



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:18 PM UTC

PDB ID : 7RYX / pdb_00007ryx
Title : S. CEREVISIAE CYP51 COMPLEXED WITH VT-1129
Authors : Ruma, Y.N.; Sagatova, A.; Keniya, M.V.; Tyndall, J.D.; Monk, B.C.
Deposited on : 2021-08-26
Resolution : 2.10 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

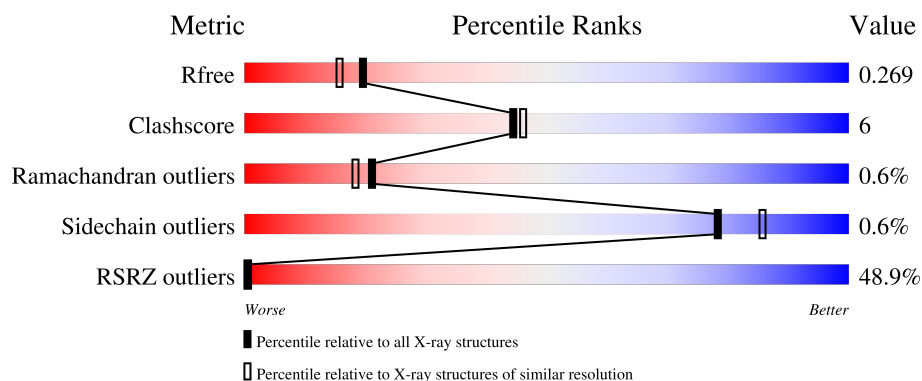
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	536	48% 84% 14%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4391 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.

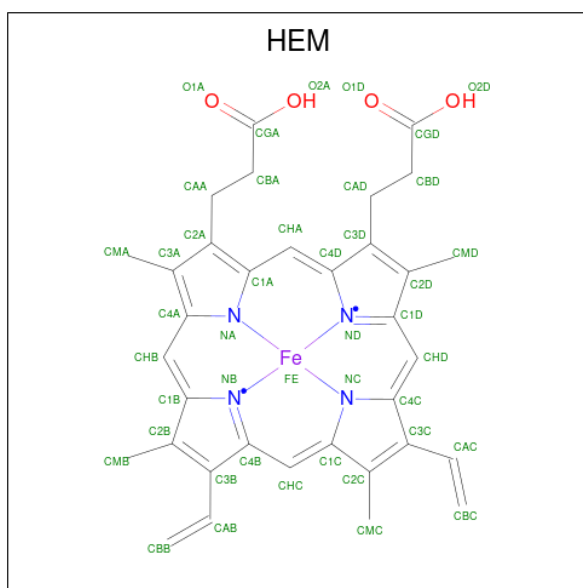
- Molecule 1 is a protein called Lanosterol 14- α demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	528	4271	2766	722	762	21	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

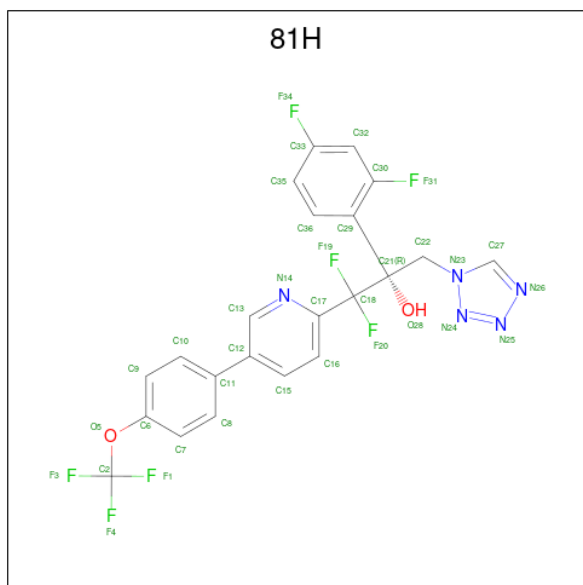
Chain	Residue	Modelled	Actual	Comment	Reference
A	531	GLY	-	expression tag	UNP A6ZSR0
A	532	GLY	-	expression tag	UNP A6ZSR0
A	533	ARG	-	expression tag	UNP A6ZSR0
A	534	HIS	-	expression tag	UNP A6ZSR0
A	535	HIS	-	expression tag	UNP A6ZSR0
A	536	HIS	-	expression tag	UNP A6ZSR0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is (2R)-2-(2,4-difluorophenyl)-1,1-difluoro-3-(1H-tetrazol-1-yl)-1-{5-[4-(trifluoromethoxy)phenyl]pyridin-2-yl}propan-2-ol (CCD ID: 81H) (formula: C₂₂H₁₄F₇N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	
			36	22	7	5	2	

