



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5V5Z / pdb_00005v5z
Title : Structure of CYP51 from the pathogen *Candida albicans*
Authors : Keniya, M.V.; Sabherwal, M.; Wilson, R.K.; Sagatova, A.A.; Tyndall, J.D.A.;
Monk, B.C.
Deposited on : 2017-03-15
Resolution : 2.90 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

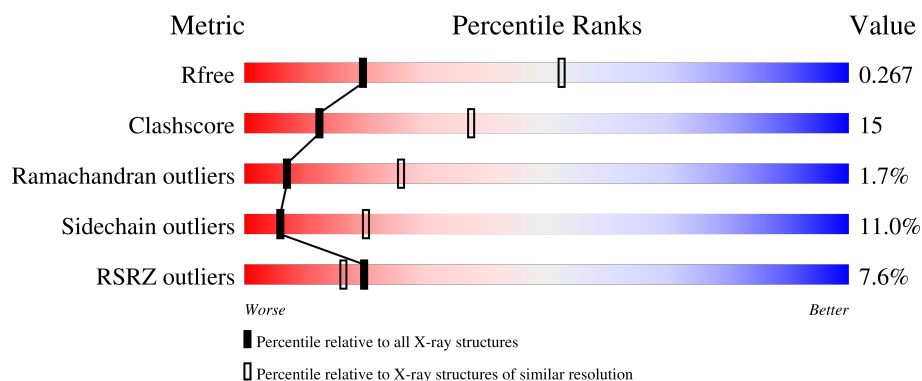
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	537	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4092 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.

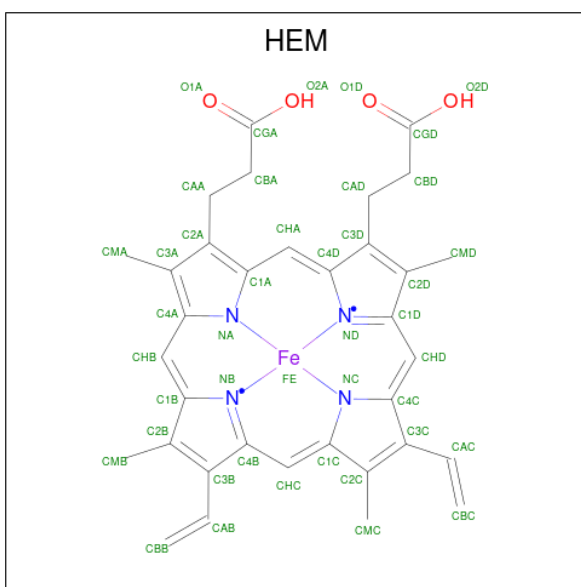
- Molecule 1 is a protein called Lanosterol 14-alpha demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	488	4000	2593	664	729	14	0	1	0

There are 9 discrepancies between the modelled and reference sequences:

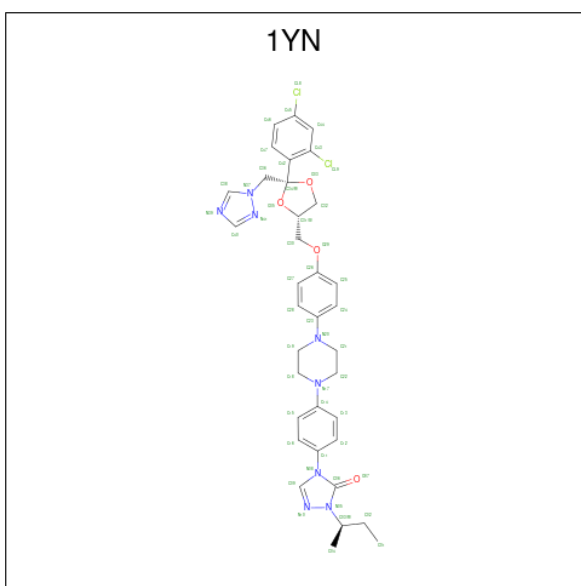
Chain	Residue	Modelled	Actual	Comment	Reference
A	529	GLY	-	expression tag	UNP P10613
A	530	GLY	-	expression tag	UNP P10613
A	531	ARG	-	expression tag	UNP P10613
A	532	HIS	-	expression tag	UNP P10613
A	533	HIS	-	expression tag	UNP P10613
A	534	HIS	-	expression tag	UNP P10613
A	535	HIS	-	expression tag	UNP P10613
A	536	HIS	-	expression tag	UNP P10613
A	537	HIS	-	expression tag	UNP P10613

