Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2024 – 03:35 PM EST

PDB ID	:	8SS0
Title	:	Human sterol 14 alpha-demethylase (CYP51) in complex with the reaction intermediate 14 alpha-aldehyde dihydrolanosterol
Authors	:	Hargrove, T.Y.; Wawrzak, Z.; Guengerich, F.P.; Lepesheva, G.I.
Deposited on	:	2023-05-08
Resolution	:	2.25 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:

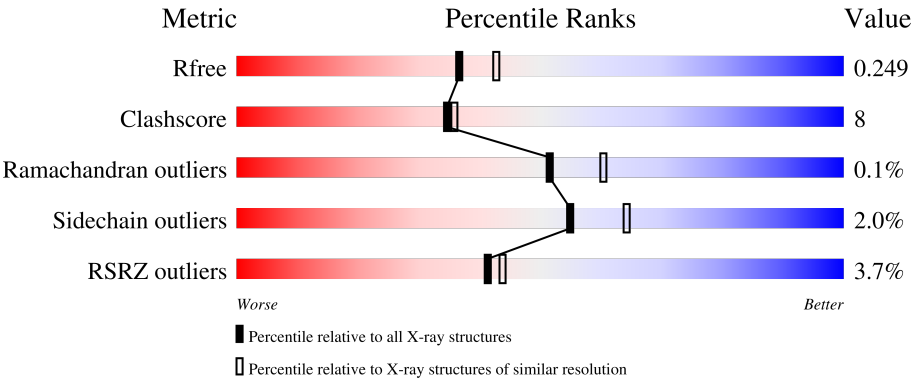
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.25 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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	458	5% 81% 16%
1	B	458	3% 79% 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7379 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	446	Total	C	N	O	S	0	0	0
			3589	2312	611	650	16			
1	B	441	Total	C	N	O	S	0	0	0
			3533	2282	595	640	16			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MET	-	expression tag	UNP Q16850
A	51	ALA	-	expression tag	UNP Q16850
A	52	LYS	-	expression tag	UNP Q16850
A	53	LYS	-	expression tag	UNP Q16850
A	54	THR	-	expression tag	UNP Q16850
A	55	SER	-	expression tag	UNP Q16850
A	56	SER	-	expression tag	UNP Q16850
A	57	LYS	-	expression tag	UNP Q16850
A	58	GLY	-	expression tag	UNP Q16850
A	59	LYS	-	expression tag	UNP Q16850
A	60	LEU	-	expression tag	UNP Q16850
A	231	ALA	ASP	engineered mutation	UNP Q16850
A	314	ALA	HIS	engineered mutation	UNP Q16850
A	504	HIS	-	expression tag	UNP Q16850
A	505	HIS	-	expression tag	UNP Q16850
A	506	HIS	-	expression tag	UNP Q16850
A	507	HIS	-	expression tag	UNP Q16850
B	50	MET	-	expression tag	UNP Q16850
B	51	ALA	-	expression tag	UNP Q16850
B	52	LYS	-	expression tag	UNP Q16850
B	53	LYS	-	expression tag	UNP Q16850
B	54	THR	-	expression tag	UNP Q16850
B	55	SER	-	expression tag	UNP Q16850
B	56	SER	-	expression tag	UNP Q16850
B	57	LYS	-	expression tag	UNP Q16850

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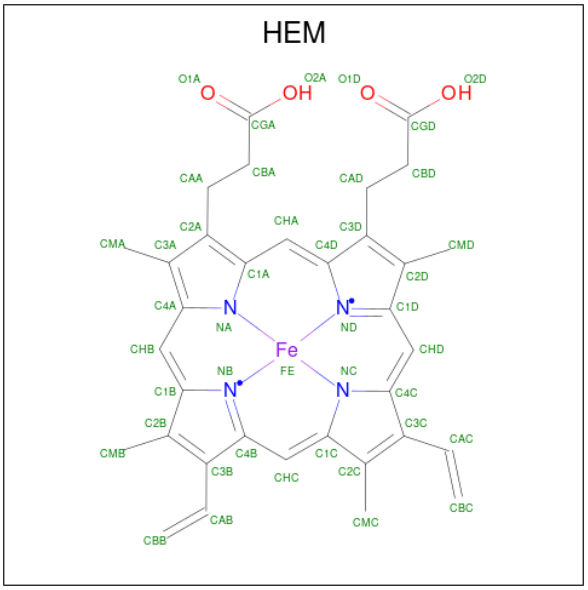
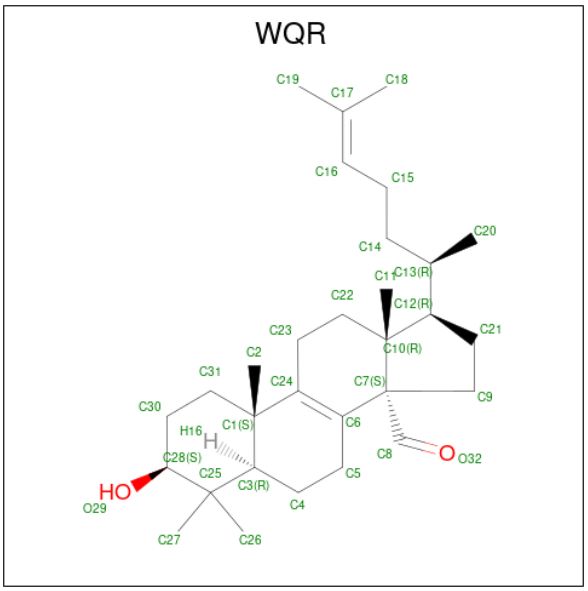
Chain	Residue	Modelled	Actual	Comment	Reference
B	58	GLY	-	expression tag	UNP Q16850
B	59	LYS	-	expression tag	UNP Q16850
B	60	LEU	-	expression tag	UNP Q16850
B	231	ALA	ASP	engineered mutation	UNP Q16850
B	314	ALA	HIS	engineered mutation	UNP Q16850
B	504	HIS	-	expression tag	UNP Q16850
B	505	HIS	-	expression tag	UNP Q16850
B	506	HIS	-	expression tag	UNP Q16850
B	507	HIS	-	expression tag	UNP Q16850

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: 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		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 3beta-hydroxy-10alpha,13alpha-lanosta-8,24-dien-30-al (three-letter code: WQR) (formula: $C_{30}H_{48}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 32 30 2	0	0
3	B	1	Total C O 32 30 2	0	0

