



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:47 PM UTC

PDB ID : 6AYC / pdb_00006ayc
Title : Naegleria fowleri CYP51-itraconazole 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 : 2017-09-08
Resolution : 2.60 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

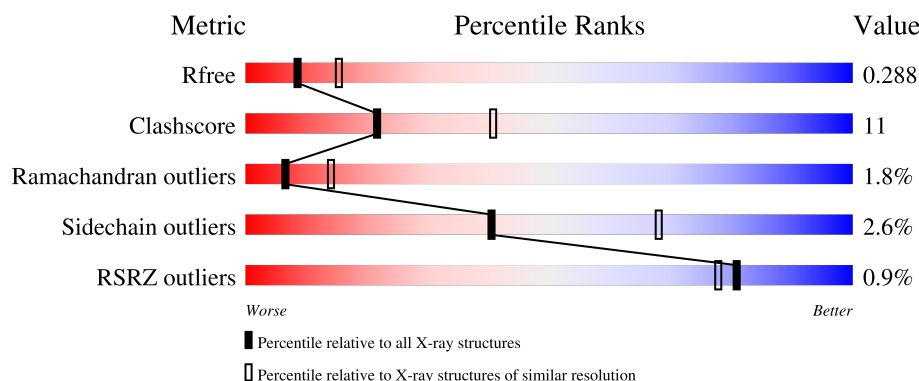
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	466	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3731 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 Protein CYP51.

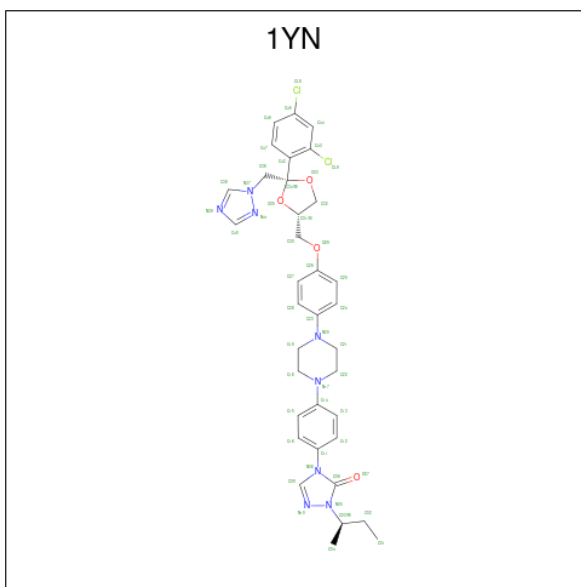
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3577	2297	604	654	22			

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



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

- Molecule 3 is 2-[(2R)-butan-2-yl]-4-{4-[4-(4-{[(2R,4S)-2-(2,4-dichlorophenyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy}phenyl)piperazin-1-yl]phenyl}-2,4-dihydro-3H-1,2,4-triazol-3-one (CCD ID: 1YN) (formula: $C_{35}H_{38}Cl_2N_8O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	1
			98	70	4	16	8		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		

- Molecule 1: Protein CYP51



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.30Å 55.19Å 72.39Å 90.00° 100.62° 90.00°	Depositor
Resolution (Å)	71.15 – 2.60 71.15 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (71.15-2.60) 99.7 (71.15-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.62Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.218 , 0.290 0.219 , 0.288	Depositor DCC
R_{free} test set	724 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	91.8	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3731	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 1YN

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	0.75	0/3655	0.95	3/4936 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ILE	CA-C-N	-7.74	112.49	120.85
1	A	44	ILE	C-N-CA	-7.74	112.49	120.85
1	A	362	MET	N-CA-C	5.33	117.93	109.50

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	3577	0	3592	74	0
2	A	43	0	30	3	0
3	A	98	0	75	8	0
4	A	13	0	0	1	0
All	All	3731	0	3697	80	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 11.