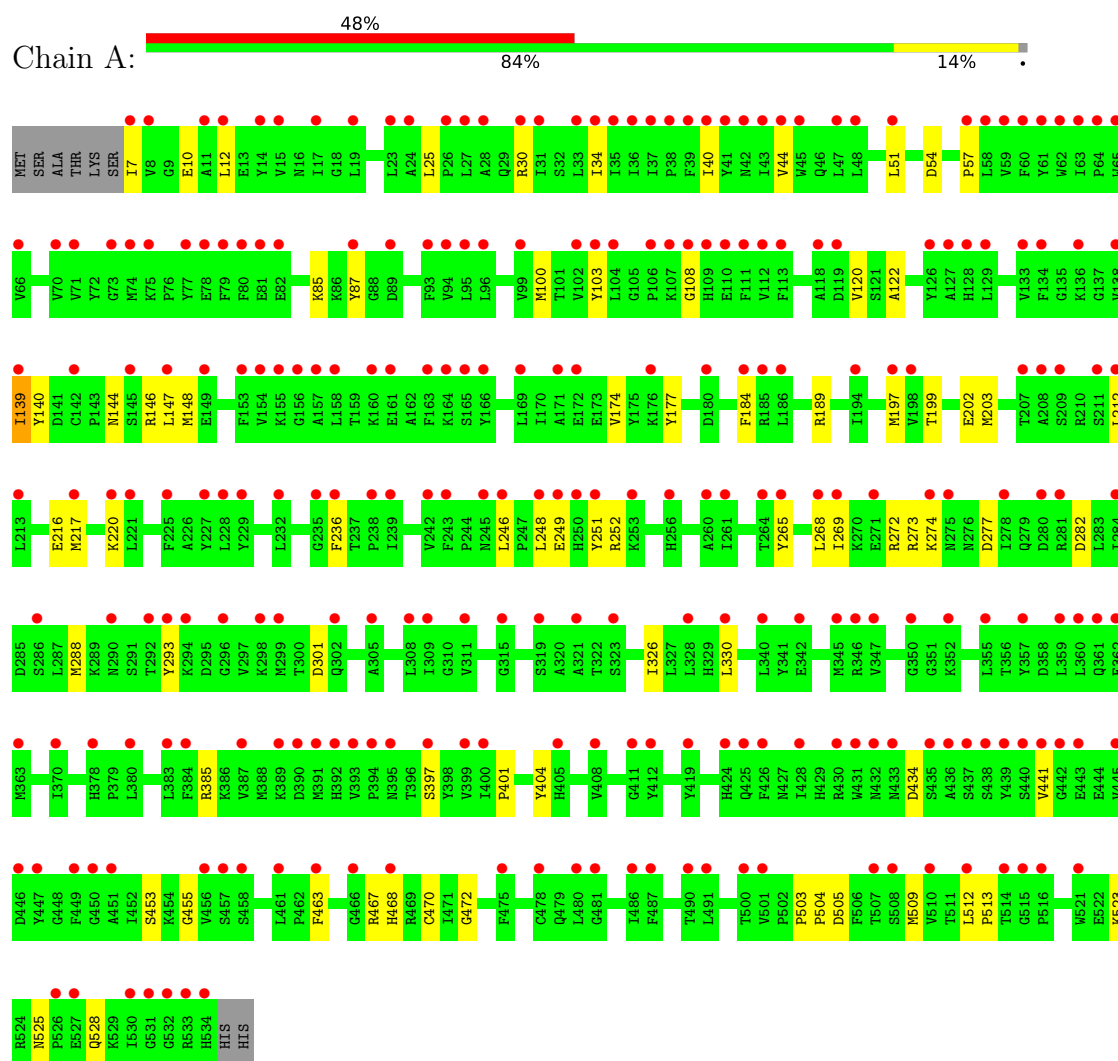
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	41	Total O 41 41	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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.40Å 67.98Å 80.30Å 90.00° 99.38° 90.00°	Depositor
Resolution (Å)	45.19 – 2.10 45.19 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.19-2.10) 99.8 (45.19-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.10Å)	Xtriage
Refinement program	PHENIX v1.19.2-4158	Depositor
R, R_{free}	0.234 , 0.268 0.235 , 0.269	Depositor DCC
R_{free} test set	2360 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.909	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4391	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 81H, 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	0.37	0/4389	0.53	0/5946