- 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
			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: C₃₅H₃₈Cl₂N₈O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0
			49	35	2	8	4	

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.94Å 92.51Å 101.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.51 – 2.90 44.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.51-2.90) 99.7 (44.51-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.219 , 0.269 0.221 , 0.267	Depositor DCC
R_{free} test set	969 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	59.2	Xtriage
Anisotropy	1.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4092	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: 1YN, 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	0.42	0/4114	0.67	1/5576 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	295	GLN	CA-CB-CG	-5.06	103.98	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	SER	Peptide

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	4000	0	3937	122	0
2	A	43	0	30	5	0
3	A	49	0	38	5	0
All	All	4092	0	4005	125	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 15.

All (125) 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:336:GLU:OE2	1:A:361:SER:OG	1.97	0.83
1:A:270:ILE:HD13	1:A:281:LEU:HD13	1.67	0.76
1:A:121:LEU:HD21	1:A:228:PHE:CE1	2.21	0.76
1:A:237:ASN:OD1	1:A:246:ARG:NH2	2.19	0.74
1:A:227:GLY:O	1:A:232:ASN:ND2	2.20	0.72
1:A:374:MET:HE3	1:A:376:LEU:O	1.91	0.70
1:A:147:LYS:HA	1:A:150:LEU:HD12	1.73	0.70
1:A:98:PRO:HB3	1:A:457:SER:O	1.93	0.69
1:A:44:ARG:HB3	1:A:46:ASP:OD1	1.93	0.68
1:A:305:LEU:O	1:A:309:GLN:HB3	1.96	0.65
1:A:121:LEU:HD21	1:A:228:PHE:HE1	1.62	0.65
1:A:121:LEU:HD12	1:A:232:ASN:HD22	1.62	0.65
1:A:267:ARG:NH2	1:A:269:ASP:OD2	2.32	0.63
1:A:493:TRP:HB2	1:A:518:ILE:HG13	1.80	0.63
1:A:101:HIS:HB3	1:A:456:VAL:HG13	1.83	0.60
1:A:344:LYS:HE3	1:A:350:ASP:O	2.01	0.60
1:A:323:LEU:HB3	1:A:330:GLN:HG3	1.86	0.58
1:A:38:GLN:HE22	1:A:53:TYR:H	1.52	0.58
1:A:261:ILE:HG23	1:A:281:LEU:HD21	1.86	0.57
1:A:29:VAL:HB	1:A:30:PRO:HD3	1.87	0.57
1:A:272:PRO:HB3	1:A:282:ILE:HD12	1.86	0.57
1:A:249:ALA:O	1:A:253:ILE:HG13	2.07	0.55
1:A:26:LEU:HD12	1:A:29:VAL:HB	1.89	0.55
1:A:147:LYS:HD3	1:A:449:PHE:O	2.06	0.55
1:A:474:GLN:O	1:A:478:VAL:HG23	2.07	0.54
