Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 04:04 PM EDT

PDB ID	:	5UYS
Title	:	Human steroidogenic cytochrome P450 17A1 with 3alphaOH-5alpha-abiraterone analog
Authors	:	Scott, E.E.; Petrunak, E.M.
Deposited on	:	2017-02-24
Resolution	:	2.39 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:

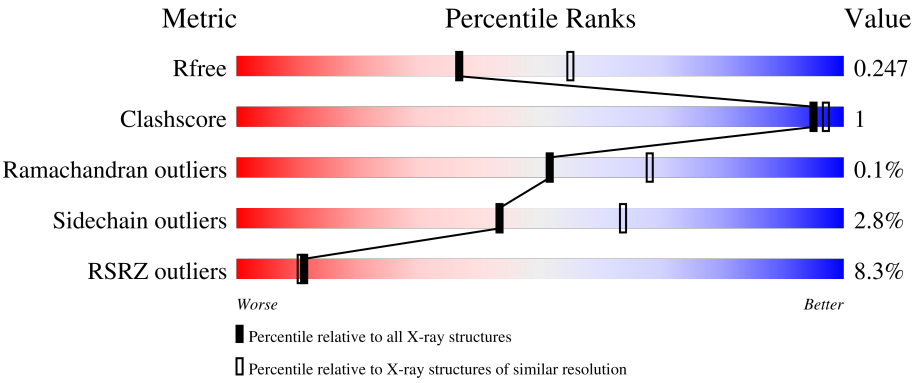
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	494	5% 90% 5% 5%
1	B	494	6% 91% • • 5%
1	C	494	7% 91% 5% •
1	D	494	13% 90% 6% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 31206 atoms, of which 15576 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 Steroid 17-alpha-hydroxylase/17,20 lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	471	Total	C	H	N	O	S	0	0	0
			7576	2403	3827	649	682	15			
1	B	470	Total	C	H	N	O	S	0	0	0
			7567	2400	3823	648	681	15			
1	C	473	Total	C	H	N	O	S	0	0	0
			7598	2409	3837	652	685	15			
1	D	473	Total	C	H	N	O	S	0	0	0
			7598	2409	3837	652	685	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP P05093
A	20	ALA	-	expression tag	UNP P05093
A	21	LYS	-	expression tag	UNP P05093
A	22	LYS	-	expression tag	UNP P05093
A	23	THR	-	expression tag	UNP P05093
A	509	HIS	-	expression tag	UNP P05093
A	510	HIS	-	expression tag	UNP P05093
A	511	HIS	-	expression tag	UNP P05093
A	512	HIS	-	expression tag	UNP P05093
B	19	MET	-	initiating methionine	UNP P05093
B	20	ALA	-	expression tag	UNP P05093
B	21	LYS	-	expression tag	UNP P05093
B	22	LYS	-	expression tag	UNP P05093
B	23	THR	-	expression tag	UNP P05093
B	509	HIS	-	expression tag	UNP P05093
B	510	HIS	-	expression tag	UNP P05093
B	511	HIS	-	expression tag	UNP P05093
B	512	HIS	-	expression tag	UNP P05093
C	19	MET	-	initiating methionine	UNP P05093
C	20	ALA	-	expression tag	UNP P05093
C	21	LYS	-	expression tag	UNP P05093

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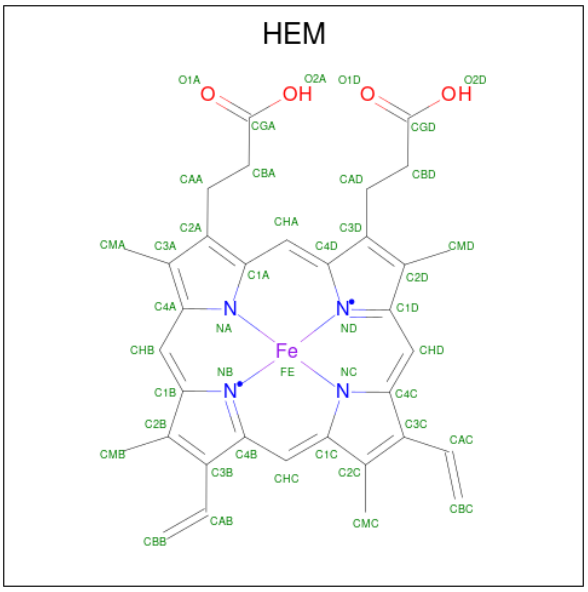
Chain	Residue	Modelled	Actual	Comment	Reference
C	22	LYS	-	expression tag	UNP P05093
C	23	THR	-	expression tag	UNP P05093
C	509	HIS	-	expression tag	UNP P05093
C	510	HIS	-	expression tag	UNP P05093
C	511	HIS	-	expression tag	UNP P05093
C	512	HIS	-	expression tag	UNP P05093
D	19	MET	-	initiating methionine	UNP P05093
D	20	ALA	-	expression tag	UNP P05093
D	21	LYS	-	expression tag	UNP P05093
D	22	LYS	-	expression tag	UNP P05093
D	23	THR	-	expression tag	UNP P05093
D	509	HIS	-	expression tag	UNP P05093
D	510	HIS	-	expression tag	UNP P05093
D	511	HIS	-	expression tag	UNP P05093
D	512	HIS	-	expression tag	UNP P05093