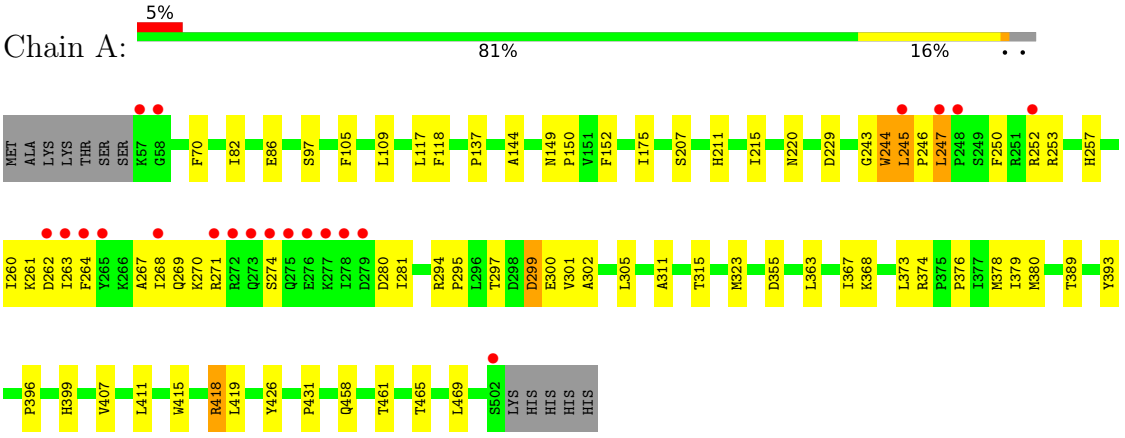
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	45	Total O 45 45	0	0
4	B	62	Total O 62 62	0	0

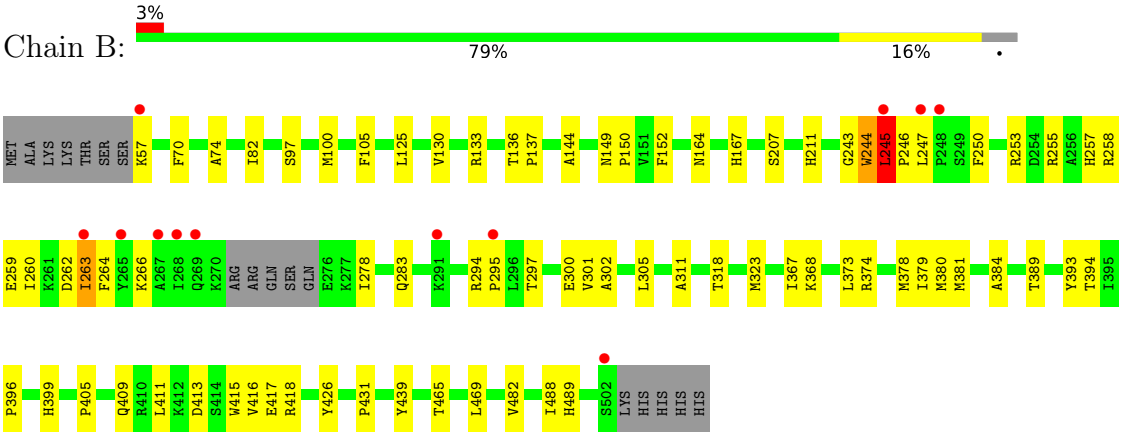
3 Residue-property plots (i)

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



• Molecule 1: Lanosterol 14-alpha demethylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	145.80Å 145.80Å 261.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 2.25 19.89 – 2.25	Depositor EDS
% Data completeness (in resolution range)	47.5 (19.89-2.25) 47.6 (19.89-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.219 , 0.249 0.223 , 0.249	Depositor DCC
R_{free} test set	1892 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 26.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7379	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7110e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: WQR, 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	0/3681	0.69	0/4985
1	B	0.41	0/3624	0.70	0/4910
All	All	0.39	0/7305	0.70	0/9895

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
1	B	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	418	ARG	Sidechain
1	B	133	ARG	Sidechain
1	B	418	ARG	Sidechain

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	3589	0	3593	59	0
1	B	3533	0	3530	51	0
2	A	43	0	30	6	0
2	B	43	0	30	6	0
3	A	32	0	0	0	0
3	B	32	0	0	0	0
4	A	45	0	0	0	0
4	B	62	0	0	1	0
All	All	7379	0	7183	120	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 8.

