Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:57 AM UTC

PDB ID	:	5ESG / pdb_00005esg
Title	:	Saccharomyces cerevisiae CYP51 (Lanosterol 14-alpha demethylase) G73E mutant complexed with itraconazole
Authors	:	Sagatova, A.; Keniya, M.V.; Wilson, R.K.; Sabherwal, M.; Tyndall, J.D.A.; Monk, B.C.
Deposited on	:	2015-11-16
Resolution	:	1.98 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:

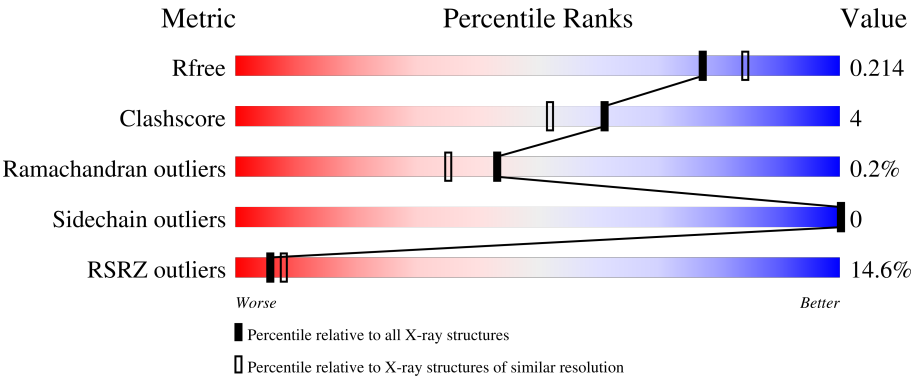
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	539	14% 88% 9% .

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4507 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.

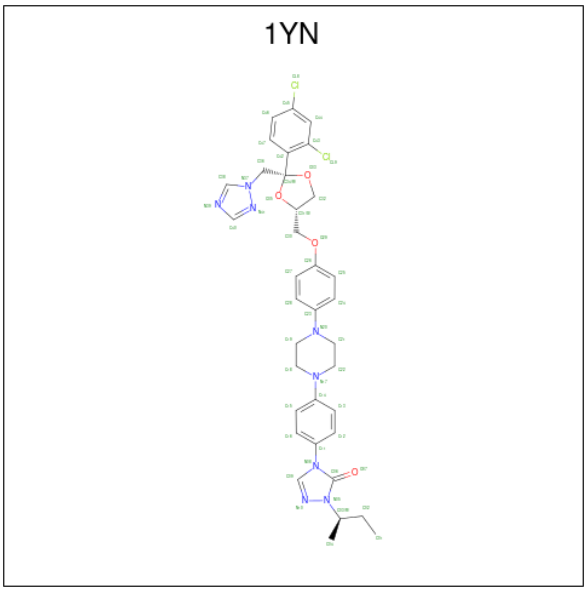
- Molecule 1 is a protein called Lanosterol 14-alpha demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	526	Total	C	N	O	S	0	0	0
			4258	2757	718	762	21			

There are 10 discrepancies between the modelled and reference sequences:

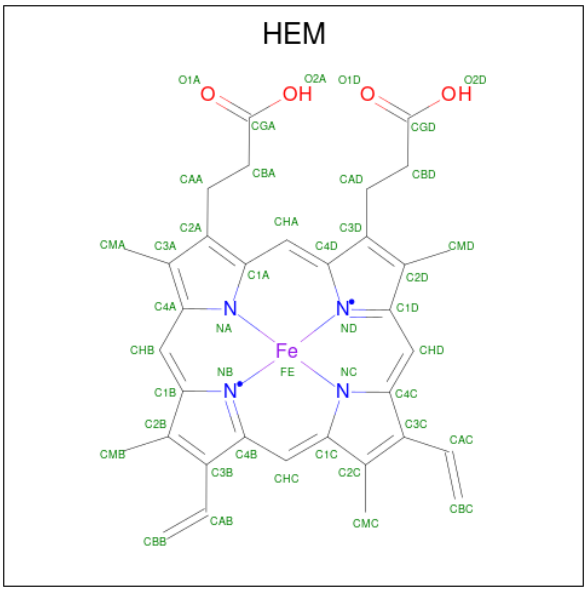
Chain	Residue	Modelled	Actual	Comment	Reference
A	73	GLU	GLY	engineered mutation	UNP A6ZSR0
A	531	GLY	-	expression tag	UNP A6ZSR0
A	532	GLY	-	expression tag	UNP A6ZSR0
A	533	ARG	-	expression tag	UNP A6ZSR0
A	534	HIS	-	expression tag	UNP A6ZSR0
A	535	HIS	-	expression tag	UNP A6ZSR0
A	536	HIS	-	expression tag	UNP A6ZSR0
A	537	HIS	-	expression tag	UNP A6ZSR0
A	538	HIS	-	expression tag	UNP A6ZSR0
A	539	HIS	-	expression tag	UNP A6ZSR0

- Molecule 2 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
2	A	1	Total	C	Cl	N	O	0	0
			49	35	2	8	4		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

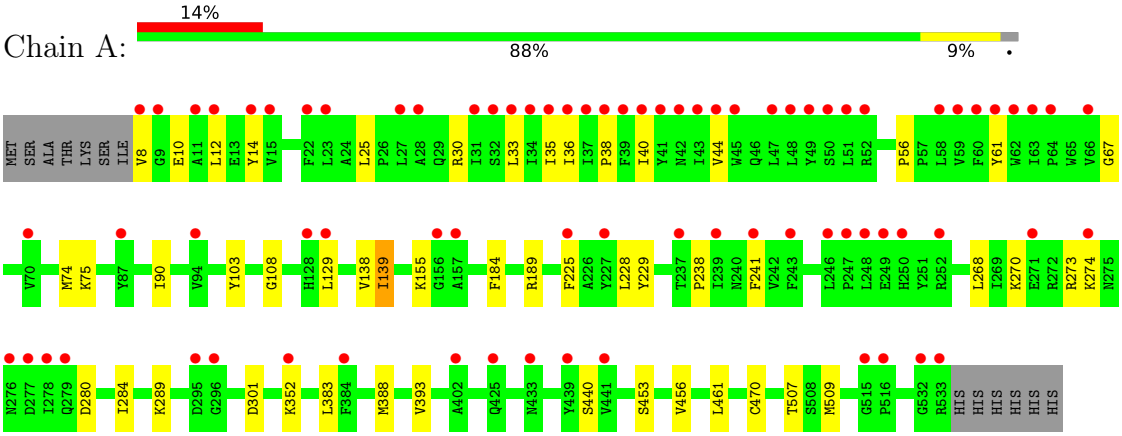
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	157	Total O 157 157	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: Lanosterol 14-alpha demethylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.24Å 67.31Å 80.83Å 90.00° 98.65° 90.00°	Depositor
Resolution (Å)	33.66 – 1.98 33.66 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.66-1.98) 93.9 (33.66-1.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.199 , 0.234 (Not available) , 0.214	Depositor DCC
R_{free} test set	2899 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.647	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4507	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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

5.1 Standard geometry

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	0.50	0/4375	0.76	1/5927 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	PRO	O-C-N	5.54	123.86	121.31

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	4258	0	4244	33	0
2	A	49	0	38	3	0
3	A	43	0	30	4	0
4	A	157	0	0	2	0
All	All	4507	0	4312	36	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 4.