- 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	H	N	O	0	0
			73	34	1	30	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
2	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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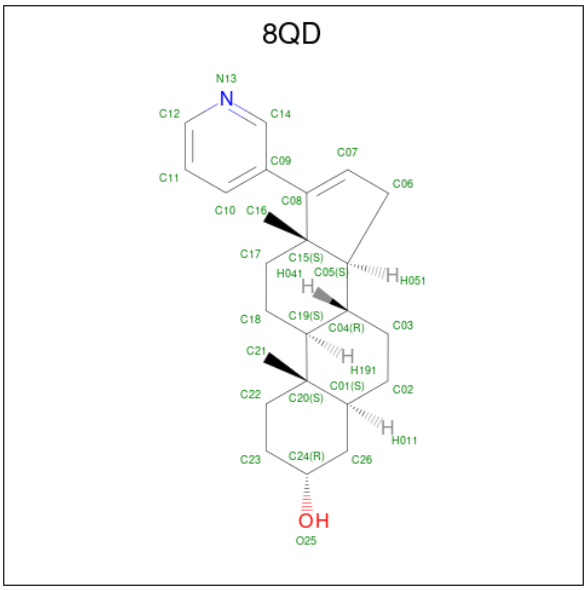
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 3 is (3alpha,5alpha,8alpha)-17-(pyridin-3-yl)androst-16-en-3-ol (three-letter code: 8QD) (formula: $C_{24}H_{33}NO$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			59	24	33	1	1		
3	B	1	Total	C	H	N	O	0	0
			59	24	33	1	1		
3	C	1	Total	C	H	N	O	0	0
			59	24	33	1	1		
3	D	1	Total	C	H	N	O	0	0
			59	24	33	1	1		

- Molecule 4 is water.

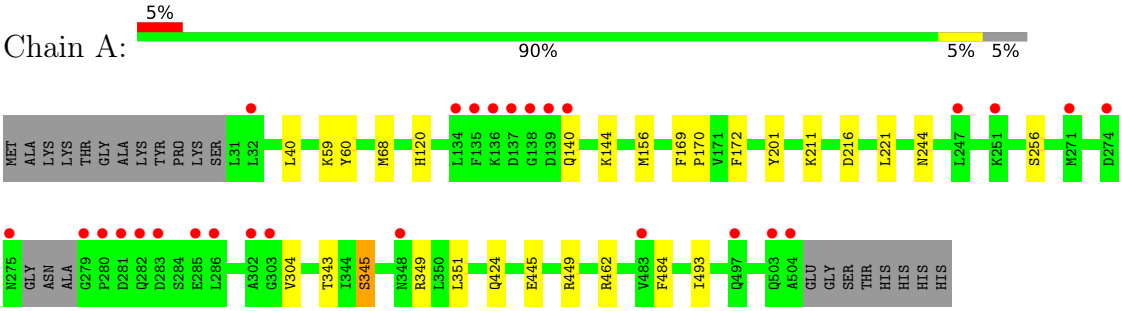
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total	O	0	0
			103	103		
4	B	93	Total	O	0	0
			93	93		
4	C	84	Total	O	0	0
			84	84		
4	D	59	Total	O	0	0
			59	59		

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.