There are no bond length outliers.

There are no bond angle outliers.

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	4271	0	4259	50	0
2	A	43	0	30	6	0
3	A	36	0	0	0	0
4	A	41	0	0	2	0
All	All	4391	0	4289	52	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 6.

All (52) 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:268:LEU:HD21	1:A:272:ARG:HH21	1.52	0.73
1:A:272:ARG:HG2	1:A:277:ASP:HB3	1.70	0.72
1:A:220:LYS:NZ	4:A:701:HOH:O	2.23	0.65
1:A:7:ILE:HG22	1:A:10:GLU:H	1.61	0.65
1:A:217:MET:HE2	1:A:265:TYR:HE1	1.62	0.65
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.84	0.58
1:A:249:GLU:HG2	1:A:252:ARG:HH12	1.69	0.58
1:A:189:ARG:NH2	4:A:703:HOH:O	2.39	0.55
1:A:470:CYS:HA	2:A:601:HEM:C4D	2.41	0.55
1:A:453:SER:OG	1:A:455:GLY:O	2.26	0.54
1:A:174:VAL:HG13	1:A:203:MET:HE1	1.90	0.54
1:A:273:ARG:NH2	1:A:301:ASP:OD2	2.43	0.52
2:A:601:HEM:HHA	2:A:601:HEM:HBD2	1.93	0.51
1:A:216:GLU:H	1:A:216:GLU:CD	2.19	0.51
1:A:217:MET:HE2	1:A:265:TYR:CE1	2.44	0.50
1:A:523:LYS:NZ	1:A:528:GLN:O	2.44	0.50
1:A:326:ILE:O	1:A:330:LEU:HG	2.12	0.49
1:A:103:TYR:O	1:A:108:GLY:HA3	2.13	0.49
1:A:199:THR:O	1:A:203:MET:HG3	2.13	0.48
1:A:246:LEU:HB2	1:A:251:TYR:CE2	2.49	0.47
1:A:30:ARG:O	1:A:34:ILE:HG13	2.15	0.47
1:A:122:ALA:HB3	1:A:468:HIS:CE1	2.50	0.47
1:A:184:PHE:O	1:A:189:ARG:HD3	2.14	0.47
1:A:236:PHE:CE1	1:A:509:MET:HE2	2.49	0.47
1:A:463:PHE:HB3	1:A:470:CYS:HB3	1.97	0.46
1:A:236:PHE:CD2	1:A:509:MET:HG2	2.51	0.46
1:A:146:ARG:HD2	1:A:293:TYR:CZ	2.50	0.45
1:A:467:ARG:HG3	1:A:468:HIS:CD2	2.52	0.45
1:A:246:LEU:O	1:A:248:LEU:N	2.45	0.45
1:A:25:LEU:HB2	1:A:30:ARG:HG3	1.98	0.44
1:A:401:PRO:HG2	1:A:404:TYR:CE1	2.52	0.44
1:A:212:LEU:O	1:A:282:ASP:HB2	2.17	0.44
1:A:268:LEU:HD21	1:A:272:ARG:NH2	2.26	0.43
1:A:470:CYS:HB2	2:A:601:HEM:NA	2.33	0.43
1:A:40:ILE:O	1:A:44:VAL:HG23	2.19	0.43
1:A:525:ASN:C	1:A:525:ASN:HD22	2.26	0.43
1:A:144:ASN:ND2	1:A:148:MET:HE3	2.33	0.43
1:A:85:LYS:HA	1:A:85:LYS:HD2	1.63	0.42
1:A:57:PRO:HG2	1:A:87:TYR:HB3	2.01	0.42
1:A:144:ASN:HD21	1:A:148:MET:HE3	1.84	0.42
1:A:100:MET:HE3	1:A:100:MET:HB3	1.80	0.42
1:A:139:ILE:HA	1:A:147:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLY:HA3	2:A:601:HEM:C3C	2.55	0.41
1:A:197:MET:SD	1:A:513:PRO:HG2	2.60	0.41
1:A:54:ASP:HA	1:A:397:SER:O	2.20	0.41
1:A:120:VAL:HB	1:A:385:ARG:HB3	2.03	0.41
1:A:177:TYR:OH	1:A:202:GLU:OE1	2.26	0.41
1:A:140:TYR:OH	2:A:601:HEM:O2D	2.19	0.41
1:A:269:ILE:HA	1:A:288:MET:HE2	2.04	0.40
1:A:505:ASP:HB3	1:A:512:LEU:HD23	2.02	0.40
1:A:217:MET:HA	1:A:217:MET:HE3	2.04	0.40
1:A:503:PRO:HA	1:A:504:PRO:HD3	1.97	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	526/536 (98%)	502 (95%)	21 (4%)	3 (1%)	21 18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	ILE
1	A	434	ASP
1	A	441	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	463/470 (98%)	460 (99%)	3 (1%)	78 86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	51	LEU
1	A	274	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	183	ASN
1	A	200	GLN
1	A	275	ASN
1	A	302	GLN
1	A	474	HIS
1	A	525	ASN
1	A	528	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	HEM	A	601	1,3	50,50,50	1.66	8 (16%)	67,82,82	1.45	10 (14%)
3	81H	A	602	2	36,39,39	0.29	0	52,59,59	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
2	HEM	A	601	1,3	-	4/14/54/54	-
3	81H	A	602	2	-	1/32/35/35	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	FE-NB	5.29	2.11	1.94
2	A	601	HEM	FE-NC	4.56	2.10	1.95
2	A	601	HEM	FE-ND	3.89	2.06	1.94
2	A	601	HEM	FE-NA	3.45	2.06	1.95
2	A	601	HEM	CAB-C3B	3.01	1.55	1.47
2	A	601	HEM	CAC-C3C	2.98	1.55	1.47
2	A	601	HEM	CMC-C2C	2.45	1.55	1.50
2	A	601	HEM	CMD-C2D	2.40	1.55	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	C1B-NB-C4B	4.01	109.96	105.21
2	A	601	HEM	C4D-ND-C1D	3.71	109.60	105.21
2	A	601	HEM	C3B-C2B-C1B	3.57	109.09	106.41
2	A	601	HEM	C2B-C1B-NB	-3.20	106.16	109.84
2	A	601	HEM	C3D-C4D-ND	-2.63	107.29	110.17
2	A	601	HEM	CMB-C2B-C1B	-2.54	121.07	125.03
2	A	601	HEM	C2D-C1D-ND	-2.50	107.02	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	CHB-C1B-NB	2.25	127.16	124.37
2	A	601	HEM	O1A-CGA-CBA	-2.18	116.17	123.09
2	A	601	HEM	CHD-C1D-ND	2.07	126.65	124.42

There are no chirality outliers.