All (36) 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:456:VAL:HG12	1:A:461:LEU:HD11	1.70	0.74
1:A:238:PRO:HD3	1:A:509:MET:HG2	1.71	0.73
1:A:33:LEU:HA	1:A:36:ILE:HG22	1.75	0.67
1:A:25:LEU:O	1:A:30:ARG:NH1	2.31	0.63
2:A:701:1YN:H20	4:A:873:HOH:O	2.05	0.57
1:A:273:ARG:NH2	1:A:301:ASP:OD2	2.38	0.56
1:A:280:ASP:OD1	1:A:289:LYS:NZ	2.29	0.54
1:A:155:LYS:NZ	4:A:804:HOH:O	2.40	0.54
1:A:470:CYS:HB2	3:A:702:HEM:NA	2.27	0.49
1:A:270:LYS:HB3	1:A:274:LYS:HE3	1.94	0.49
1:A:129:LEU:HD11	1:A:241:PHE:HD1	1.78	0.49
3:A:702:HEM:HBB2	3:A:702:HEM:HMB2	1.96	0.48
1:A:138:VAL:HG23	1:A:139:ILE:HG12	1.95	0.48
1:A:103:TYR:O	1:A:108:GLY:HA3	2.14	0.47
1:A:184:PHE:O	1:A:189:ARG:HD3	2.13	0.47
1:A:388:MET:HA	1:A:388:MET:HE2	1.96	0.47
1:A:238:PRO:HG2	1:A:507:THR:O	2.15	0.46
1:A:383:LEU:HD22	3:A:702:HEM:HBA2	1.98	0.46
1:A:440:SER:HB2	1:A:453:SER:HB2	1.98	0.46
1:A:470:CYS:HA	3:A:702:HEM:C4D	2.51	0.45
2:A:701:1YN:O07	2:A:701:1YN:H1	2.16	0.45
1:A:268:LEU:HD23	1:A:284:ILE:HD13	2.00	0.44
1:A:225:PHE:CD1	1:A:228:LEU:HD12	2.53	0.44
1:A:36:ILE:O	1:A:40:ILE:HG12	2.18	0.43
1:A:35:ILE:O	1:A:38:PRO:HD2	2.18	0.43
1:A:129:LEU:HD11	1:A:241:PHE:CD1	2.53	0.43
1:A:352:LYS:HA	1:A:352:LYS:HD3	1.88	0.43
1:A:509:MET:HE2	2:A:701:1YN:H23	2.01	0.43
1:A:10:GLU:O	1:A:14:TYR:HD2	2.03	0.42
1:A:225:PHE:CE2	1:A:229:TYR:HE1	2.38	0.42
1:A:8:VAL:O	1:A:12:LEU:HD12	2.20	0.41
1:A:40:ILE:O	1:A:44:VAL:HG23	2.21	0.41
1:A:61:TYR:CD2	1:A:67:GLY:HA2	2.56	0.41
1:A:74:MET:O	1:A:75:LYS:HD2	2.20	0.41
1:A:90:ILE:HD13	1:A:393:VAL:HG11	2.02	0.40
1:A:238:PRO:CA	1:A:509:MET:HE3	2.52	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	524/539 (97%)	505 (96%)	18 (3%)	1 (0%)	43 35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ILE

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	462/474 (98%)	462 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

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	276	ASN
1	A	302	GLN
1	A	368	GLN

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)

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	$\#\|Z\| > 2$
2	1YN	A	701	3	54,55,55	0.53	2 (3%)	76,79,79	0.98	4 (5%)
3	HEM	A	702	2,1	50,50,50	1.89	9 (18%)	67,82,82	1.30	5 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1YN	A	701	3	-	14/34/55/55	0/7/7/7
3	HEM	A	702	2,1	-	1/14/54/54	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	HEM	C3D-C2D	7.63	1.53	1.36
3	A	702	HEM	FE-ND	5.94	2.13	1.94
3	A	702	HEM	FE-NB	3.98	2.07	1.94
3	A	702	HEM	CAB-C3B	2.90	1.55	1.47
2	A	701	1YN	C09-N10	2.80	1.34	1.30
3	A	702	HEM	CAC-C3C	2.78	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	HEM	CMD-C2D	2.71	1.56	1.50
3	A	702	HEM	FE-NA	2.27	2.02	1.95
3	A	702	HEM	FE-NC	2.09	2.02	1.95
2	A	701	1YN	C36-C34	2.05	1.55	1.52
3	A	702	HEM	CMB-C2B	2.00	1.54	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	HEM	C4D-ND-C1D	5.32	111.50	105.21
2	A	701	1YN	C36-C34-C42	3.87	115.03	109.59
2	A	701	1YN	C34-C36-N37	-3.60	108.35	112.81
2	A	701	1YN	C09-N08-C06	3.57	109.91	107.27
3	A	702	HEM	C1B-NB-C4B	2.53	108.21	105.21
3	A	702	HEM	CAD-C3D-C4D	2.22	128.56	124.70
3	A	702	HEM	CMD-C2D-C1D	2.11	128.33	125.03
2	A	701	1YN	O33-C34-C42	-2.08	107.81	111.37
3	A	702	HEM	CAD-CBD-CGD	-2.05	108.24	113.67