All (120) 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)
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.59	0.82
2:A:601:HEM:HBB2	2:A:601:HEM:HMB2	1.62	0.79
1:B:297:THR:HG23	1:B:300:GLU:H	1.47	0.79
1:A:229:ASP:HB2	1:A:252:ARG:HG3	1.73	0.70
1:A:294:ARG:HG2	1:A:295:PRO:HD2	1.74	0.69
2:B:601:HEM:HBB2	2:B:601:HEM:CMB	2.22	0.69
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.23	0.68
1:A:378:MET:HG2	1:A:379:ILE:HG23	1.77	0.67
1:B:294:ARG:HG2	1:B:295:PRO:HD2	1.77	0.67
1:B:260:ILE:O	1:B:263:ILE:HG22	1.96	0.66
1:A:229:ASP:CB	1:A:252:ARG:HG3	2.27	0.65
1:A:215:ILE:HG12	1:A:263:ILE:HG21	1.80	0.63
1:A:137:PRO:HB3	1:A:250:PHE:CE1	2.34	0.62
1:A:264:PHE:HZ	1:A:302:ALA:HA	1.65	0.62
1:A:297:THR:HG23	1:A:299:ASP:H	1.65	0.62
1:A:215:ILE:HG12	1:A:263:ILE:HD13	1.82	0.60
1:A:269:GLN:OE1	1:A:270:LYS:HG2	2.01	0.60
1:A:297:THR:HG23	1:A:300:GLU:H	1.66	0.59
1:B:253:ARG:NH2	1:B:257:HIS:CE1	2.72	0.58
1:A:268:ILE:HA	1:A:271:ARG:HB3	1.86	0.58
1:B:311:ALA:HB1	2:B:601:HEM:C3C	2.39	0.58
1:A:260:ILE:HG22	1:A:264:PHE:CZ	2.39	0.57
1:B:245:LEU:HB3	1:B:246:PRO:HD2	1.86	0.57
1:B:415:TRP:CE2	1:B:431:PRO:HG2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:PHE:HZ	1:B:302:ALA:HA	1.70	0.57
1:B:263:ILE:HD12	1:B:266:LYS:HB3	1.85	0.57
1:A:261:LYS:HA	1:A:264:PHE:CE2	2.40	0.57
1:B:264:PHE:CZ	1:B:301:VAL:HG12	2.41	0.56
1:A:297:THR:CG2	1:A:300:GLU:H	2.19	0.56
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.87	0.55
1:B:264:PHE:HE2	1:B:302:ALA:HB2	1.72	0.55
2:B:601:HEM:CMC	2:B:601:HEM:HBC2	2.37	0.55
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.88	0.55
1:A:415:TRP:CE2	1:A:431:PRO:HG2	2.42	0.54
1:B:253:ARG:O	1:B:257:HIS:HB2	2.07	0.54
1:B:373:LEU:O	1:B:374:ARG:HD3	2.07	0.54
1:A:396:PRO:HG2	1:A:399:HIS:CD2	2.43	0.53
1:A:268:ILE:HA	1:A:271:ARG:CB	2.38	0.53
1:B:368:LYS:HD3	1:B:426:TYR:CZ	2.44	0.52
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.40	0.52
1:A:264:PHE:CE2	1:A:302:ALA:HB2	2.45	0.52
1:B:264:PHE:CE2	1:B:302:ALA:HB2	2.45	0.52
1:A:137:PRO:HB3	1:A:250:PHE:HE1	1.73	0.52
1:A:253:ARG:O	1:A:257:HIS:HB2	2.10	0.52
1:A:267:ALA:O	1:A:271:ARG:N	2.42	0.52
1:A:323:MET:CE	1:A:367:ILE:HG12	2.40	0.52
1:B:278:ILE:O	1:B:283:GLN:HG3	2.10	0.52
1:A:109:LEU:HD13	1:A:407:VAL:HG11	1.90	0.52
1:B:396:PRO:HG2	1:B:399:HIS:CD2	2.45	0.52
1:A:297:THR:HG23	1:A:299:ASP:N	2.25	0.51
2:B:601:HEM:HMB2	2:B:601:HEM:CBB	2.35	0.51
1:B:207:SER:O	1:B:211:HIS:HB2	2.12	0.50
1:A:243:GLY:C	1:A:244:TRP:CD1	2.85	0.50
1:B:137:PRO:HB3	1:B:250:PHE:HE1	1.75	0.50
1:B:243:GLY:C	1:B:244:TRP:CD1	2.85	0.50
1:A:118:PHE:CE1	1:A:380:MET:HE3	2.46	0.50
1:A:264:PHE:CE1	1:A:301:VAL:HG12	2.47	0.50
1:B:245:LEU:HD22	1:B:246:PRO:HD3	1.94	0.49
1:B:137:PRO:HB3	1:B:250:PHE:CE1	2.48	0.49
1:B:245:LEU:HD13	1:B:246:PRO:HD2	1.94	0.49
1:A:465:THR:O	1:A:469:LEU:HG	2.13	0.49
1:B:246:PRO:HG2	4:B:761:HOH:O	2.12	0.49
1:B:260:ILE:HG21	1:B:305:LEU:HB2	1.95	0.48
1:A:261:LYS:HA	1:A:264:PHE:CD2	2.49	0.47
2:A:601:HEM:HMB2	2:A:601:HEM:CBB	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ILE:HD13	1:A:458:GLN:HA	1.97	0.47
1:B:409:GLN:HG2	1:B:439:TYR:HA	1.95	0.47
1:B:97:SER:HA	1:B:105:PHE:O	2.15	0.47
1:B:368:LYS:HD3	1:B:426:TYR:CE2	2.49	0.46
1:A:245:LEU:HB3	1:A:246:PRO:CD	2.45	0.46
1:A:373:LEU:O	1:A:374:ARG:HD3	2.15	0.46
1:A:144:ALA:HA	1:A:152:PHE:CD1	2.51	0.46
1:A:118:PHE:CE1	1:A:380:MET:CE	2.99	0.45
1:B:323:MET:CE	1:B:367:ILE:HG12	2.47	0.44
1:A:418:ARG:HG3	1:A:419:LEU:HG	1.99	0.44
1:B:482:VAL:HG13	1:B:489:HIS:HB3	2.00	0.44
1:B:144:ALA:HA	1:B:152:PHE:CD1	2.52	0.44
1:A:368:LYS:HD3	1:A:426:TYR:CE2	2.53	0.44
1:A:270:LYS:O	1:A:274:SER:HB3	2.17	0.44
1:B:380:MET:CE	1:B:405:PRO:CG	2.96	0.44
1:A:82:ILE:O	1:A:86:GLU:HG3	2.18	0.44
1:A:264:PHE:HE1	1:A:305:LEU:HD12	1.83	0.44
1:B:378:MET:HG3	1:B:379:ILE:HG12	1.99	0.44
1:A:247:LEU:H	1:A:247:LEU:HG	1.40	0.43
1:B:416:VAL:O	1:B:417:GLU:C	2.56	0.43
1:B:318:THR:HG21	1:B:488:ILE:HG22	2.00	0.43
1:A:389:THR:HA	1:A:393:TYR:O	2.18	0.43
1:A:97:SER:HA	1:A:105:PHE:O	2.18	0.43
1:A:411:LEU:HD12	1:A:411:LEU:HA	1.91	0.43
1:B:164:ASN:OD1	1:B:167:HIS:ND1	2.51	0.43
1:A:207:SER:O	1:A:211:HIS:HB2	2.19	0.43
1:A:260:ILE:HG21	1:A:305:LEU:HB2	2.01	0.43
1:A:363:LEU:O	1:A:367:ILE:HG13	2.19	0.43
1:B:389:THR:HA	1:B:393:TYR:O	2.19	0.42
1:B:415:TRP:CD2	1:B:431:PRO:HG2	2.54	0.42
1:A:315:THR:HG22	1:A:376:PRO:HB2	2.02	0.42
1:B:465:THR:O	1:B:469:LEU:HG	2.19	0.42
1:A:118:PHE:HE1	1:A:380:MET:CE	2.33	0.42
1:A:270:LYS:HB3	1:A:274:SER:HB3	2.00	0.42
1:B:74:ALA:N	1:B:100:MET:HG2	2.34	0.42
1:B:411:LEU:HD12	1:B:411:LEU:HA	1.88	0.42
1:B:136:THR:N	1:B:137:PRO:CD	2.83	0.42
1:A:323:MET:HE1	1:A:367:ILE:HG12	2.01	0.42
1:A:82:ILE:HD11	1:A:378:MET:HG3	2.02	0.42
1:A:311:ALA:HB1	2:A:601:HEM:C3C	2.55	0.42
1:B:82:ILE:HD13	1:B:378:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ILE:HA	1:A:263:ILE:HD12	2.02	0.42
1:A:149:ASN:N	1:A:150:PRO:CD	2.83	0.41
1:B:130:VAL:HG11	1:B:381:MET:CB	2.49	0.41
1:B:149:ASN:HB3	1:B:150:PRO:HD3	2.02	0.41
1:B:57:LYS:N	1:B:394:THR:HG21	2.35	0.41
1:B:130:VAL:HG11	1:B:381:MET:HB3	2.02	0.41
1:A:297:THR:HG22	1:A:300:GLU:HG3	2.03	0.41
1:A:280:ASP:CG	1:A:281:ILE:H	2.25	0.41
1:B:125:LEU:HD23	1:B:384:ALA:HA	2.03	0.40
1:B:255:ARG:O	1:B:259:GLU:HG3	2.21	0.40
1:A:175:ILE:HB	1:A:461:THR:HG21	2.03	0.40
1:B:258:ARG:HD3	1:B:258:ARG:HA	1.84	0.40
1:B:297:THR:HG22	1:B:300:GLU:OE2	2.22	0.40
1:A:117:LEU:C	1:A:117:LEU:HD23	2.41	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	444/458 (97%)	426 (96%)	18 (4%)	0	100 100
1	B	437/458 (95%)	421 (96%)	15 (3%)	1 (0%)	47 55
All	All	881/916 (96%)	847 (96%)	33 (4%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	245	LEU