1:A:470:CYS:HB2	2:A:601:HEM:NA	2.21	0.54
1:A:262:LYS:O	1:A:266:GLU:HG3	2.08	0.54
1:A:412:SER:OG	1:A:414:ARG:HG3	2.07	0.54
1:A:31:PHE:O	1:A:35:LEU:HB2	2.08	0.54
1:A:265:ARG:HA	1:A:270:ILE:HD11	1.90	0.53
1:A:388:ARG:HA	1:A:395:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:HD11	1:A:491:LEU:HD21	1.89	0.53
1:A:25:ILE:C	1:A:27:LEU:H	2.17	0.53
1:A:321:LEU:HD13	1:A:501:PRO:HD2	1.91	0.53
1:A:333:ILE:HD11	1:A:484:LEU:HG	1.91	0.53
1:A:26:LEU:HD12	1:A:30:PRO:HD3	1.91	0.52
1:A:304:ILE:HG23	2:A:601:HEM:HBC1	1.91	0.52
1:A:403:LEU:HD23	1:A:404:VAL:O	2.10	0.51
1:A:309:GLN:HG3	1:A:310:HIS:N	2.26	0.51
1:A:114:ALA:HB3	1:A:468:HIS:CE1	2.46	0.50
1:A:130:VAL:HG21	1:A:300:LEU:N	2.26	0.50
1:A:121:LEU:HD12	1:A:232:ASN:HB2	1.92	0.50
1:A:237:ASN:HA	1:A:243:TYR:HD2	1.76	0.50
1:A:469:ARG:NH2	1:A:473:GLU:OE1	2.44	0.49
1:A:410:HIS:CD2	1:A:460:TYR:HA	2.48	0.49
1:A:466:GLY:O	1:A:469:ARG:HB2	2.13	0.49
3:A:602:1YN:O07	3:A:602:1YN:H1	2.14	0.48
1:A:164:GLU:CD	1:A:202:ARG:HH22	2.21	0.48
1:A:73:GLU:C	1:A:75:CYS:H	2.22	0.47
1:A:492:ARG:HG3	1:A:523:ARG:CZ	2.44	0.47
1:A:298:ALA:O	1:A:301:LEU:HB2	2.14	0.47
1:A:298:ALA:HA	1:A:301:LEU:HD12	1.96	0.47
1:A:410:HIS:NE2	1:A:460:TYR:HA	2.30	0.47
1:A:126:PHE:CE1	1:A:303:GLY:HA2	2.50	0.47
1:A:497:GLY:C	1:A:499:LYS:H	2.22	0.47
1:A:333:ILE:CD1	1:A:484:LEU:HG	2.45	0.47
1:A:278:ASP:O	1:A:281:LEU:N	2.47	0.47
1:A:319:PHE:CE1	1:A:484:LEU:HD13	2.50	0.46
1:A:364:ASN:O	1:A:368:GLU:N	2.36	0.46
1:A:67:GLN:HB3	1:A:70:GLU:HG3	1.97	0.46
1:A:237:ASN:HA	1:A:243:TYR:CD2	2.50	0.46
1:A:165:GLU:CD	1:A:210:ARG:HE	2.24	0.46
1:A:344:LYS:NZ	1:A:355:ASP:OD2	2.48	0.46
1:A:31:PHE:HE2	1:A:35:LEU:HD13	1.81	0.46
1:A:323:LEU:HD22	1:A:329:LEU:HB2	1.97	0.46
1:A:225:ASP:O	1:A:227:GLY:N	2.49	0.45
1:A:233:PHE:HE2	1:A:380:PHE:HE2	1.63	0.45
1:A:64:TYR:O	1:A:68:PRO:HB3	2.16	0.45
1:A:235:PHE:O	1:A:243:TYR:OH	2.32	0.45
1:A:319:PHE:O	1:A:323:LEU:HG	2.15	0.45
1:A:31:PHE:CE2	1:A:35:LEU:HD22	2.51	0.45
1:A:362:VAL:O	1:A:366:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASN:OD1	1:A:140:MET:HE3	2.16	0.45
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.53	0.45
1:A:97:GLY:O	1:A:100:GLY:N	2.49	0.45
1:A:209:MET:HA	1:A:209:MET:HE2	1.99	0.45
1:A:130:VAL:HG11	1:A:300:LEU:HB2	1.99	0.44
1:A:470:CYS:HB2	2:A:601:HEM:C1A	2.52	0.44