All (80) 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:395:THR:CG2	1:A:396:TYR:CE1	2.07	1.37
1:A:395:THR:HG21	1:A:396:TYR:CE1	1.70	1.23
1:A:395:THR:HG22	1:A:396:TYR:CE1	1.83	1.11
1:A:395:THR:HG22	1:A:396:TYR:CD1	1.93	1.03
1:A:46:TYR:OH	1:A:218:TYR:OH	1.74	0.99
1:A:395:THR:CG2	1:A:396:TYR:CD1	2.48	0.94
1:A:395:THR:HG21	1:A:396:TYR:HE1	1.21	0.92
1:A:120:TYR:OH	3:A:502[B]:1YN:CL9	2.23	0.92
1:A:353:ARG:HD2	1:A:396:TYR:CD2	2.05	0.90
1:A:291:LEU:O	1:A:295:GLN:HG3	1.75	0.86
1:A:395:THR:CB	1:A:396:TYR:CD1	2.73	0.72
1:A:395:THR:HB	1:A:396:TYR:CD1	2.25	0.71
1:A:44:ILE:HG22	1:A:45:PRO:O	1.90	0.71
1:A:373:GLN:OE1	1:A:373:GLN:N	2.16	0.71
1:A:395:THR:HB	1:A:396:TYR:HD1	1.59	0.68
3:A:502[B]:1YN:CL9	3:A:502[B]:1YN:O35	2.50	0.67
1:A:373:GLN:H	1:A:373:GLN:CD	2.03	0.67
1:A:44:ILE:HG22	1:A:45:PRO:N	2.10	0.67
1:A:324:GLU:OE1	4:A:601:HOH:O	2.12	0.66
1:A:353:ARG:HD2	1:A:396:TYR:CE2	2.32	0.65
1:A:353:ARG:CD	1:A:396:TYR:CD2	2.79	0.64
1:A:42:ASN:HB3	1:A:44:ILE:O	1.98	0.64
1:A:395:THR:CB	1:A:396:TYR:CE1	2.81	0.64
1:A:433:GLU:O	1:A:436:ALA:N	2.31	0.63
1:A:353:ARG:CD	1:A:396:TYR:CE2	2.81	0.63
1:A:403:ASP:O	1:A:406:ARG:HG2	1.99	0.62
1:A:96:ALA:O	1:A:427:ARG:NH1	2.25	0.61
1:A:308:ASN:HB3	1:A:402:PHE:CE2	2.36	0.60
1:A:44:ILE:HG22	1:A:45:PRO:CD	2.32	0.59
3:A:502[A]:1YN:CL9	3:A:502[A]:1YN:H33	2.41	0.58
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.85	0.57
1:A:110:MET:HE3	1:A:114:PHE:CZ	2.39	0.57
1:A:37:PRO:HA	1:A:374:TYR:CD1	2.40	0.56
1:A:396:TYR:CD1	1:A:396:TYR:N	2.74	0.54
1:A:250:LYS:C	1:A:251:HIS:CD2	2.86	0.53
1:A:44:ILE:CG2	1:A:45:PRO:CD	2.87	0.53
1:A:248:HIS:CE1	1:A:255:LEU:HD21	2.44	0.53
1:A:353:ARG:HD3	1:A:396:TYR:CE2	2.44	0.52
1:A:114:PHE:HZ	3:A:502[A]:1YN:CL9	2.29	0.52
1:A:44:ILE:HG22	1:A:45:PRO:HD2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:MET:O	1:A:330:ASP:HB2	2.10	0.51
1:A:372:GLU:C	1:A:374:TYR:H	2.19	0.51
1:A:37:PRO:HA	1:A:374:TYR:CE1	2.46	0.51
1:A:372:GLU:HB3	1:A:373:GLN:OE1	2.11	0.50
1:A:292:PHE:CD2	3:A:502[A]:1YN:CL9	3.02	0.50
1:A:294:GLY:HA2	2:A:501:HEM:HMC2	1.94	0.50
1:A:373:GLN:HG2	1:A:374:TYR:CE2	2.47	0.50
1:A:308:ASN:HB3	1:A:402:PHE:CD2	2.46	0.50
1:A:104:ARG:O	1:A:108:ARG:HB2	2.13	0.49
1:A:372:GLU:O	1:A:374:TYR:N	2.45	0.49
1:A:302:SER:OG	1:A:440:VAL:HG22	2.14	0.48
1:A:327:MET:O	1:A:328:GLY:C	2.57	0.48
1:A:370:GLU:O	1:A:371:CYS:HB2	2.14	0.47
1:A:188:GLY:O	1:A:191:VAL:HG12	2.15	0.47
1:A:360:MET:HG2	1:A:383:VAL:CG1	2.45	0.46
1:A:395:THR:C	1:A:396:TYR:CD1	2.93	0.46
1:A:333:LEU:HD11	1:A:341:MET:HE1	1.98	0.46
1:A:45:PRO:O	1:A:46:TYR:HB3	2.16	0.45
1:A:169:ASP:HA	1:A:475:THR:O	2.17	0.45
1:A:296:HIS:O	1:A:297:THR:C	2.58	0.45
1:A:44:ILE:CG2	1:A:45:PRO:N	2.77	0.45
1:A:372:GLU:C	1:A:374:TYR:N	2.75	0.45
1:A:465:THR:O	1:A:465:THR:HG22	2.17	0.45
1:A:321:LYS:HE2	1:A:325:GLU:OE2	2.17	0.44
1:A:44:ILE:CG2	1:A:45:PRO:HD2	2.48	0.44
3:A:502[A]:1YN:H26	3:A:502[A]:1YN:H18	1.75	0.44
1:A:373:GLN:HG2	1:A:374:TYR:CD2	2.52	0.43
1:A:250:LYS:O	1:A:251:HIS:CG	2.72	0.43
1:A:250:LYS:O	1:A:251:HIS:CD2	2.71	0.43
1:A:360:MET:HG2	1:A:383:VAL:HG13	2.00	0.43
1:A:421:VAL:N	1:A:422:PRO:CD	2.82	0.43
3:A:502[B]:1YN:H26	3:A:502[B]:1YN:H18	1.74	0.43
1:A:333:LEU:HD22	1:A:446:ILE:HG13	1.99	0.43
1:A:246:GLU:O	1:A:249:LYS:HB2	2.19	0.42
1:A:250:LYS:HB2	1:A:251:HIS:CD2	2.54	0.42
1:A:327:MET:HE3	1:A:330:ASP:O	2.20	0.42
1:A:292:PHE:HD2	3:A:502[A]:1YN:CL9	2.40	0.41
1:A:250:LYS:C	1:A:251:HIS:CG	2.99	0.41
1:A:433:GLU:O	1:A:435:PHE:N	2.55	0.40
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.51	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	447/466 (96%)	428 (96%)	11 (2%)	8 (2%)	6	14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	371	CYS
1	A	373	GLN
1	A	433	GLU
1	A	109	PHE
1	A	46	TYR
1	A	119	VAL
1	A	434	ASN
1	A	372	GLU