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	388/399 (97%)	380 (98%)	8 (2%)	53 62
1	B	381/399 (96%)	374 (98%)	7 (2%)	59 68
All	All	769/798 (96%)	754 (98%)	15 (2%)	55 64

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	PHE
1	A	220	ASN
1	A	244	TRP
1	A	245	LEU
1	A	247	LEU
1	A	262	ASP
1	A	299	ASP
1	A	355	ASP
1	B	70	PHE
1	B	244	TRP
1	B	245	LEU
1	B	247	LEU
1	B	262	ASP
1	B	263	ILE
1	B	413	ASP

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	73	HIS
1	B	408	ASN
1	B	483	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	B	601	1	41,50,50	1.44	4 (9%)	45,82,82	2.08	15 (33%)
3	WQR	A	602	-	31,35,35	2.91	6 (19%)	49,57,57	1.93	11 (22%)
2	HEM	A	601	1	41,50,50	1.47	8 (19%)	45,82,82	2.24	18 (40%)
3	WQR	B	602	-	31,35,35	2.90	6 (19%)	49,57,57	1.87	9 (18%)

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	B	601	1	-	2/12/54/54	-
3	WQR	A	602	-	-	4/13/85/85	0/4/4/4
2	HEM	A	601	1	-	4/12/54/54	-
3	WQR	B	602	-	-	4/13/85/85	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	WQR	C1-C24	-10.32	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	WQR	C1-C24	-10.16	1.38	1.53
3	A	602	WQR	C16-C17	7.34	1.53	1.32
3	B	602	WQR	C16-C17	7.24	1.53	1.32
3	A	602	WQR	C23-C24	-6.48	1.40	1.51
3	B	602	WQR	C23-C24	-6.39	1.40	1.51
3	B	602	WQR	C5-C6	-6.10	1.41	1.51
3	A	602	WQR	C5-C6	-5.78	1.41	1.51
2	A	601	HEM	C1B-NB	-4.46	1.32	1.40
2	B	601	HEM	C1B-NB	-4.38	1.32	1.40
3	A	602	WQR	C24-C6	3.42	1.41	1.34
3	B	602	WQR	C24-C6	3.41	1.41	1.34
2	B	601	HEM	C1D-ND	-3.05	1.32	1.38
2	A	601	HEM	C4D-ND	-2.95	1.35	1.40
2	A	601	HEM	C1D-ND	-2.50	1.33	1.38
2	B	601	HEM	C4D-ND	-2.39	1.36	1.40
2	B	601	HEM	FE-NB	2.38	2.08	1.96
2	A	601	HEM	C4B-NB	-2.38	1.33	1.38
2	A	601	HEM	FE-NB	2.17	2.07	1.96
3	B	602	WQR	C4-C3	-2.17	1.50	1.53
2	A	601	HEM	CHB-C1B	2.13	1.40	1.35
2	A	601	HEM	C1B-C2B	-2.12	1.40	1.44
3	A	602	WQR	C4-C3	-2.11	1.50	1.53
2	A	601	HEM	C1A-CHA	-2.00	1.35	1.41

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	HEM	CHC-C4B-NB	7.44	132.51	124.43
2	B	601	HEM	CHC-C4B-NB	5.57	130.48	124.43
3	A	602	WQR	C15-C16-C17	-4.97	110.75	127.75
2	A	601	HEM	C1B-NB-C4B	4.89	110.13	105.07
3	B	602	WQR	C15-C16-C17	-4.88	111.08	127.75
3	A	602	WQR	C10-C12-C13	-4.80	113.07	119.30
3	B	602	WQR	C19-C17-C16	-4.78	108.84	122.65
3	A	602	WQR	C19-C17-C16	-4.63	109.26	122.65
2	B	601	HEM	CHA-C4D-ND	4.55	130.00	124.38
3	A	602	WQR	C18-C17-C16	-4.37	110.01	122.65
2	A	601	HEM	CHD-C1D-ND	4.32	129.12	124.43
3	B	602	WQR	C5-C4-C3	-4.31	103.92	110.87
3	B	602	WQR	C18-C17-C16	-4.30	110.22	122.65
2	B	601	HEM	C1B-NB-C4B	4.03	109.24	105.07
3	B	602	WQR	C10-C12-C13	-3.98	114.14	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	HEM	CHA-C4D-ND	3.97	129.28	124.38
3	A	602	WQR	C5-C4-C3	-3.93	104.53	110.87
2	A	601	HEM	CHB-C1B-NB	3.87	129.16	124.38
2	B	601	HEM	CAD-C3D-C4D	3.86	131.40	124.66
2	B	601	HEM	CHD-C1D-ND	3.46	128.19	124.43
3	A	602	WQR	C30-C28-C25	-3.44	109.79	113.32
3	A	602	WQR	C21-C12-C13	-3.39	106.90	112.15
3	B	602	WQR	C21-C12-C13	-3.36	106.94	112.15
2	B	601	HEM	CHB-C1B-NB	3.23	128.37	124.38
3	B	602	WQR	C30-C28-C25	-3.21	110.02	113.32
2	A	601	HEM	CAD-C3D-C4D	3.13	130.13	124.66
2	B	601	HEM	CHA-C4D-C3D	-3.03	119.64	125.33
2	B	601	HEM	CMD-C2D-C1D	2.84	129.37	125.04
2	A	601	HEM	CHD-C1D-C2D	-2.76	120.66	124.98
2	B	601	HEM	O2D-CGD-CBD	2.73	122.81	114.03
3	A	602	WQR	C4-C3-C1	-2.62	106.67	110.61
2	A	601	HEM	O2A-CGA-O1A	-2.58	116.88	123.30
3	B	602	WQR	C4-C3-C1	-2.56	106.76	110.61
3	A	602	WQR	C18-C17-C19	-2.54	108.99	114.60
2	A	601	HEM	O2D-CGD-CBD	2.54	122.18	114.03
2	B	601	HEM	O2A-CGA-O1A	-2.53	116.99	123.30
2	A	601	HEM	CHA-C4D-C3D	-2.42	120.79	125.33
3	B	602	WQR	C18-C17-C19	-2.39	109.33	114.60
3	A	602	WQR	C21-C9-C7	-2.38	100.62	104.16
2	A	601	HEM	CHC-C4B-C3B	-2.32	121.02	124.57
2	B	601	HEM	C4D-ND-C1D	2.23	107.38	105.07
2	A	601	HEM	O2A-CGA-CBA	2.15	120.94	114.03
2	B	601	HEM	CAD-C3D-C2D	-2.13	123.90	127.88
2	A	601	HEM	CHB-C1B-C2B	-2.12	120.85	126.72
2	A	601	HEM	O1D-CGD-CBD	-2.12	116.29	123.08
2	A	601	HEM	CMA-C3A-C4A	-2.10	125.23	128.46
2	A	601	HEM	C4D-ND-C1D	2.09	107.23	105.07
3	A	602	WQR	C15-C14-C13	-2.06	110.65	114.62
2	B	601	HEM	CBD-CAD-C3D	2.04	118.30	112.63
2	B	601	HEM	CHB-C1B-C2B	-2.04	121.08	126.72
2	B	601	HEM	O2A-CGA-CBA	2.03	120.56	114.03
2	A	601	HEM	CBA-CAA-C2A	2.01	116.04	112.62
2	A	601	HEM	CAD-C3D-C2D	-2.00	124.14	127.88