1:A:95:TYR:OH	1:A:99:LYS:HB3	2.17	0.44
1:A:215:ARG:C	1:A:217:PHE:H	2.25	0.44
1:A:215:ARG:HG2	1:A:217:PHE:H	1.82	0.44
1:A:229:THR:H	1:A:232:ASN:ND2	2.15	0.44
1:A:333:ILE:HG23	1:A:488:VAL:HG11	1.99	0.43
1:A:173:ASP:OD1	1:A:190:LYS:NZ	2.50	0.43
1:A:135:PRO:HG2	1:A:138:ARG:HG2	2.00	0.43
1:A:376:LEU:HD23	3:A:602:1YN:C26	2.48	0.43
1:A:118:TYR:CE1	3:A:602:1YN:H25	2.53	0.43
3:A:602:1YN:CL9	3:A:602:1YN:H33	2.56	0.43
1:A:319:PHE:C	1:A:319:PHE:CD1	2.96	0.43
1:A:367:LYS:HE3	1:A:460:TYR:HE2	1.82	0.43
1:A:388:ARG:CZ	1:A:395:ILE:HD11	2.48	0.43
1:A:231:ILE:HD12	1:A:231:ILE:HA	1.70	0.43
1:A:255:ALA:HA	1:A:258:MET:HE3	2.00	0.43
1:A:235:PHE:HB3	1:A:238:LEU:HD21	2.01	0.42
1:A:389:ILE:HG13	1:A:394:TYR:O	2.20	0.42
1:A:423:ASP:OD1	1:A:425:THR:OG1	2.34	0.42
2:A:601:HEM:HHA	2:A:601:HEM:HBD2	2.01	0.42
1:A:101:HIS:HA	1:A:404:VAL:HG21	2.01	0.42
1:A:292:MET:HE2	1:A:297:ILE:HG12	2.01	0.42
1:A:33:TYR:HA	1:A:36:VAL:HG12	2.01	0.42
1:A:299:ASN:N	1:A:299:ASN:OD1	2.52	0.42
1:A:225:ASP:C	1:A:227:GLY:H	2.28	0.41
1:A:405:SER:C	1:A:407:GLY:N	2.78	0.41
1:A:101:HIS:O	1:A:105:PHE:HB2	2.20	0.41
1:A:52:PHE:HE2	1:A:54:TRP:CE2	2.38	0.41
1:A:96:LEU:HD22	1:A:408:TYR:CD2	2.54	0.41
1:A:73:GLU:C	1:A:75:CYS:N	2.78	0.41
1:A:57:TRP:O	1:A:89:GLY:N	2.54	0.41
1:A:198:PHE:HE1	1:A:213:PHE:CD2	2.39	0.41
1:A:470:CYS:HA	2:A:601:HEM:C4D	2.55	0.41
1:A:53:TYR:CD2	1:A:59:GLY:HA2	2.55	0.41
1:A:233:PHE:CE2	1:A:380:PHE:HE2	2.38	0.41
1:A:319:PHE:CZ	1:A:484:LEU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLU:HG2	1:A:116:ASP:N	2.36	0.41
1:A:118:TYR:CZ	3:A:602:1YN:H27	2.55	0.41
1:A:480:LEU:H	1:A:480:LEU:HG	1.66	0.41
1:A:166:ILE:HD13	1:A:483:ILE:HA	2.03	0.41
1:A:405:SER:C	1:A:407:GLY:H	2.29	0.41
1:A:497:GLY:C	1:A:499:LYS:N	2.78	0.40
1:A:28:GLY:O	1:A:32:VAL:HG13	2.20	0.40
1:A:260:GLU:O	1:A:264:ARG:HG2	2.21	0.40
1:A:235:PHE:HB3	1:A:238:LEU:CD2	2.52	0.40
1:A:374:MET:SD	1:A:462:PRO:HA	2.62	0.40
1:A:392:THR:OG1	1:A:394:TYR:N	2.50	0.40
1:A:122:THR:HB	1:A:126:PHE:CE2	2.57	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	485/537 (90%)	425 (88%)	52 (11%)	8 (2%)	7	27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	ILE
1	A	74	SER
1	A	496	ASP
1	A	282	ILE
1	A	226	LYS
1	A	284	SER
1	A	426	ARG
1	A	241	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	438/478 (92%)	390 (89%)	48 (11%)	6 20