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	390/418 (93%)	380 (97%)	10 (3%)	40	68

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	THR
1	A	111	ARG
1	A	277	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	329	SER
1	A	349	LYS
1	A	360	MET
1	A	370	GLU
1	A	393	THR
1	A	396	TYR
1	A	459	ILE

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

Mol	Chain	Res	Type
1	A	251	HIS
1	A	266	HIS
1	A	380	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	1,3	50,50,50	2.50	22 (44%)	67,82,82	2.79	28 (41%)
3	1YN	A	502[B]	2	54,55,55	1.76	9 (16%)	76,79,79	2.10	26 (34%)
3	1YN	A	502[A]	2	54,55,55	1.82	10 (18%)	76,79,79	2.36	24 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	501	1,3	-	0/14/54/54	-
3	1YN	A	502[B]	2	-	17/34/55/55	0/7/7/7
3	1YN	A	502[A]	2	-	11/34/55/55	0/7/7/7

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502[A]	1YN	C43-C42	6.07	1.49	1.39
3	A	502[B]	1YN	C11-N08	-5.43	1.34	1.44
3	A	502[A]	1YN	C11-N08	-5.32	1.35	1.44
3	A	502[B]	1YN	C43-C42	5.06	1.47	1.39
3	A	502[B]	1YN	C06-N08	-4.80	1.33	1.39
2	A	501	HEM	C4A-NA	-4.65	1.30	1.39
2	A	501	HEM	C3B-C2B	4.64	1.46	1.37
3	A	502[A]	1YN	C06-N08	-4.61	1.33	1.39
2	A	501	HEM	C4D-ND	-4.16	1.33	1.40
2	A	501	HEM	FE-NB	4.15	2.07	1.94
3	A	502[B]	1YN	C09-N10	4.14	1.36	1.30
3	A	502[A]	1YN	C09-N10	4.13	1.36	1.30
2	A	501	HEM	C1A-NA	-4.13	1.31	1.39
2	A	501	HEM	C4C-NC	-4.06	1.32	1.39
2	A	501	HEM	CBB-CAB	4.00	1.49	1.30
2	A	501	HEM	C4B-NB	-3.98	1.31	1.38
2	A	501	HEM	C1C-NC	-3.89	1.32	1.39
3	A	502[A]	1YN	O07-C06	3.82	1.29	1.22
2	A	501	HEM	C1D-ND	-3.76	1.31	1.38
3	A	502[A]	1YN	C34-C42	-3.75	1.49	1.53
3	A	502[B]	1YN	O07-C06	3.72	1.29	1.22
2	A	501	HEM	C3C-C2C	3.71	1.44	1.37
2	A	501	HEM	C3D-C2D	3.67	1.44	1.36
3	A	502[B]	1YN	C34-C42	-3.53	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	CHC-C1C	3.52	1.45	1.38
2	A	501	HEM	C1B-NB	-3.45	1.34	1.40
2	A	501	HEM	CHD-C4C	3.10	1.44	1.38
3	A	502[B]	1YN	C43-CL9	2.90	1.80	1.73
2	A	501	HEM	FE-ND	2.88	2.03	1.94
2	A	501	HEM	CHB-C4A	2.87	1.45	1.39
3	A	502[A]	1YN	C43-CL9	2.81	1.80	1.73
2	A	501	HEM	FE-NC	2.61	2.03	1.95
2	A	501	HEM	CHD-C1D	2.38	1.44	1.39
2	A	501	HEM	CHB-C1B	2.38	1.43	1.38
3	A	502[A]	1YN	C45-CL8	2.36	1.79	1.74
2	A	501	HEM	CHA-C4D	2.33	1.43	1.38
2	A	501	HEM	CHC-C4B	2.22	1.44	1.39
3	A	502[B]	1YN	N05-N10	2.20	1.41	1.37
3	A	502[B]	1YN	C45-CL8	2.20	1.79	1.74
3	A	502[A]	1YN	C09-N08	-2.10	1.34	1.37
3	A	502[A]	1YN	N05-N10	2.02	1.40	1.37