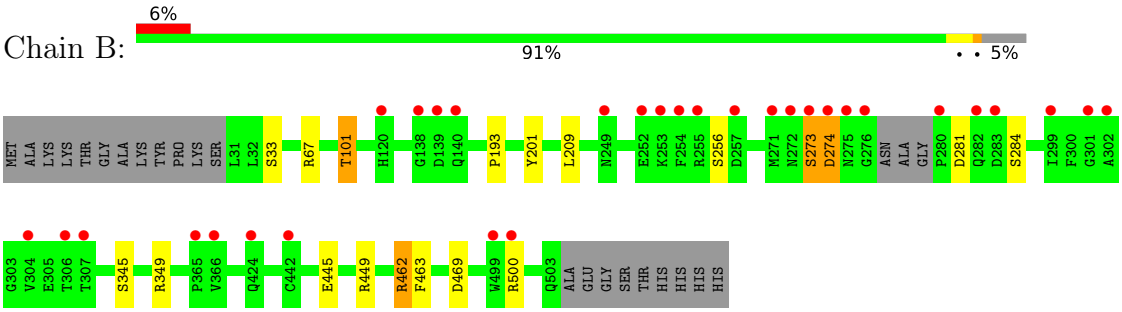
• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain A:



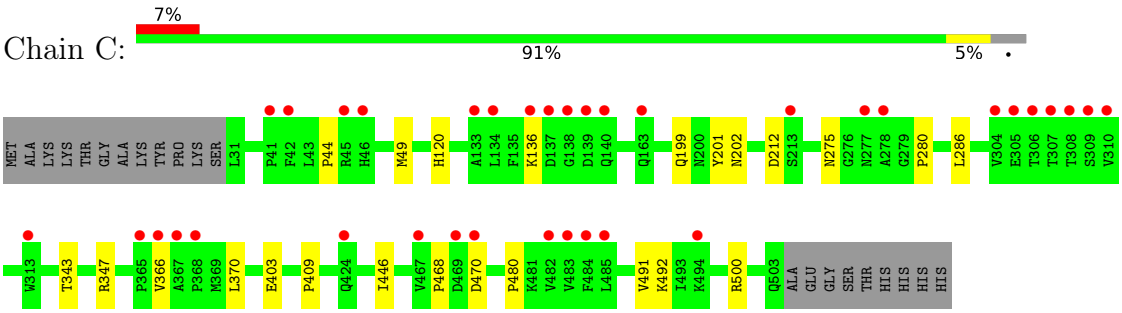
• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain B:



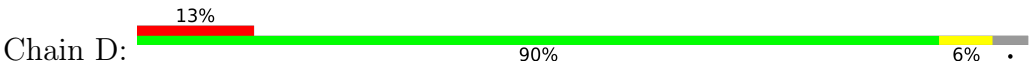
• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

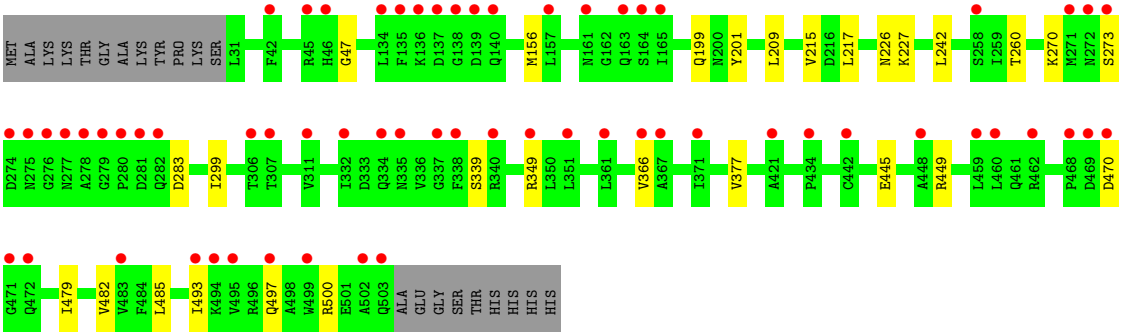
Chain C:



• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain D:




MET ALA LYS LYS THR GLY ALA LYS TYR PRO LYS SER L31 F42 R45 H46 G47 L134 F135 K136 D137 G138 D139 Q140 M156 L157 N161 G162 Q163 S164 I165 Q199 N200 Y201 L209 V215 D216 L217 N226 K227 L242 S258 I259 T260 K270 M271 N272 S273
D274 N275 G276 N277 A278 G279 P280 D281 Q282 D283 I299 T306 T307 V311 I332 D333 Q334 N335 V336 G337 F338 S339 R340 R349 L350 L351 L361 V366 A367 I371 V377 A421 P434 C442 E445 A448 R449 L459 L460 Q461 R462 P468 D469 D470
G471 Q472 I479 V482 V483 F484 L485 I493 K494 V495 R496 Q497 A498 W499 R500 E501 A502 Q503 ALA GLU GLY SER THR HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.76Å 153.18Å 168.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.29 – 2.39 39.29 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.29-2.39) 90.2 (39.29-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.190 , 0.245 0.191 , 0.247	Depositor DCC
R_{free} test set	4613 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31206	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: HEM, 8QD