All (5) torsion outliers are listed below:

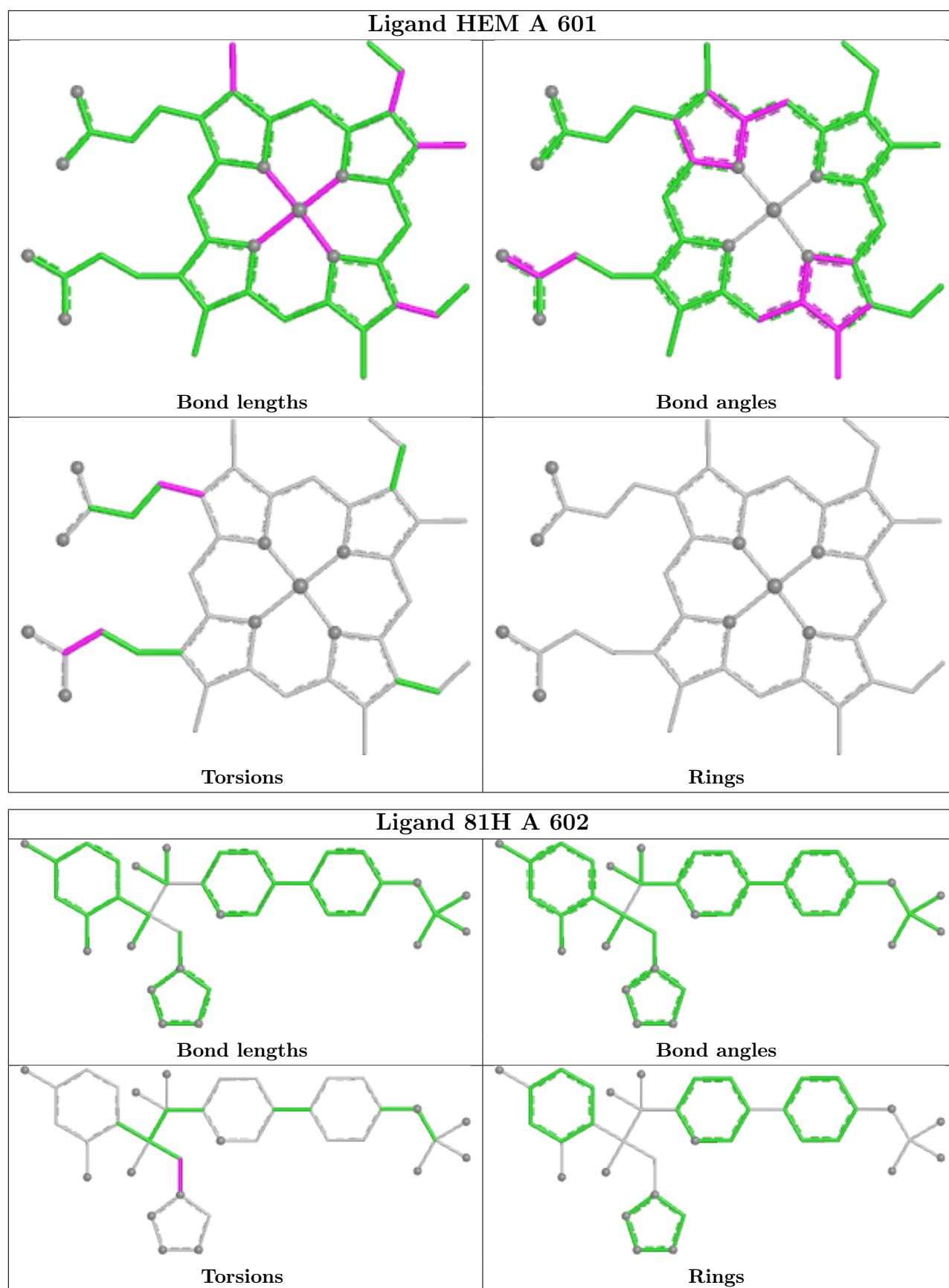
Mol	Chain	Res	Type	Atoms
2	A	601	HEM	C4D-C3D-CAD-CBD
2	A	601	HEM	C2D-C3D-CAD-CBD
3	A	602	81H	C21-C22-N23-C27
2	A	601	HEM	CAA-CBA-CGA-O1A
2	A	601	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	6	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	528/536 (98%)	2.09	258 (48%) 0 0	40, 59, 86, 104	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	441	VAL	6.0
1	A	227	TYR	5.4
1	A	221	LEU	5.3
1	A	451	ALA	5.2
1	A	111	PHE	4.5
1	A	399	VAL	4.4
1	A	118	ALA	4.4
1	A	457	SER	4.4
1	A	71	VAL	4.3
1	A	389	LYS	4.3
1	A	40	ILE	4.3
1	A	78	GLU	4.3
1	A	7	ILE	4.3
1	A	456	VAL	4.2
1	A	27	LEU	4.2
1	A	439	TYR	4.1
1	A	36	ILE	4.1
1	A	166	TYR	4.0
1	A	534	HIS	4.0
1	A	23	LEU	4.0
1	A	275	ASN	3.9
1	A	265	TYR	3.9
1	A	119	ASP	3.9
1	A	342	GLU	3.9
1	A	311	VAL	3.9
1	A	134	PHE	3.9
1	A	156	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	446	ASP	3.8
1	A	274	LYS	3.7
1	A	394	PRO	3.7
1	A	108	GLY	3.7
1	A	278	ILE	3.6
1	A	31	ILE	3.6
1	A	35	ILE	3.6
1	A	12	LEU	3.6
1	A	82	GLU	3.5
1	A	51	LEU	3.5
1	A	186	LEU	3.5
1	A	62	TRP	3.4
1	A	34	ILE	3.4
1	A	197	MET	3.4
1	A	286	SER	3.4
1	A	395	ASN	3.4
1	A	532	GLY	3.4
1	A	107	LYS	3.4
1	A	133	VAL	3.4
1	A	481	GLY	3.4
1	A	475	PHE	3.4
1	A	507	THR	3.3
1	A	357	TYR	3.3
1	A	39	PHE	3.3
1	A	65	TRP	3.3
1	A	390	ASP	3.3
1	A	533	ARG	3.3
1	A	225	PHE	3.2
1	A	437	SER	3.2
1	A	8	VAL	3.2
1	A	436	ALA	3.2
1	A	248	LEU	3.2
1	A	392	HIS	3.2
1	A	490	THR	3.2
1	A	26	PRO	3.2
1	A	360	LEU	3.2
1	A	171	ALA	3.1
1	A	269	ILE	3.1
1	A	126	TYR	3.1
1	A	294	LYS	3.1
1	A	58	LEU	3.1
1	A	424	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	66	VAL	3.1