There are no chirality outliers.

All (15) torsion outliers are listed below:

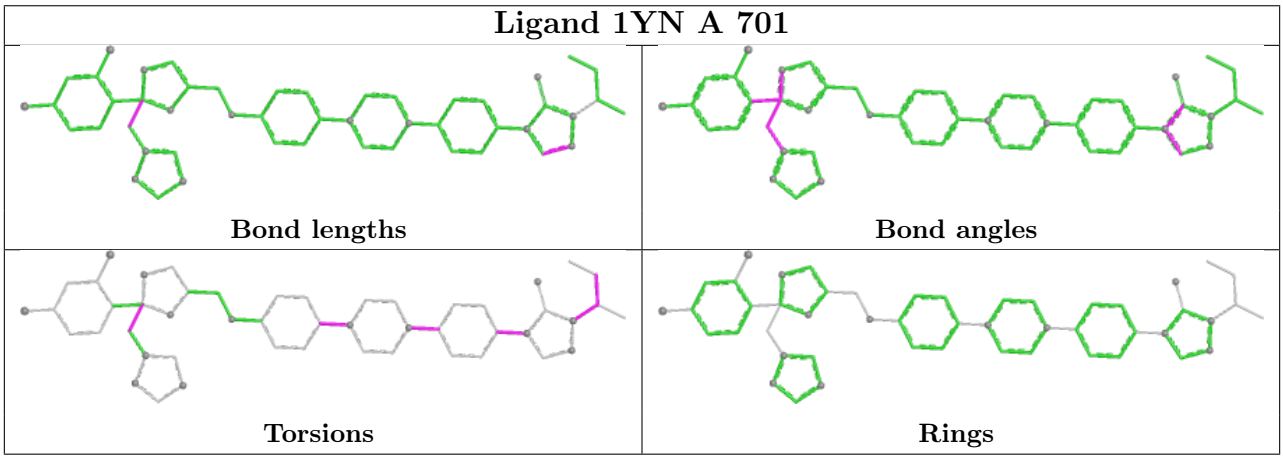
Mol	Chain	Res	Type	Atoms
2	A	701	1YN	C04-C03-N05-N10
2	A	701	1YN	O33-C34-C36-N37
2	A	701	1YN	C42-C34-C36-N37
2	A	701	1YN	C12-C11-N08-C09
2	A	701	1YN	C16-C11-N08-C09
2	A	701	1YN	C01-C02-C03-N05
2	A	701	1YN	C04-C03-N05-C06
2	A	701	1YN	C12-C11-N08-C06
2	A	701	1YN	C16-C11-N08-C06
2	A	701	1YN	O35-C34-C36-N37
2	A	701	1YN	C01-C02-C03-C04
2	A	701	1YN	C28-C23-N20-C21
2	A	701	1YN	C15-C14-N17-C22
2	A	701	1YN	C24-C23-N20-C21
3	A	702	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