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	0.36	0/3830	0.53	0/5186
1	B	0.37	0/3825	0.54	0/5178
1	C	0.36	0/3843	0.55	0/5205
1	D	0.35	0/3843	0.54	1/5205 (0.0%)
All	All	0.36	0/15341	0.54	1/20774 (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	D	47	GLY	N-CA-C	-5.65	98.97	113.10

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	3749	3827	3812	9	0
1	B	3744	3823	3808	7	0
1	C	3761	3837	3822	7	0
1	D	3761	3837	3822	11	0
2	A	43	30	30	1	0
2	B	43	30	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	30	30	4	0
2	D	43	30	30	3	0
3	A	26	33	0	0	0
3	B	26	33	0	0	0
3	C	26	33	0	0	0
3	D	26	33	0	0	0
4	A	103	0	0	1	0
4	B	93	0	0	1	0
4	C	84	0	0	0	0
4	D	59	0	0	2	0
All	All	15630	15576	15384	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 1.

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:B:445:GLU:OE2	1:B:449:ARG:NH2	2.25	0.69
1:A:120:HIS:ND1	4:A:701:HOH:O	2.28	0.66
1:A:445:GLU:OE2	1:A:449:ARG:NH2	2.29	0.65
2:C:600:HEM:HHC	2:C:600:HEM:HBB2	1.80	0.64
1:B:274:ASP:N	1:B:274:ASP:OD1	2.34	0.60
2:A:600:HEM:HBC2	2:A:600:HEM:HHD	1.84	0.58
2:D:600:HEM:HBC2	2:D:600:HEM:HHD	1.88	0.56
1:A:343:THR:HG22	1:A:345:SER:H	1.74	0.52
1:D:366:VAL:CG2	2:D:600:HEM:HMB2	2.39	0.52
2:C:600:HEM:HBC2	2:C:600:HEM:HHD	1.93	0.50
1:B:101:THR:HG21	1:B:209:LEU:O	2.12	0.49
1:B:273:SER:OG	1:B:284:SER:N	2.47	0.47
1:A:351:LEU:HD13	1:A:424:GLN:HA	1.96	0.47
1:B:469:ASP:N	4:B:705:HOH:O	2.47	0.47
1:C:212:ASP:HA	1:C:480:PRO:HB2	1.96	0.46
1:D:445:GLU:OE2	1:D:449:ARG:NH2	2.49	0.46
1:C:403:GLU:HG2	1:C:409:PRO:HG3	1.96	0.46
1:D:479:ILE:N	1:D:485:LEU:O	2.40	0.46
1:D:299:ILE:HG23	2:D:600:HEM:HBC1	1.98	0.46
1:B:462:ARG:HG2	1:B:463:PHE:CZ	2.51	0.45
1:D:226:ASN:HB2	4:D:702:HOH:O	2.15	0.45
1:C:366:VAL:CG2	2:C:600:HEM:HMB2	2.47	0.44
1:A:59:LYS:HE3	1:A:60:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PHE:CE1	1:A:304:VAL:HG11	2.53	0.43
1:C:370:LEU:HD22	2:C:600:HEM:HMA1	2.01	0.43
1:D:273:SER:HB3	1:D:283:ASP:HB2	2.00	0.42
1:A:156:MET:SD	1:B:193:PRO:HB3	2.59	0.42
1:A:169:PHE:HB3	1:A:170:PRO:HD3	2.01	0.42
1:D:215:VAL:HG12	1:D:217:LEU:H	1.85	0.41
1:D:227:LYS:N	4:D:702:HOH:O	2.37	0.41
1:C:468:PRO:HA	1:C:492:LYS:HB2	2.03	0.41
1:D:209:LEU:HD23	1:D:482:VAL:HG11	2.02	0.41
1:C:120:HIS:CD2	1:C:286:LEU:HD22	2.57	0.40
1:C:280:PRO:CD	1:D:377:VAL:HG12	2.51	0.40
1:A:40:LEU:HD21	1:A:68:MET:HE2	2.04	0.40
1:D:470:ASP:OD1	1:D:470:ASP:N	2.54	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	467/494 (94%)	451 (97%)	16 (3%)	0	100 100
1	B	466/494 (94%)	451 (97%)	15 (3%)	0	100 100
1	C	471/494 (95%)	454 (96%)	15 (3%)	2 (0%)	34 48
1	D	471/494 (95%)	450 (96%)	21 (4%)	0	100 100
All	All	1875/1976 (95%)	1806 (96%)	67 (4%)	2 (0%)	51 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	44	PRO
1	C	275	ASN