1	A	37	ILE	3.1
1	A	74	MET	3.1
1	A	447	TYR	3.0
1	A	463	PHE	3.0
1	A	63	ILE	3.0
1	A	315	GLY	3.0
1	A	249	GLU	3.0
1	A	362	GLU	3.0
1	A	250	HIS	3.0
1	A	129	LEU	3.0
1	A	211	SER	3.0
1	A	43	ILE	3.0
1	A	433	ASN	3.0
1	A	531	GLY	3.0
1	A	512	LEU	3.0
1	A	103	TYR	3.0
1	A	243	PHE	3.0
1	A	384	PHE	3.0
1	A	514	THR	2.9
1	A	41	TYR	2.9
1	A	80	PHE	2.9
1	A	15	VAL	2.9
1	A	113	PHE	2.9
1	A	155	LYS	2.9
1	A	242	VAL	2.8
1	A	75	LYS	2.8
1	A	391	MET	2.8
1	A	44	VAL	2.8
1	A	61	TYR	2.8
1	A	305	ALA	2.8
1	A	95	LEU	2.8
1	A	461	LEU	2.8
1	A	59	VAL	2.8
1	A	102	VAL	2.8
1	A	438	SER	2.8
1	A	425	GLN	2.8
1	A	70	VAL	2.8
1	A	94	VAL	2.8
1	A	443	GLU	2.7
1	A	308	LEU	2.7
1	A	393	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	435	SER	2.7
1	A	153	PHE	2.7
1	A	185	ARG	2.7
1	A	516	PRO	2.7
1	A	521	TRP	2.7
1	A	346	ARG	2.7
1	A	19	LEU	2.7
1	A	292	THR	2.7
1	A	412	TYR	2.7
1	A	432	ASN	2.7
1	A	164	LYS	2.7
1	A	350	GLY	2.7
1	A	149	GLU	2.6
1	A	208	ALA	2.6
1	A	491	LEU	2.6
1	A	293	TYR	2.6
1	A	154	VAL	2.6
1	A	142	CYS	2.6
1	A	207	THR	2.6
1	A	500	THR	2.6
1	A	106	PRO	2.6
1	A	138	VAL	2.6
1	A	136	LYS	2.6
1	A	158	LEU	2.6
1	A	180	ASP	2.6
1	A	508	SER	2.6
1	A	515	GLY	2.6
1	A	264	THR	2.6
1	A	38	PRO	2.6
1	A	73	GLY	2.5
1	A	251	TYR	2.5
1	A	217	MET	2.5
1	A	411	GLY	2.5
1	A	165	SER	2.5
1	A	323	SER	2.5
1	A	47	LEU	2.5
1	A	104	LEU	2.5
1	A	284	ILE	2.5
1	A	400	ILE	2.5
1	A	298	LYS	2.5
1	A	147	LEU	2.5
1	A	383	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	160	LYS	2.5
1	A	347	VAL	2.5
1	A	486	ILE	2.5
1	A	42	ASN	2.5
1	A	89	ASP	2.5
1	A	440	SER	2.5
1	A	321	ALA	2.5
1	A	48	LEU	2.5
1	A	232	LEU	2.5
1	A	378	HIS	2.5
1	A	45	TRP	2.5
1	A	478	CYS	2.4