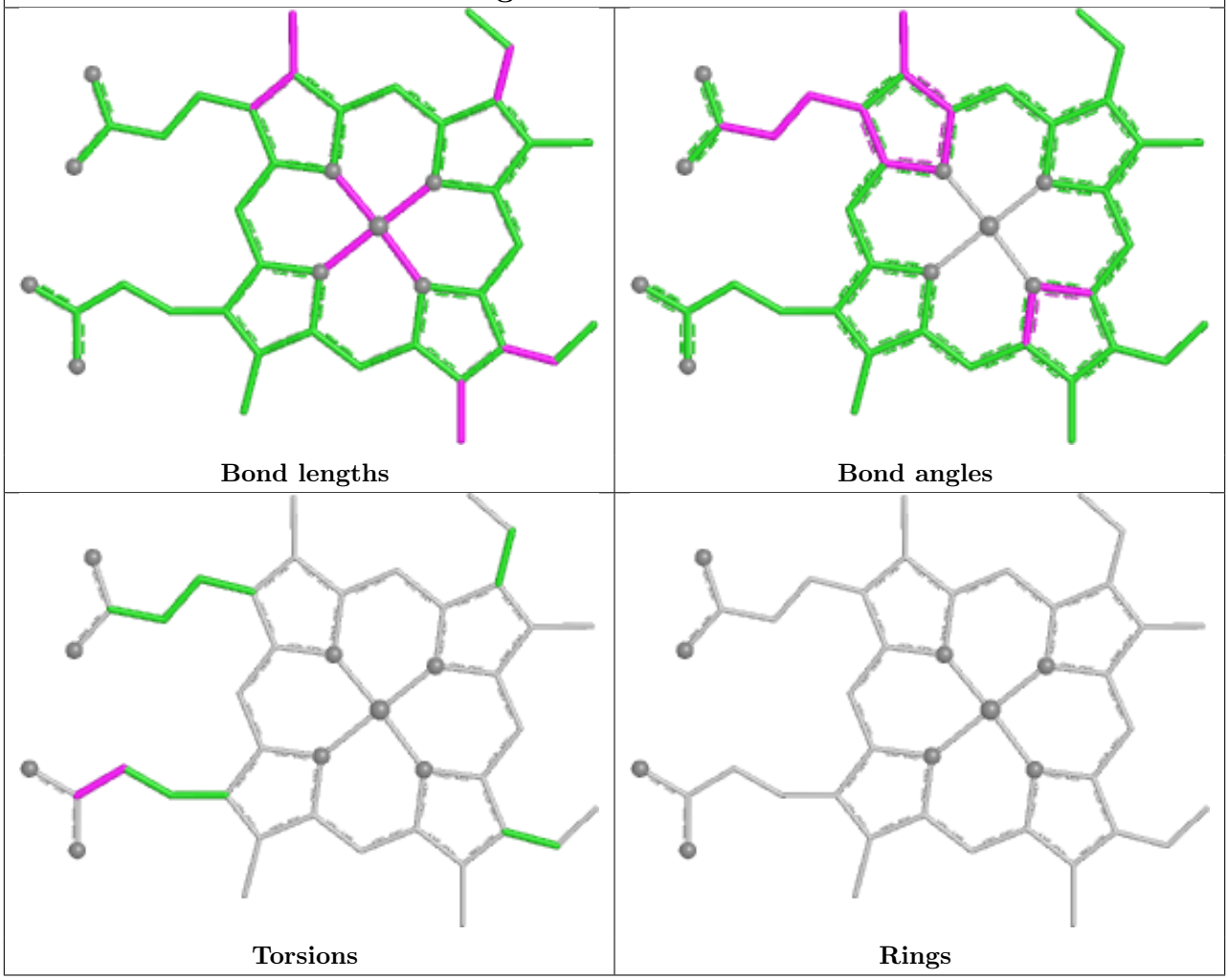
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	1YN	3	0
3	A	702	HEM	4	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 702