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C3B-C2B-C1B	-8.31	100.17	106.41
2	A	501	HEM	C3B-C4B-NB	7.65	114.96	109.47
3	A	502[A]	1YN	C34-C42-C43	-7.62	118.32	123.72
2	A	501	HEM	C2B-C1B-NB	6.29	117.07	109.84
3	A	502[A]	1YN	C06-N05-N10	-6.19	108.00	112.87
3	A	502[B]	1YN	C06-N05-N10	-6.08	108.09	112.87
3	A	502[A]	1YN	C47-C42-C34	6.03	123.17	119.18
3	A	502[A]	1YN	O33-C34-C42	-5.84	101.36	111.37
2	A	501	HEM	CHD-C1D-C2D	-5.83	115.82	125.03
2	A	501	HEM	C3C-C2C-C1C	-5.51	101.83	107.05
3	A	502[B]	1YN	C16-C11-N08	5.27	126.50	119.62
2	A	501	HEM	C2D-C1D-ND	4.87	115.54	109.90
2	A	501	HEM	C1D-C2D-C3D	-4.79	101.95	106.98
3	A	502[A]	1YN	C16-C11-N08	4.71	125.78	119.62
3	A	502[A]	1YN	C09-N08-C06	4.71	110.75	107.27
3	A	502[B]	1YN	C09-N08-C06	4.70	110.75	107.27
3	A	502[B]	1YN	C21-N20-C19	4.68	122.10	111.57
3	A	502[B]	1YN	N08-C06-N05	4.52	107.98	102.88
2	A	501	HEM	CMA-C3A-C4A	4.46	132.21	125.42
3	A	502[A]	1YN	N08-C06-N05	4.39	107.83	102.88
3	A	502[A]	1YN	C03-N05-C06	4.31	136.74	125.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502[A]	1YN	C21-N20-C19	4.29	121.22	111.57
3	A	502[B]	1YN	O33-C34-C42	-4.24	104.10	111.37
3	A	502[B]	1YN	C19-C18-N17	-4.19	101.96	110.78
3	A	502[A]	1YN	C19-C18-N17	-4.08	102.20	110.78
2	A	501	HEM	CHC-C1C-C2C	-3.96	117.25	125.49
2	A	501	HEM	CHA-C1A-C2A	-3.87	116.82	125.30
2	A	501	HEM	CHA-C1A-NA	3.83	130.80	123.86
2	A	501	HEM	CHD-C1D-ND	3.69	128.39	124.42
3	A	502[B]	1YN	C03-N05-C06	3.67	135.03	125.26
3	A	502[B]	1YN	C44-C43-C42	-3.57	118.40	121.97
3	A	502[B]	1YN	C36-N37-N41	-3.47	116.21	121.25
3	A	502[A]	1YN	C36-N37-N41	-3.40	116.31	121.25
2	A	501	HEM	C4B-C3B-C2B	-3.32	104.22	107.28
2	A	501	HEM	CHC-C1C-NC	3.31	128.06	124.45
2	A	501	HEM	CAD-C3D-C4D	3.30	130.44	124.70
2	A	501	HEM	CAA-C2A-C1A	3.29	131.37	124.94
2	A	501	HEM	CAD-CBD-CGD	-2.98	105.76	113.67
3	A	502[A]	1YN	C30-C31-C32	-2.91	104.06	112.95
2	A	501	HEM	CHB-C4A-NA	2.84	129.01	123.86
2	A	501	HEM	C2C-C1C-NC	2.73	114.69	109.64
3	A	502[A]	1YN	C30-O29-C26	2.71	123.81	117.85
3	A	502[B]	1YN	C30-C31-C32	-2.62	104.94	112.95
2	A	501	HEM	CHB-C1B-C2B	-2.62	119.52	126.95
2	A	501	HEM	C1A-CHA-C4D	-2.59	120.16	126.25
3	A	502[A]	1YN	C09-N10-N05	2.58	106.23	103.68
3	A	502[B]	1YN	C21-C22-N17	-2.54	105.44	110.78
3	A	502[B]	1YN	C47-C42-C43	2.53	119.21	116.51
3	A	502[B]	1YN	C13-C12-C11	2.51	123.48	120.30
3	A	502[B]	1YN	C28-C23-N20	-2.48	117.95	121.39
2	A	501	HEM	C3D-C4D-ND	2.47	112.88	110.17
3	A	502[A]	1YN	C13-C12-C11	2.43	123.38	120.30
3	A	502[B]	1YN	C09-N10-N05	2.42	106.07	103.68
2	A	501	HEM	CBB-CAB-C3B	-2.41	115.47	127.53
3	A	502[B]	1YN	C34-C42-C43	-2.39	122.03	123.72
3	A	502[A]	1YN	C28-C23-N20	-2.37	118.10	121.39
3	A	502[B]	1YN	C36-N37-C38	2.36	133.45	128.82
3	A	502[B]	1YN	C44-C43-CL9	2.36	122.31	118.45
3	A	502[A]	1YN	C36-N37-C38	2.35	133.42	128.82
3	A	502[B]	1YN	N08-C09-N10	-2.33	107.03	111.42
3	A	502[B]	1YN	C30-O29-C26	2.30	122.92	117.85
2	A	501	HEM	CHB-C4A-C3A	-2.29	120.77	127.43
2	A	501	HEM	C1A-C2A-C3A	-2.27	103.36	106.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502[A]	1YN	O35-C31-C30	2.27	114.36	108.58
3	A	502[A]	1YN	N08-C09-N10	-2.27	107.14	111.42
3	A	502[B]	1YN	C38-N39-C40	2.24	108.91	102.85
3	A	502[B]	1YN	C22-N17-C18	2.23	116.59	111.57
3	A	502[A]	1YN	C38-N39-C40	2.23	108.87	102.85
2	A	501	HEM	C4C-C3C-C2C	-2.23	104.88	106.81
3	A	502[A]	1YN	C16-C11-C12	-2.22	114.94	119.18
3	A	502[A]	1YN	C47-C46-C45	2.20	121.46	119.24
3	A	502[B]	1YN	C16-C11-C12	-2.12	115.14	119.18
3	A	502[A]	1YN	N41-C40-N39	-2.08	108.95	114.90
3	A	502[B]	1YN	N41-C40-N39	-2.08	108.95	114.90
3	A	502[A]	1YN	C36-C34-C42	2.04	112.46	109.59
3	A	502[B]	1YN	C36-C34-C42	2.03	112.44	109.59
2	A	501	HEM	CMD-C2D-C1D	2.02	128.19	125.03
2	A	501	HEM	CMB-C2B-C1B	2.01	128.17	125.03