1	A	157	ALA	2.4
1	A	30	ARG	2.4
1	A	468	HIS	2.4
1	A	81	GLU	2.4
1	A	112	VAL	2.4
1	A	238	PRO	2.4
1	A	480	LEU	2.4
1	A	510	VAL	2.4
1	A	458	SER	2.4
1	A	57	PRO	2.4
1	A	526	PRO	2.4
1	A	256	HIS	2.4
1	A	268	LEU	2.4
1	A	176	LYS	2.4
1	A	345	MET	2.4
1	A	228	LEU	2.3
1	A	290	ASN	2.3
1	A	239	ILE	2.3
1	A	370	ILE	2.3
1	A	428	ILE	2.3
1	A	445	VAL	2.3
1	A	501	VAL	2.3
1	A	109	HIS	2.3
1	A	302	GLN	2.3
1	A	361	GLN	2.3
1	A	299	MET	2.3
1	A	145	SER	2.3
1	A	99	VAL	2.3
1	A	28	ALA	2.3
1	A	14	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	212	LEU	2.3
1	A	213	LEU	2.3
1	A	431	TRP	2.3
1	A	281	ARG	2.3
1	A	209	SER	2.3
1	A	79	PHE	2.3
1	A	93	PHE	2.3
1	A	236	PHE	2.3
1	A	198	VAL	2.3
1	A	169	LEU	2.3
1	A	330	LEU	2.3
1	A	340	LEU	2.3
1	A	77	TYR	2.3
1	A	397	SER	2.2
1	A	184	PHE	2.2
1	A	194	ILE	2.2
1	A	11	ALA	2.2
1	A	260	ALA	2.2
1	A	296	GLY	2.2
1	A	450	GLY	2.2
1	A	110	GLU	2.2
1	A	229	TYR	2.2
1	A	60	PHE	2.2
1	A	220	LYS	2.2
1	A	245	ASN	2.2
1	A	139	ILE	2.2
1	A	380	LEU	2.2
1	A	319	SER	2.2
1	A	87	TYR	2.2
1	A	261	ILE	2.1
1	A	530	ILE	2.1
1	A	387	VAL	2.1
1	A	127	ALA	2.1
1	A	96	LEU	2.1
1	A	355	LEU	2.1
1	A	419	TYR	2.1
1	A	161	GLU	2.1
1	A	64	PRO	2.1
1	A	163	PHE	2.1
1	A	442	GLY	2.1
1	A	430	ARG	2.1
1	A	405	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	17	ILE	2.1
1	A	309	ILE	2.1
1	A	487	PHE	2.1
1	A	33	LEU	2.1
1	A	246	LEU	2.1
1	A	328	LEU	2.1
1	A	363	MET	2.1
1	A	527	GLU	2.1
1	A	466	GLY	2.1
1	A	253	LYS	2.1
1	A	408	VAL	2.1
1	A	24	ALA	2.1
1	A	172	GLU	2.0
1	A	271	GLU	2.0
1	A	128	HIS	2.0
1	A	352	LYS	2.0
1	A	426	PHE	2.0
1	A	449	PHE	2.0
1	A	359	LEU	2.0
1	A	280	ASP	2.0
1	A	235	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