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	60	SER
1	A	70	GLU
1	A	109	LEU
1	A	121	LEU
1	A	123	THR
1	A	141	GLU
1	A	152	THR
1	A	154	SER
1	A	162	ILE
1	A	164	GLU
1	A	168	ASN
1	A	175	SER
1	A	178	LEU
1	A	196	THR
1	A	213	PHE
1	A	219	GLN
1	A	238	LEU
1	A	270	ILE
1	A	282	ILE
1	A	306	MET
1	A	309	GLN
1	A	319	PHE
1	A	333	ILE
1	A	336	GLU
1	A	337	VAL
1	A	338	VAL
1	A	341	LEU
1	A	347	ASP
1	A	361	SER

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Mol	Chain	Res	Type
1	A	372	MET
1	A	388	ARG
1	A	389	ILE
1	A	402	VAL
1	A	411	THR
1	A	412	SER
1	A	414	ARG
1	A	417	ASP
1	A	451	LYS
1	A	456	VAL
1	A	471	ILE
1	A	474	GLN
1	A	482	THR
1	A	506	SER
1	A	507	SER
1	A	511	LEU
1	A	518	ILE
1	A	524	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	192	GLN
1	A	232	ASN
1	A	328	HIS
1	A	490	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	1YN	A	602	2	54,55,55	0.65	2 (3%)	76,79,79	1.27	9 (11%)
2	HEM	A	601	3,1	50,50,50	1.84	8 (16%)	67,82,82	1.24	9 (13%)

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	1YN	A	602	2	-	11/34/55/55	0/7/7/7
2	HEM	A	601	3,1	-	2/14/54/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	FE-NA	7.75	2.20	1.95
2	A	601	HEM	FE-ND	5.50	2.11	1.94
3	A	602	1YN	C09-N10	3.05	1.35	1.30
2	A	601	HEM	CAC-C3C	3.03	1.55	1.47
2	A	601	HEM	FE-NB	-2.74	1.86	1.94
2	A	601	HEM	CAB-C3B	2.72	1.54	1.47
2	A	601	HEM	CMB-C2B	2.39	1.55	1.50
2	A	601	HEM	CMC-C2C	2.24	1.55	1.50
2	A	601	HEM	FE-NC	-2.16	1.88	1.95
3	A	602	1YN	C34-C42	2.07	1.56	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	1YN	C34-C36-N37	-4.74	106.94	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	1YN	C09-N08-C06	4.54	110.62	107.27
3	A	602	1YN	O35-C34-C36	-3.61	104.22	109.00
2	A	601	HEM	CHC-C4B-NB	2.99	127.64	124.42
3	A	602	1YN	C36-C34-C42	2.90	113.67	109.59
3	A	602	1YN	O33-C34-C42	-2.86	106.47	111.37
3	A	602	1YN	C47-C42-C34	2.78	121.02	119.18
2	A	601	HEM	CAD-CBD-CGD	-2.71	106.48	113.67
2	A	601	HEM	O2A-CGA-CBA	2.69	122.50	114.00
2	A	601	HEM	O1A-CGA-CBA	-2.62	114.79	123.09
3	A	602	1YN	O35-C34-C42	2.46	118.01	111.00
2	A	601	HEM	C4C-C3C-C2C	2.45	108.94	106.81
3	A	602	1YN	C34-C42-C43	-2.43	122.00	123.72
2	A	601	HEM	CHD-C1D-ND	2.19	126.78	124.42
3	A	602	1YN	C11-N08-C06	-2.08	123.79	125.87
2	A	601	HEM	C2B-C1B-NB	-2.07	107.46	109.84
2	A	601	HEM	C3B-C2B-C1B	2.03	107.94	106.41
2	A	601	HEM	C4A-C3A-C2A	2.01	109.11	106.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	1YN	O33-C34-C36-N37
3	A	602	1YN	C42-C34-C36-N37
3	A	602	1YN	C12-C11-N08-C09
2	A	601	HEM	C2D-C3D-CAD-CBD
2	A	601	HEM	C4D-C3D-CAD-CBD
3	A	602	1YN	C12-C11-N08-C06
3	A	602	1YN	O35-C34-C36-N37
3	A	602	1YN	C36-C34-C42-C47
3	A	602	1YN	C34-C36-N37-N41
3	A	602	1YN	C16-C11-N08-C09
3	A	602	1YN	C36-C34-C42-C43
3	A	602	1YN	C04-C03-N05-C06
3	A	602	1YN	C04-C03-N05-N10