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502[A]	1YN	C04-C03-N05-C06
3	A	502[A]	1YN	C04-C03-N05-N10
3	A	502[A]	1YN	O33-C34-C36-N37
3	A	502[A]	1YN	C42-C34-C36-N37
3	A	502[B]	1YN	C02-C03-N05-N10
3	A	502[B]	1YN	O33-C34-C36-N37
3	A	502[B]	1YN	C42-C34-C36-N37
3	A	502[B]	1YN	O33-C34-C42-C43
3	A	502[B]	1YN	O33-C34-C42-C47
3	A	502[B]	1YN	O35-C34-C42-C43
3	A	502[B]	1YN	O35-C34-C42-C47
3	A	502[B]	1YN	C36-C34-C42-C43
3	A	502[B]	1YN	C36-C34-C42-C47
3	A	502[A]	1YN	C34-C36-N37-C38
3	A	502[A]	1YN	O29-C30-C31-O35
3	A	502[B]	1YN	O29-C30-C31-O35
3	A	502[A]	1YN	C34-C36-N37-N41
3	A	502[B]	1YN	C34-C36-N37-N41
3	A	502[A]	1YN	O29-C30-C31-C32
3	A	502[B]	1YN	O29-C30-C31-C32
3	A	502[B]	1YN	C34-C36-N37-C38
3	A	502[A]	1YN	C01-C02-C03-C04

Continued on next page...