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	WQR	C9-C7-C8-O32
3	B	602	WQR	C9-C7-C8-O32
3	B	602	WQR	C15-C16-C17-C18
3	A	602	WQR	C15-C16-C17-C18
3	A	602	WQR	C10-C12-C13-C20
2	A	601	HEM	C2D-C3D-CAD-CBD
3	A	602	WQR	C10-C7-C8-O32
3	B	602	WQR	C10-C7-C8-O32
2	A	601	HEM	C4D-C3D-CAD-CBD
3	B	602	WQR	C10-C12-C13-C20
2	A	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAD-CBD-CGD-O1D
2	B	601	HEM	C2D-C3D-CAD-CBD
2	B	601	HEM	CAA-CBA-CGA-O2A

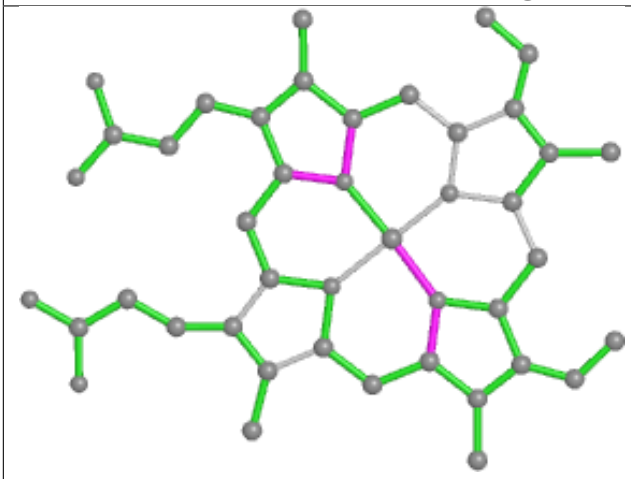
There are no ring outliers.

2 monomers are involved in 12 short contacts:

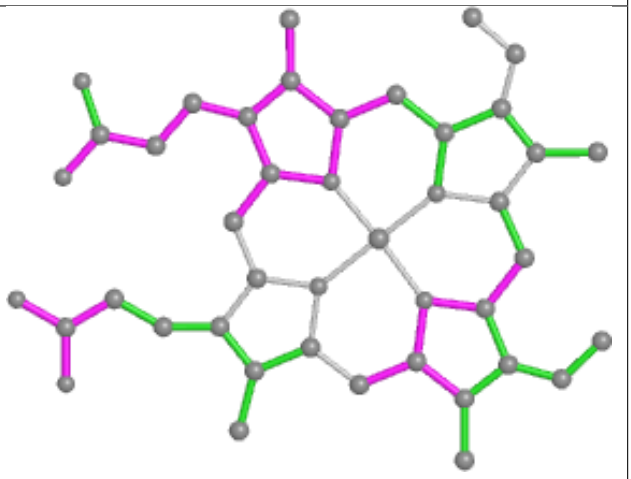
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HEM	6	0
2	A	601	HEM	6	0

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 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.