There are no ring outliers.

2 monomers are involved in 10 short contacts:

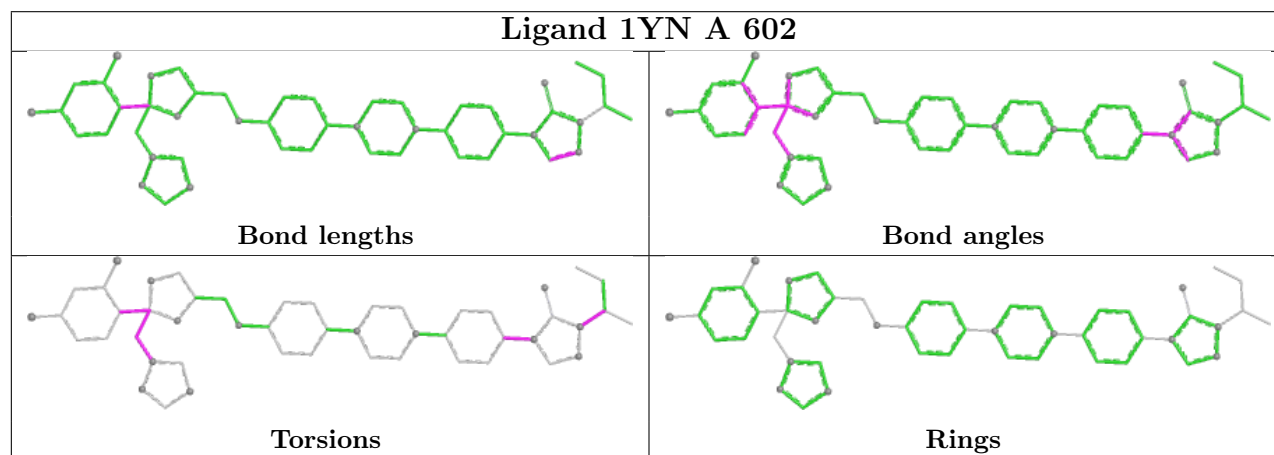
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	1YN	5	0