Continued from previous page...

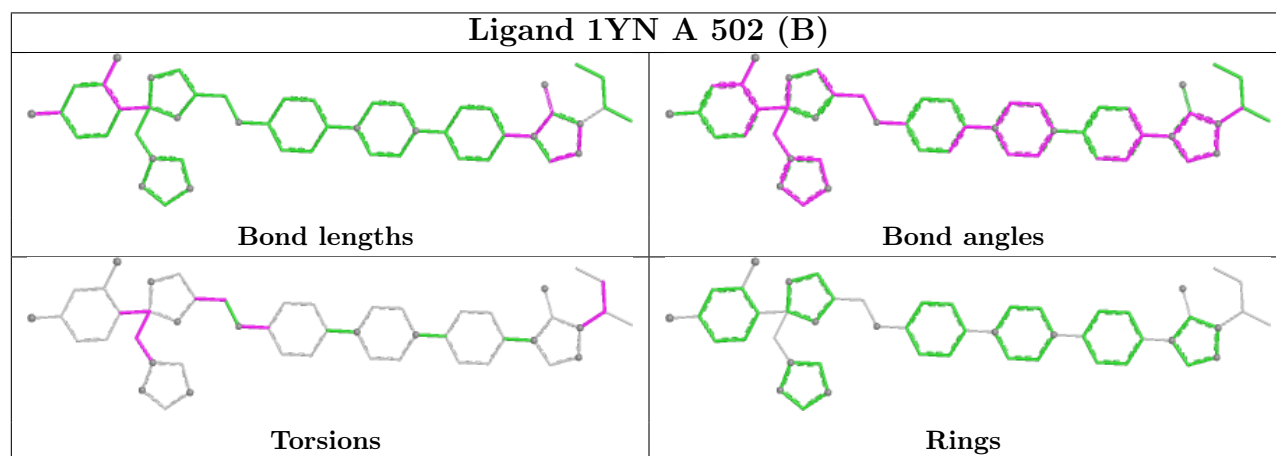
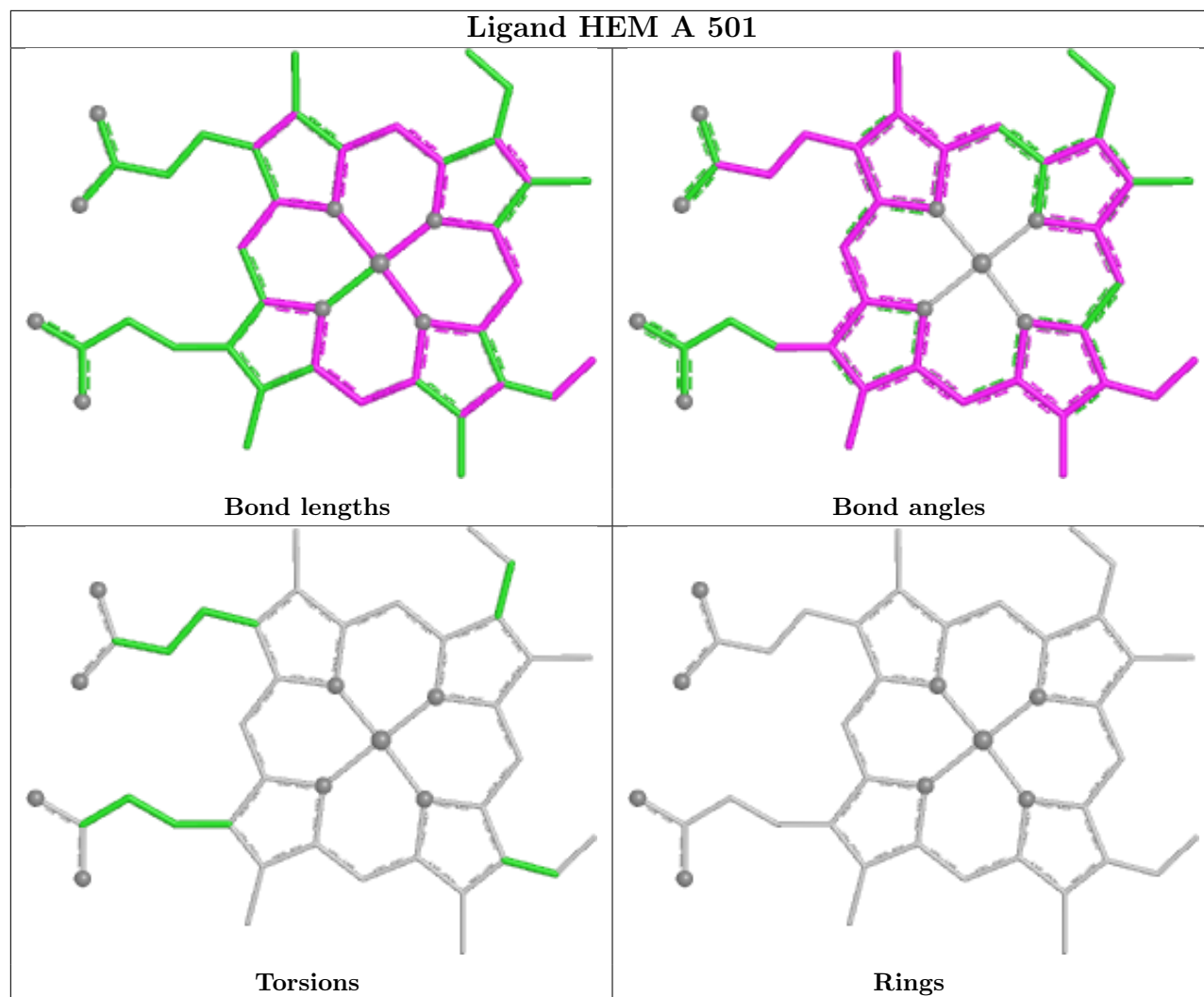
Mol	Chain	Res	Type	Atoms
3	A	502[A]	1YN	O35-C34-C36-N37
3	A	502[B]	1YN	C01-C02-C03-C04
3	A	502[B]	1YN	C01-C02-C03-N05
3	A	502[B]	1YN	C27-C26-O29-C30
3	A	502[B]	1YN	C25-C26-O29-C30
3	A	502[A]	1YN	C01-C02-C03-N05