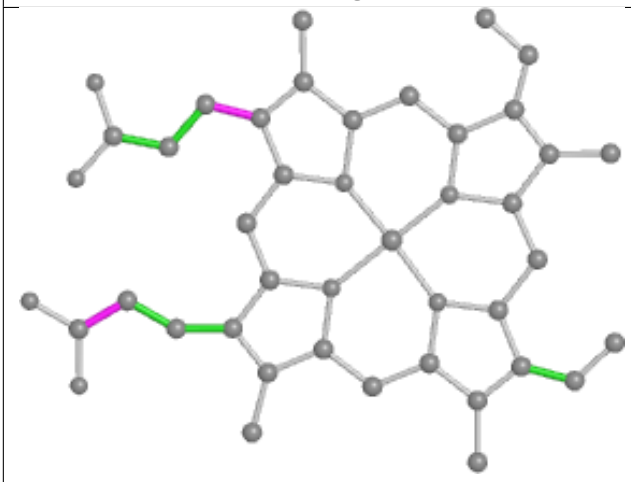
Ligand HEM B 601



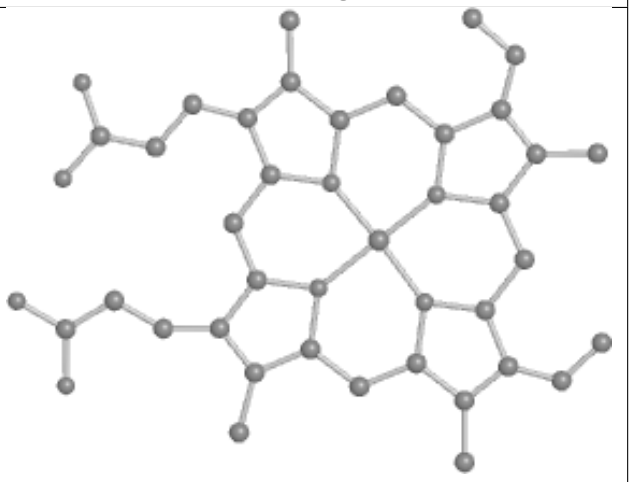
Bond lengths



Bond angles

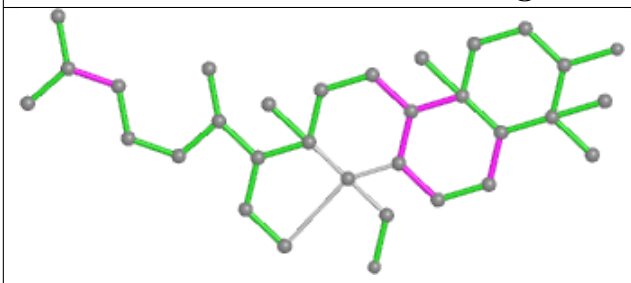


Torsions

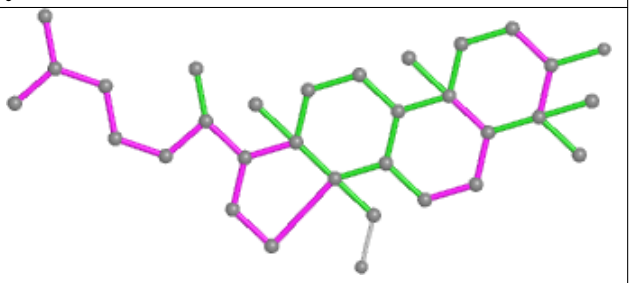


Rings

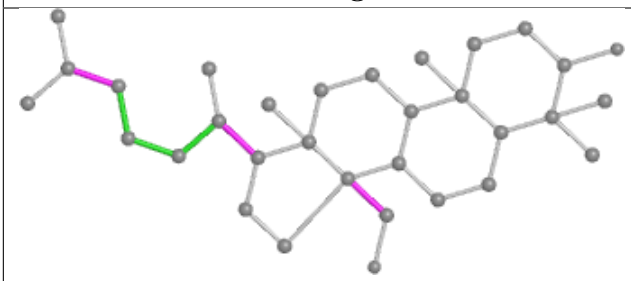
Ligand WQR A 602



Bond lengths



Bond angles



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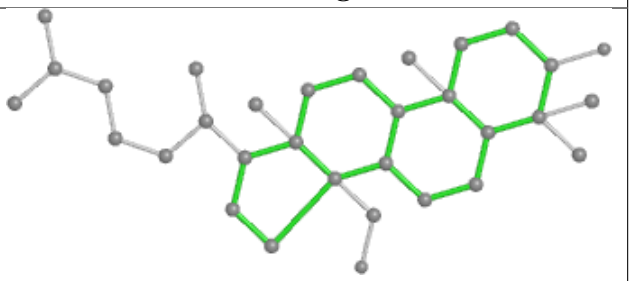
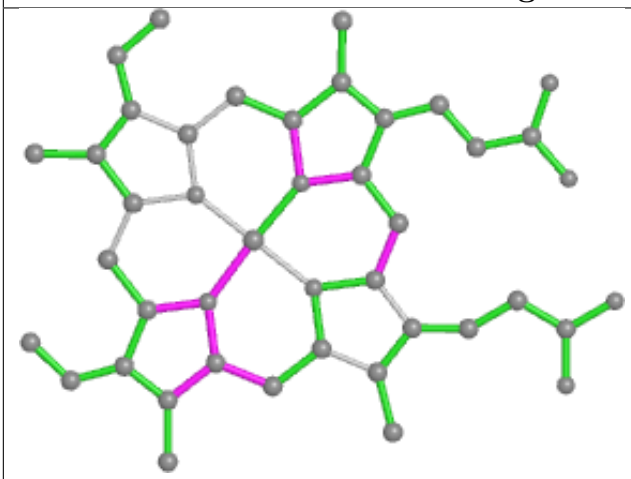
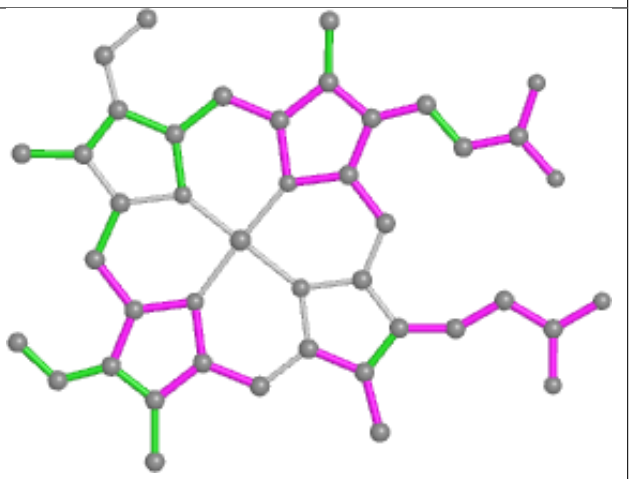