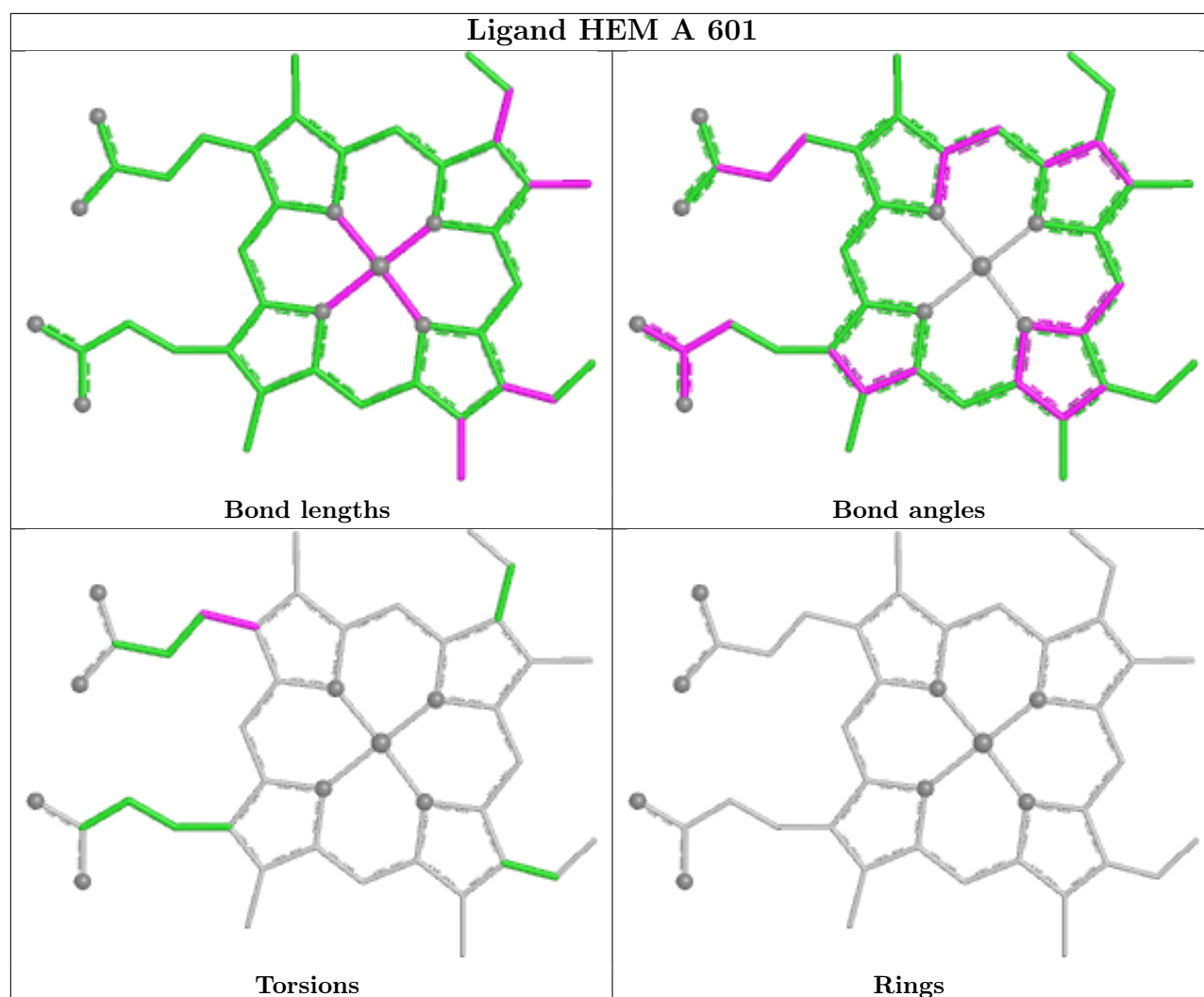
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	5	0

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.