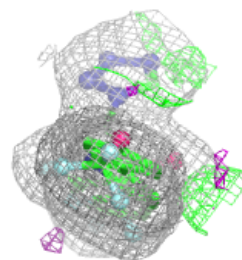
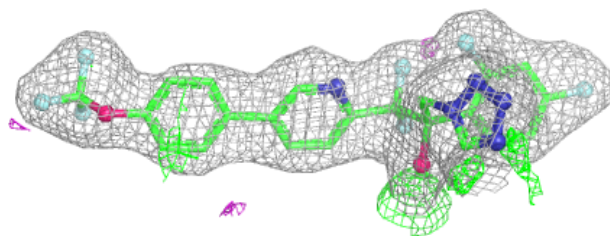
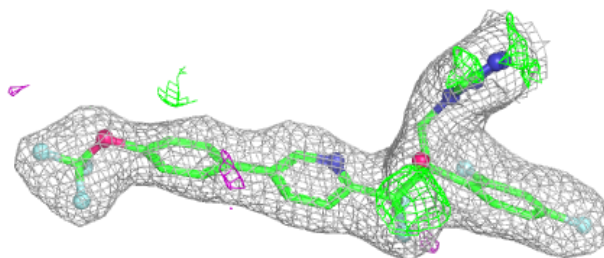
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	81H	A	602	36/36	0.92	0.12	42,50,63,66	0
2	HEM	A	601	43/43	0.95	0.13	41,47,51,53	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.