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	526/539 (97%)	0.80	77 (14%)	6	8	23, 39, 68, 82	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	PHE	5.9
1	A	27	LEU	5.5
1	A	63	ILE	4.7
1	A	36	ILE	4.6
1	A	439	TYR	4.5
1	A	12	LEU	4.4
1	A	40	ILE	4.3
1	A	43	ILE	4.2
1	A	225	PHE	4.1
1	A	35	ILE	4.1
1	A	37	ILE	3.9
1	A	66	VAL	3.8
1	A	8	VAL	3.7
1	A	441	VAL	3.7
1	A	47	LEU	3.7
1	A	31	ILE	3.7
1	A	532	GLY	3.7
1	A	44	VAL	3.6
1	A	41	TYR	3.6
1	A	249	GLU	3.4
1	A	246	LEU	3.3
1	A	28	ALA	3.3
1	A	70	VAL	3.3
1	A	515	GLY	3.3
1	A	274	LYS	3.1
1	A	156	GLY	3.1
1	A	276	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	247	PRO	3.0
1	A	384	PHE	3.0
1	A	11	ALA	2.9
1	A	48	LEU	2.9
1	A	248	LEU	2.9
1	A	352	LYS	2.9
1	A	45	TRP	2.9
1	A	23	LEU	2.9
1	A	34	ILE	2.9
1	A	49	TYR	2.8
1	A	250	HIS	2.8
1	A	516	PRO	2.8
1	A	62	TRP	2.8
1	A	32	SER	2.8
1	A	402	ALA	2.8
1	A	129	LEU	2.7
1	A	128	HIS	2.7
1	A	38	PRO	2.7
1	A	271	GLU	2.6
1	A	239	ILE	2.6
1	A	9	GLY	2.6
1	A	243	PHE	2.5
1	A	58	LEU	2.5
1	A	60	PHE	2.5
1	A	52	ARG	2.4
1	A	533	ARG	2.4
1	A	296	GLY	2.4
1	A	51	LEU	2.4
1	A	14	TYR	2.4
1	A	22	PHE	2.4
1	A	252	ARG	2.4
1	A	157	ALA	2.4
1	A	279	GLN	2.4
1	A	15	VAL	2.3
1	A	39	PHE	2.3
1	A	87	TYR	2.3
1	A	227	TYR	2.2
1	A	295	ASP	2.2
1	A	278	ILE	2.2
1	A	425	GLN	2.2
1	A	277	ASP	2.2
1	A	61	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	237	THR	2.1
1	A	50	SER	2.1
1	A	59	VAL	2.1
1	A	94	VAL	2.1
1	A	42	ASN	2.0
1	A	433	ASN	2.0
1	A	64	PRO	2.0
1	A	33	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)

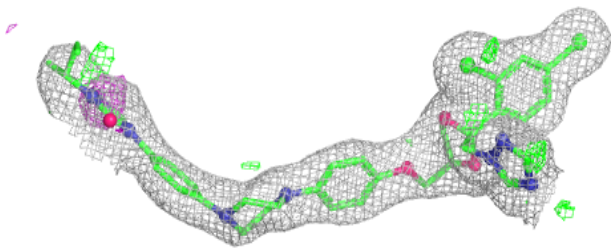
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

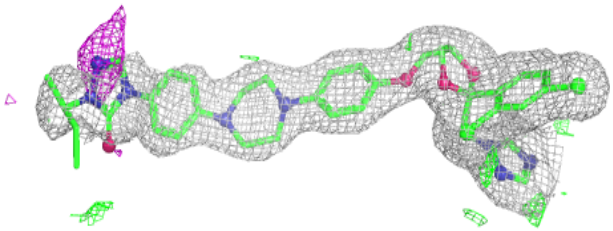
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	1YN	A	701	49/49	0.94	0.12	26,39,75,77	0
3	HEM	A	702	43/43	0.98	0.07	24,27,30,34	0

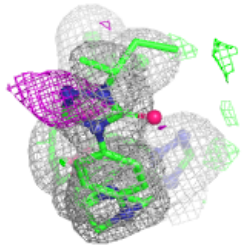
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1YN A 701:

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

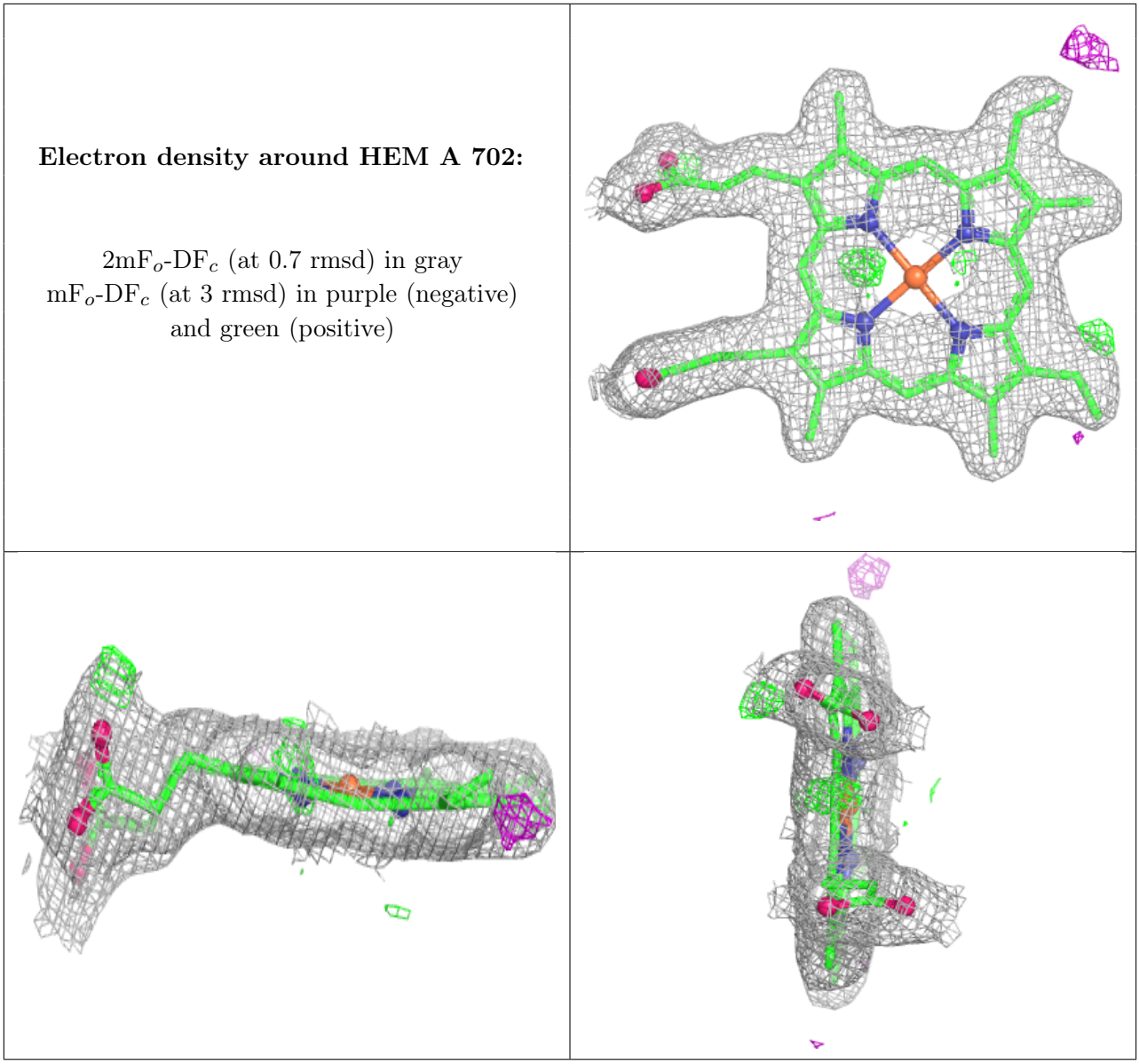






Electron density around HEM A 702:

$2mF_o$-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.