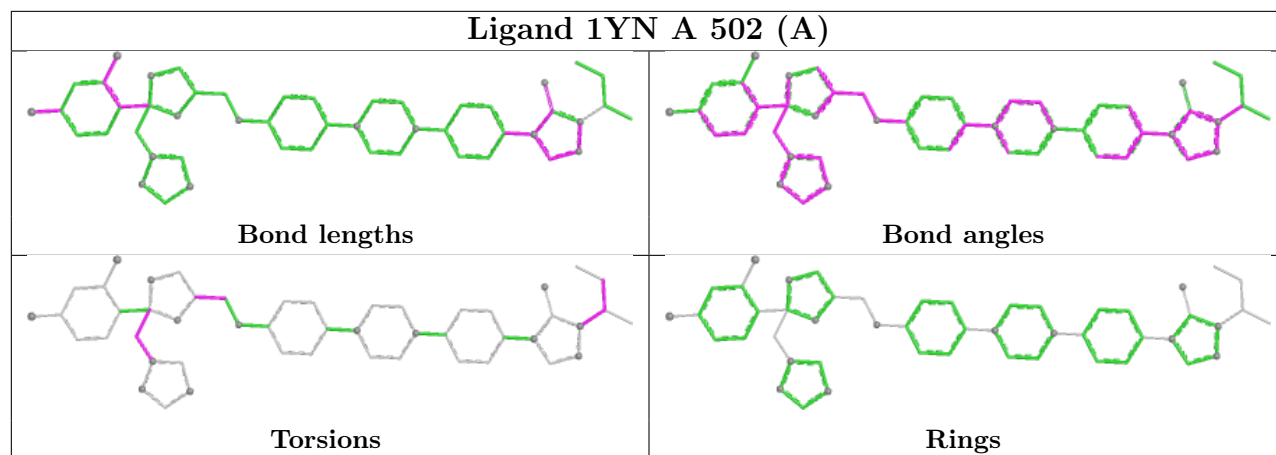
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	3	0
3	A	502[B]	1YN	3	0
3	A	502[A]	1YN	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.