Rings

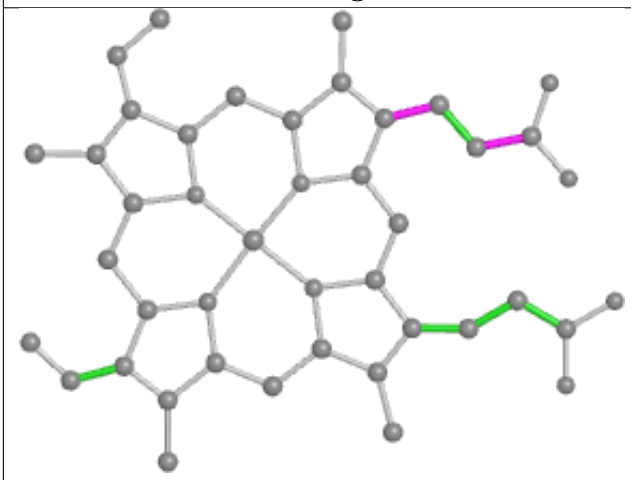
Ligand HEM A 601



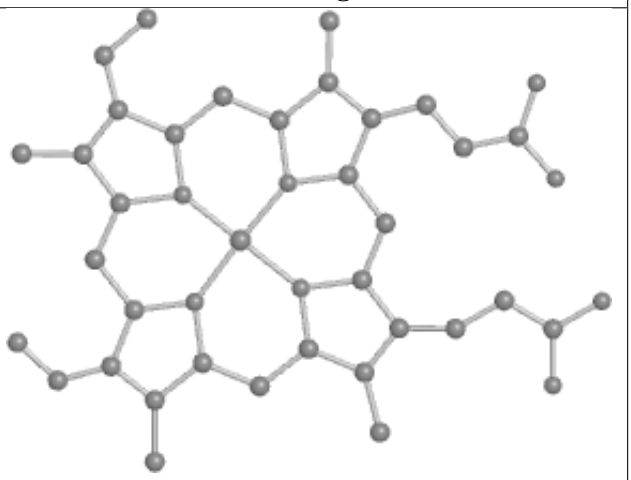
Bond lengths



Bond angles

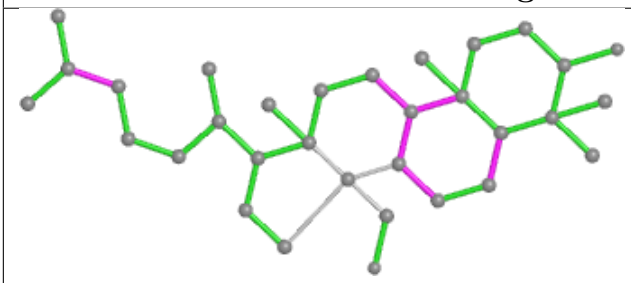


Torsions

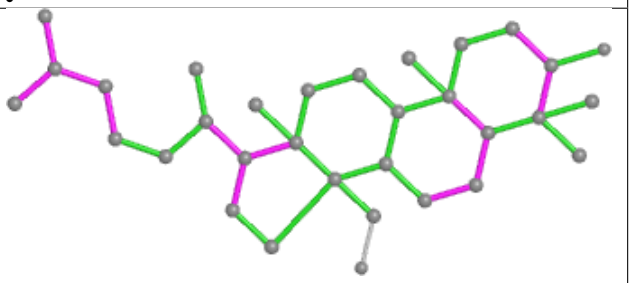


Rings

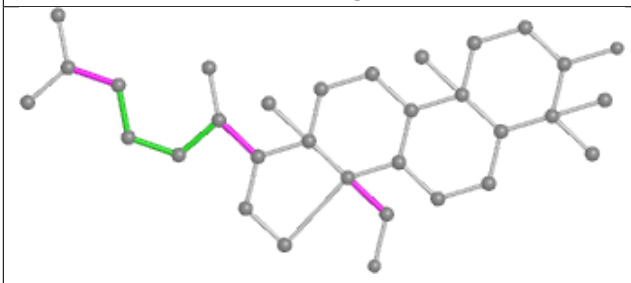
Ligand WQR B 602



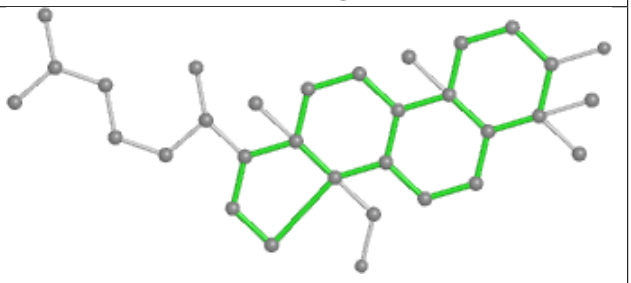
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	446/458 (97%)	-0.13	21 (4%)	31	34	16, 32, 83, 163	0
1	B	441/458 (96%)	-0.38	12 (2%)	54	57	17, 30, 74, 110	0
All	All	887/916 (96%)	-0.26	33 (3%)	41	44	16, 31, 78, 163	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	ILE	17.5
1	A	272	ARG	14.9
1	A	271	ARG	14.8
1	A	275	GLN	12.1
1	A	277	LYS	9.4
1	A	273	GLN	9.1
1	A	245	LEU	6.8
1	A	274	SER	4.6
1	A	57	LYS	4.4
1	A	265	TYR	4.1
1	B	502	SER	4.0
1	B	245	LEU	3.9
1	A	502	SER	3.8
1	B	295	PRO	3.6
1	B	265	TYR	3.4
1	A	276	GLU	3.0
1	A	268	ILE	2.9
1	A	264	PHE	2.9
1	B	57	LYS	2.8
1	A	279	ASP	2.7
1	B	247	LEU	2.7
1	A	247	LEU	2.6
1	A	248	PRO	2.5
1	B	248	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	263	ILE	2.4
1	A	252	ARG	2.3
1	B	269	GLN	2.3
1	B	267	ALA	2.2
1	B	268	ILE	2.1
1	B	291	LYS	2.1
1	A	58	GLY	2.1
1	B	263	ILE	2.1
1	A	262	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

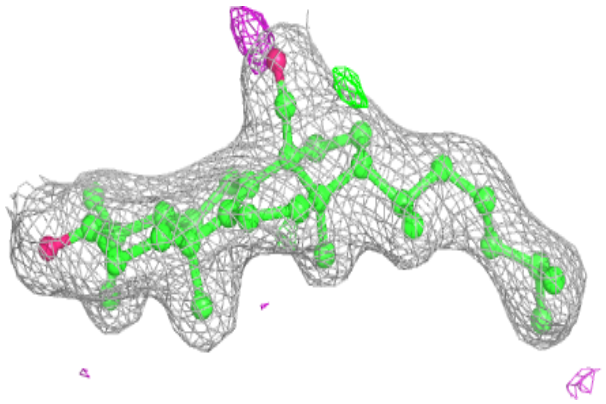
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

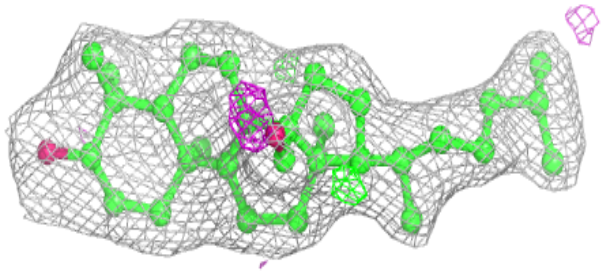
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	WQR	A	602	32/32	0.94	0.13	21,28,32,33	0
3	WQR	B	602	32/32	0.94	0.12	19,22,25,26	0
2	HEM	A	601	43/43	0.98	0.08	18,25,33,34	0
2	HEM	B	601	43/43	0.99	0.07	18,23,36,40	0

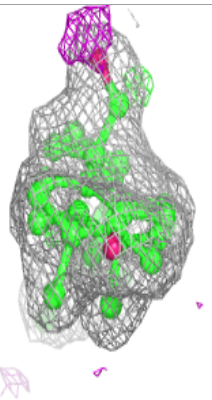
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WQR 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)