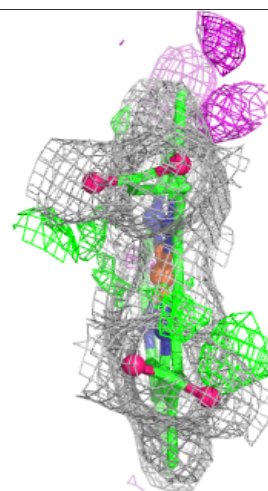
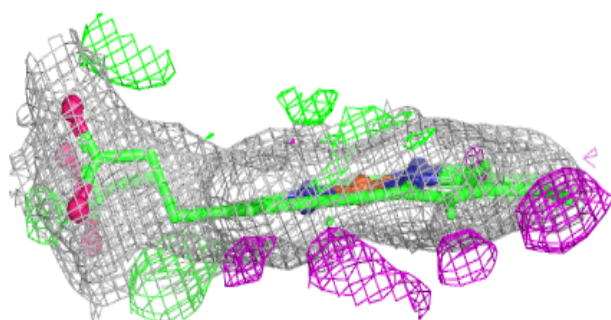
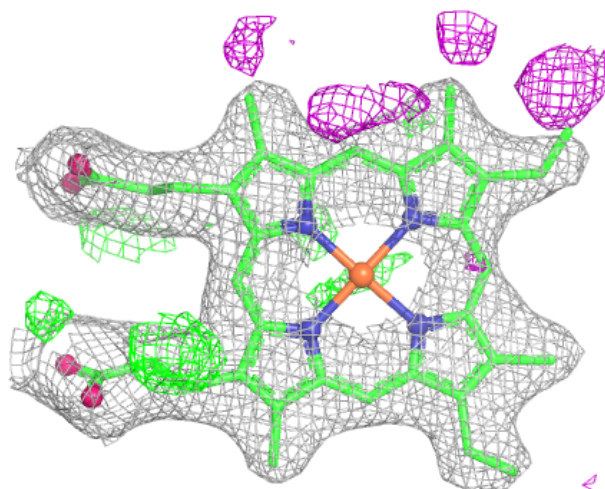
Electron density around 81H A 602:

$2mF_o-DF_c$ (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.