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	488/537 (90%)	0.54	37 (7%) 20 16	40, 66, 112, 130	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	HIS	6.3
1	A	25	ILE	5.6
1	A	43	LEU	4.8
1	A	510	VAL	4.8
1	A	77[A]	GLN	4.3
1	A	174	GLU	4.0
1	A	214	ASP	3.7
1	A	289	GLY	3.2
1	A	52	PHE	3.2
1	A	29	VAL	3.0
1	A	41	TYR	3.0
1	A	27	LEU	2.9
1	A	318	TRP	2.8
1	A	216	SER	2.8
1	A	420	GLU	2.7
1	A	233	PHE	2.7
1	A	347	ASP	2.7
1	A	50	LEU	2.7
1	A	40	LEU	2.6
1	A	272	PRO	2.6
1	A	335	GLN	2.6
1	A	339	GLU	2.6
1	A	26	LEU	2.6
1	A	28	GLY	2.5
1	A	72	PHE	2.5
1	A	185	VAL	2.5
1	A	422	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	215	ARG	2.3
1	A	310	HIS	2.3
1	A	39	TYR	2.2
1	A	511	LEU	2.2
1	A	411	THR	2.2
1	A	267	ARG	2.1
1	A	179	LYS	2.1
1	A	505	TYR	2.1
1	A	372	MET	2.0
1	A	341	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](#)

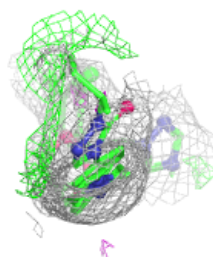
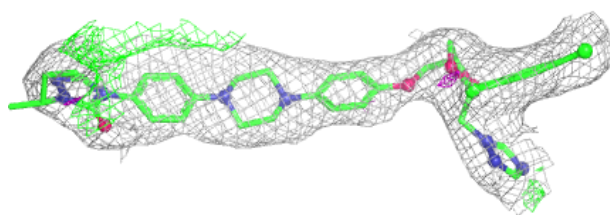
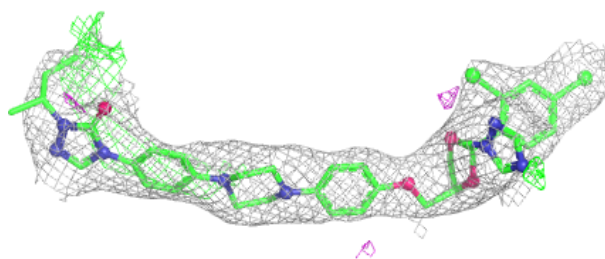
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	1YN	A	602	49/49	0.86	0.16	46,76,112,120	0
2	HEM	A	601	43/43	0.98	0.09	34,49,55,57	0

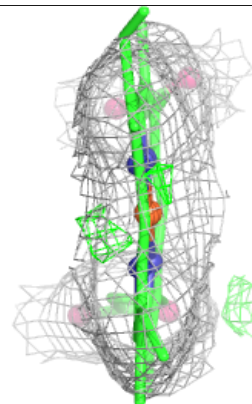
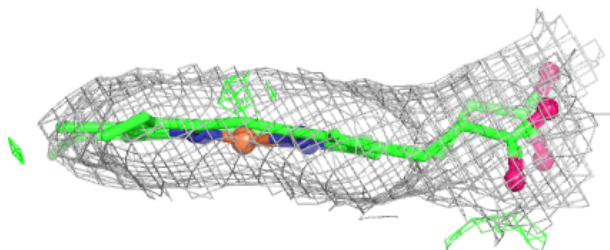
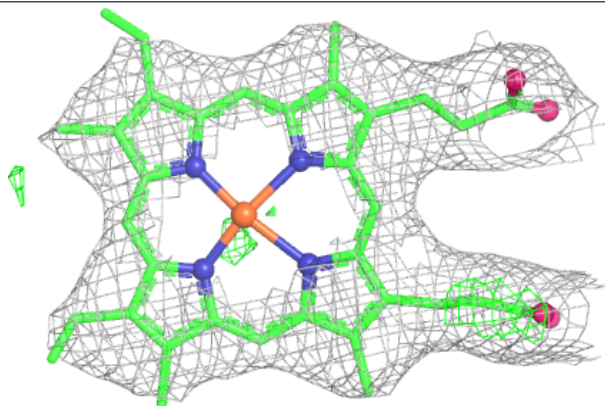
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1YN A 602:

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

**Electron density around HEM A 601:**

$2mF_o-DF_c$ (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.