2.1
1	A	174	MET	2.1
1	A	171	ALA	2.1
1	A	413	HIS	2.1
1	A	132	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	81	MET	2.1
1	A	84	LEU	2.1
1	A	292	PHE	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)

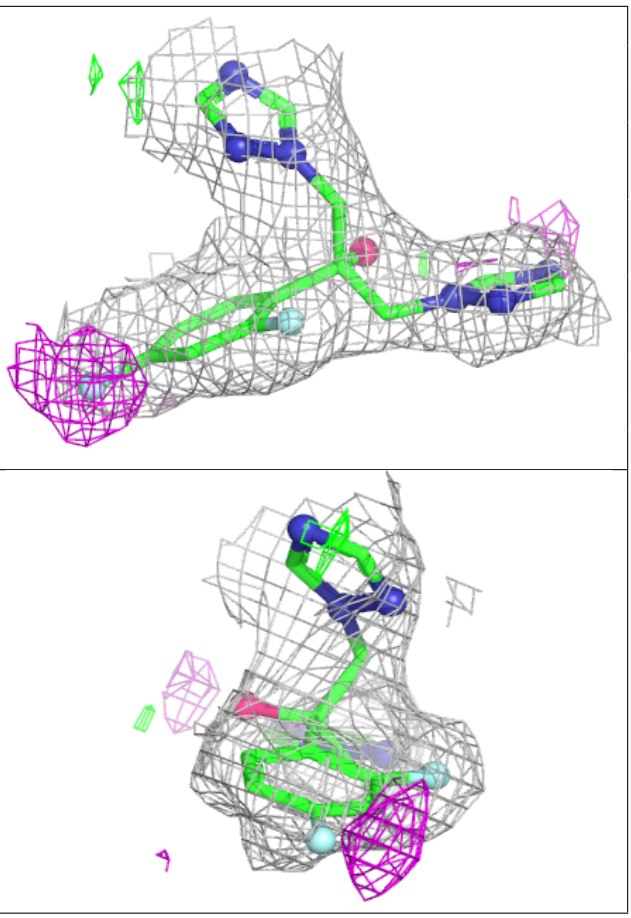
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	A	502	4/4	0.75	0.18	104,114,114,114	0
3	EDO	A	503	4/4	0.78	0.16	68,69,70,79	0
3	EDO	A	504	4/4	0.79	0.24	118,121,124,124	0
3	EDO	A	505	4/4	0.85	0.41	124,128,131,134	0
4	TPF	A	506	22/22	0.87	0.13	67,74,99,106	0
2	HEM	A	501	43/43	0.93	0.19	76,90,113,119	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.

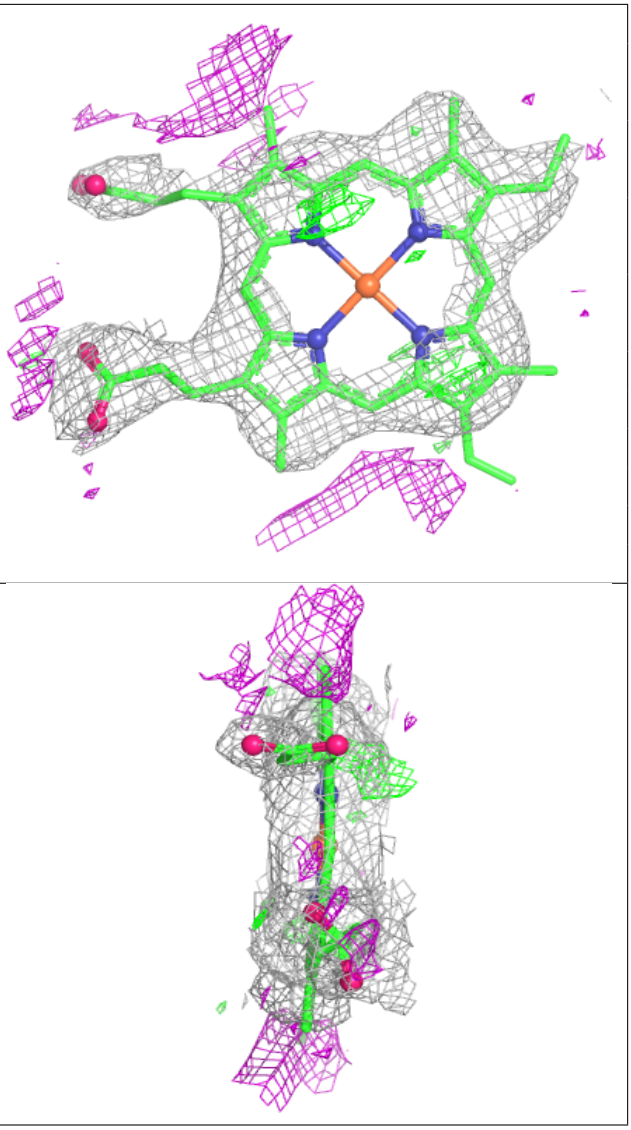
Electron density around TPF A 506:

$2mF_o$-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.