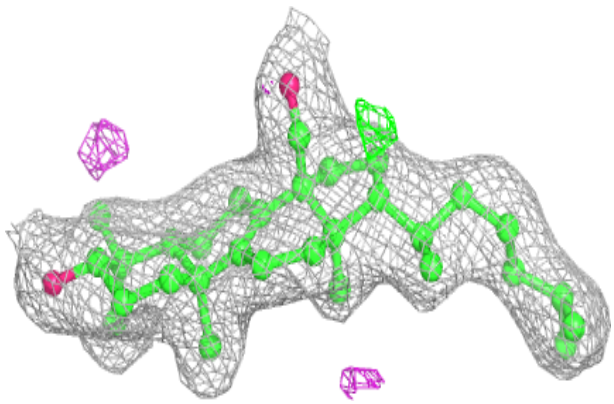


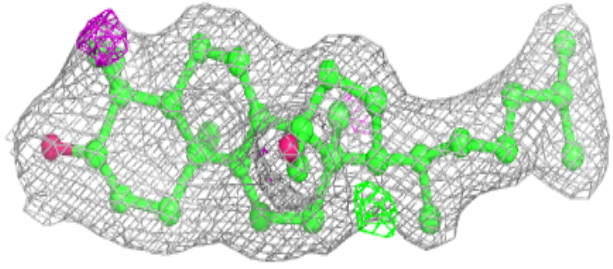


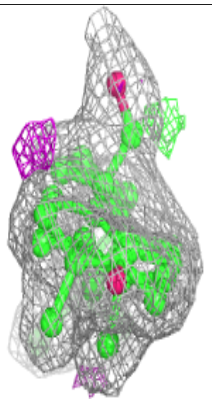


Electron density around WQR B 602:

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

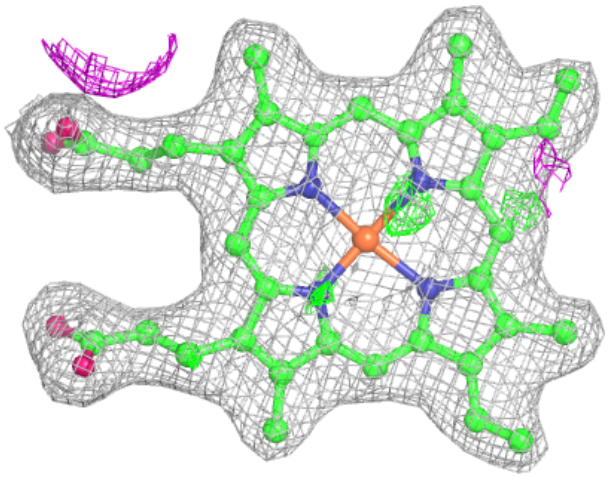


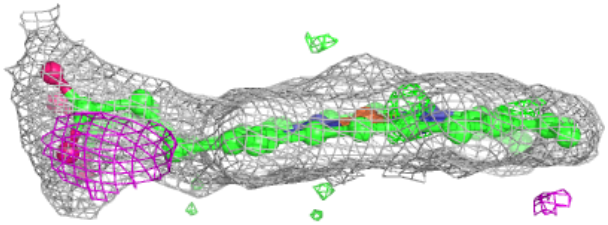


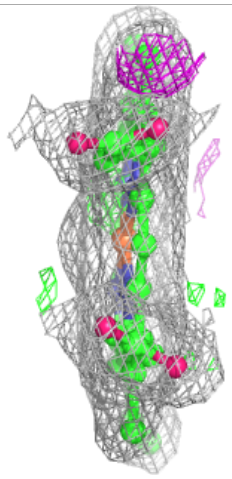


Electron density around HEM A 601:

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

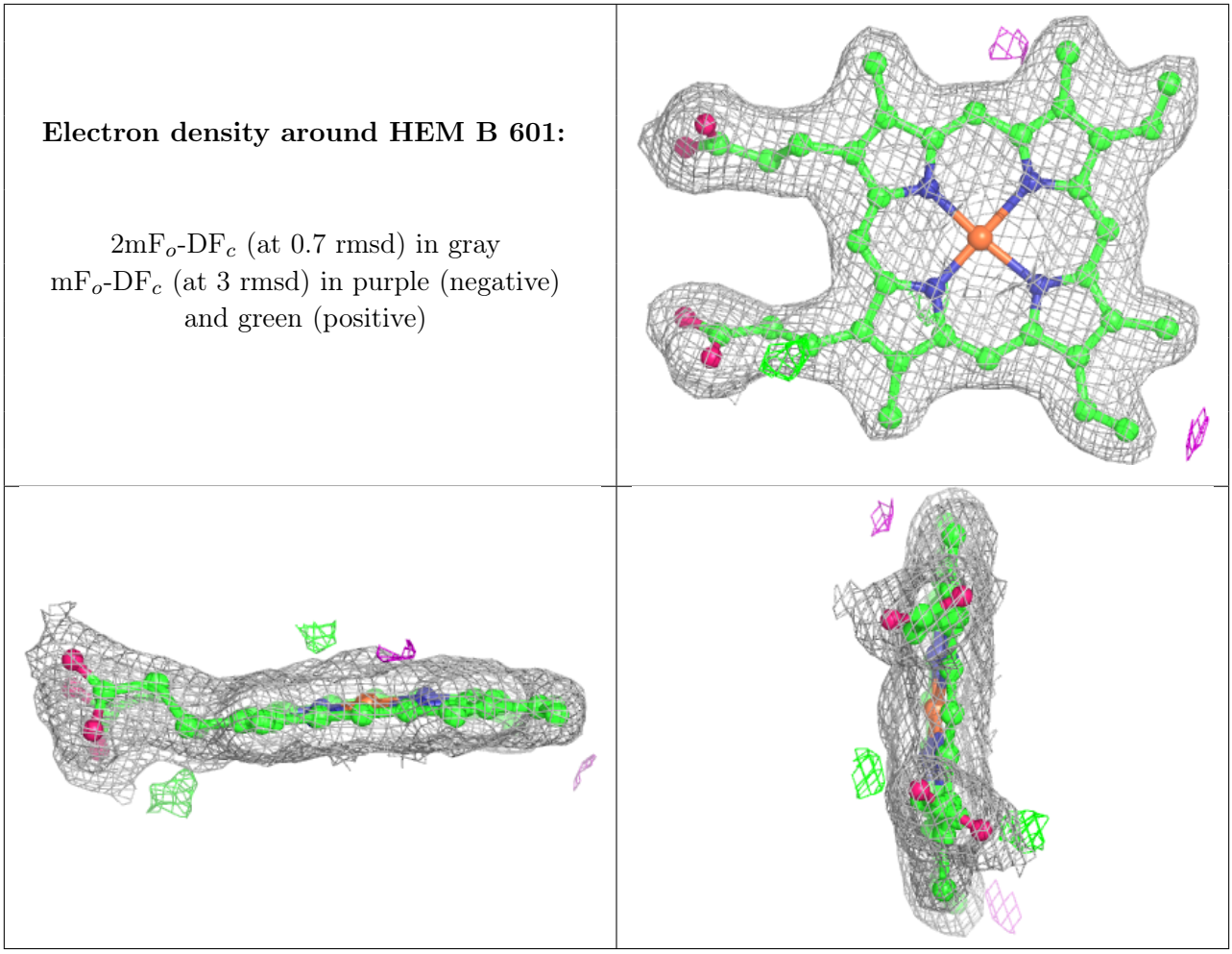






Electron density around HEM B 601:

$2mF_o$-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

There are no such residues in this entry.