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	449/466 (96%)	0.08	4 (0%) 81 78	63, 96, 124, 150	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	LEU	3.2
1	A	135	VAL	2.2
1	A	58	VAL	2.2
1	A	302	SER	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](#)

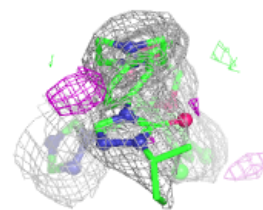
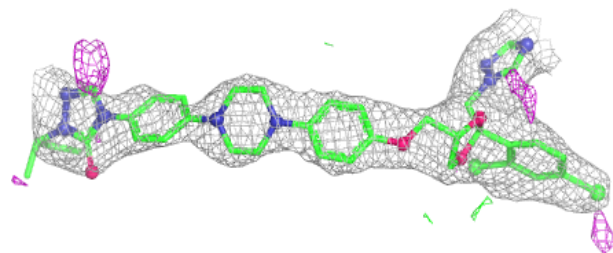
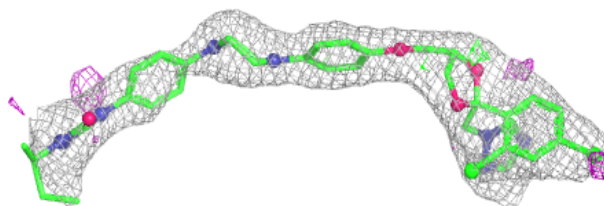
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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	1YN	A	502[A]	49/49	0.93	0.10	56,81,116,123	49
3	1YN	A	502[B]	49/49	0.93	0.10	68,98,120,126	49
2	HEM	A	501	43/43	0.97	0.10	67,78,92,95	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.

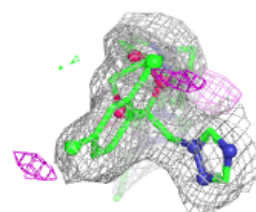
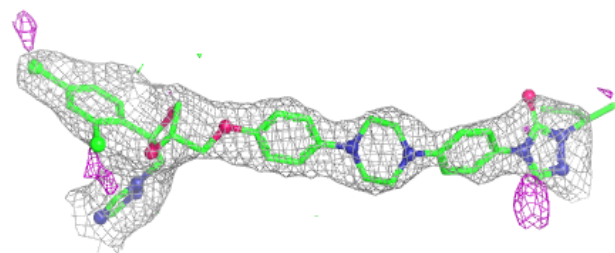
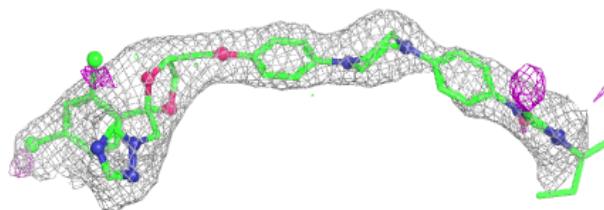
Electron density around 1YN A 502 (A):

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



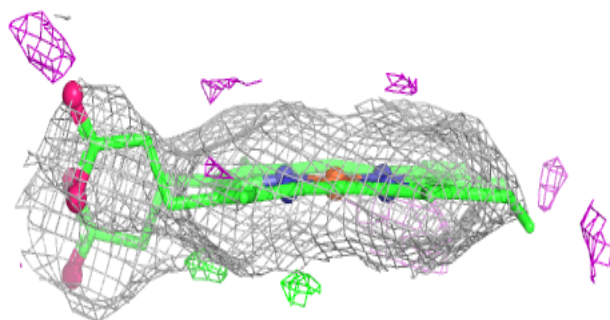
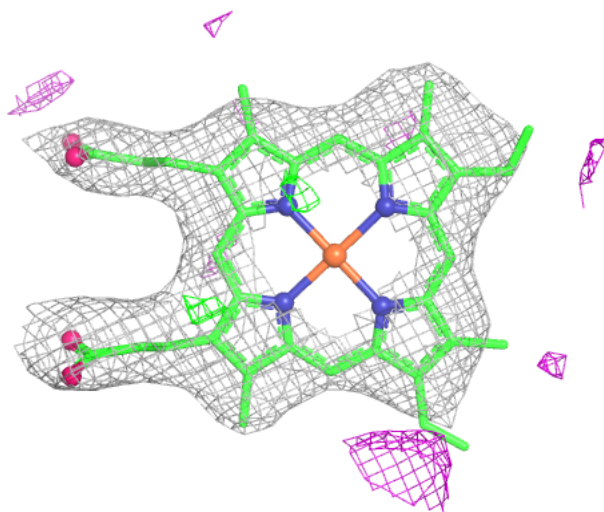
Electron density around 1YN A 502 (B):

$2mF_o-DF_c$ (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.