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	419/436 (96%)	406 (97%)	13 (3%)	40	60
1	B	419/436 (96%)	407 (97%)	12 (3%)	42	62
1	C	420/436 (96%)	409 (97%)	11 (3%)	46	66
1	D	420/436 (96%)	409 (97%)	11 (3%)	46	66
All	All	1678/1744 (96%)	1631 (97%)	47 (3%)	43	63

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	144	LYS
1	A	201	TYR
1	A	211	LYS
1	A	216	ASP
1	A	221	LEU
1	A	244	ASN
1	A	256	SER
1	A	345	SER
1	A	349	ARG
1	A	462	ARG
1	A	484	PHE
1	A	493	ILE
1	B	33	SER
1	B	67	ARG
1	B	101	THR
1	B	201	TYR
1	B	256	SER
1	B	273	SER
1	B	274	ASP
1	B	281	ASP
1	B	345	SER
1	B	349	ARG
1	B	462	ARG

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Mol	Chain	Res	Type
1	B	500	ARG
1	C	49	MET
1	C	136	LYS
1	C	199	GLN
1	C	201	TYR
1	C	202	ASN
1	C	343	THR
1	C	347	ARG
1	C	446	ILE
1	C	470	ASP
1	C	491	VAL
1	C	500	ARG
1	D	156	MET
1	D	199	GLN
1	D	201	TYR
1	D	242	LEU
1	D	260	THR
1	D	270	LYS
1	D	339	SER
1	D	349	ARG
1	D	493	ILE
1	D	497	GLN
1	D	500	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	79	HIS

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)

8 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	8QD	C	601	2	30,30,30	6.10	20 (66%)	44,47,47	2.94	13 (29%)
2	HEM	D	600	3,1	41,50,50	1.92	6 (14%)	45,82,82	1.70	7 (15%)
3	8QD	A	601	2	30,30,30	6.30	21 (70%)	44,47,47	2.96	15 (34%)
3	8QD	D	601	2	30,30,30	6.27	20 (66%)	44,47,47	2.95	18 (40%)
3	8QD	B	601	2	30,30,30	6.17	21 (70%)	44,47,47	2.98	14 (31%)
2	HEM	C	600	3,1	41,50,50	1.88	6 (14%)	45,82,82	1.81	14 (31%)
2	HEM	B	600	3,1	41,50,50	1.89	6 (14%)	45,82,82	1.66	8 (17%)
2	HEM	A	600	3,1	41,50,50	1.95	5 (12%)	45,82,82	1.60	7 (15%)

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	8QD	C	601	2	-	0/4/62/62	0/5/5/5
2	HEM	D	600	3,1	-	1/12/54/54	-
3	8QD	A	601	2	-	0/4/62/62	0/5/5/5
3	8QD	D	601	2	-	1/4/62/62	0/5/5/5
3	8QD	B	601	2	-	1/4/62/62	0/5/5/5
2	HEM	C	600	3,1	-	3/12/54/54	-
2	HEM	B	600	3,1	-	2/12/54/54	-
2	HEM	A	600	3,1	-	0/12/54/54	-

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	8QD	C07-C08	18.33	1.66	1.33
3	D	601	8QD	C07-C08	18.24	1.65	1.33
3	B	601	8QD	C07-C08	17.83	1.65	1.33
3	C	601	8QD	C07-C08	17.76	1.65	1.33
3	D	601	8QD	C06-C07	16.14	1.74	1.50
3	A	601	8QD	C06-C07	15.81	1.73	1.50
3	B	601	8QD	C06-C07	15.79	1.73	1.50
3	C	601	8QD	C06-C07	14.99	1.72	1.50
3	A	601	8QD	C15-C08	-14.74	1.39	1.53
3	D	601	8QD	C15-C08	-14.57	1.39	1.53
3	B	601	8QD	C15-C08	-14.20	1.39	1.53
3	C	601	8QD	C15-C08	-13.89	1.40	1.53
3	A	601	8QD	C06-C05	-8.59	1.41	1.54
3	B	601	8QD	C06-C05	-8.51	1.41	1.54
3	C	601	8QD	C06-C05	-8.39	1.42	1.54
3	D	601	8QD	C06-C05	-8.12	1.42	1.54
2	B	600	HEM	C3D-C2D	7.80	1.53	1.36
2	D	600	HEM	C3D-C2D	7.75	1.53	1.36
2	A	600	HEM	C3D-C2D	7.72	1.53	1.36
3	D	601	8QD	C14-C09	7.60	1.51	1.39
3	C	601	8QD	C14-C09	7.45	1.50	1.39
3	A	601	8QD	C14-C09	7.41	1.50	1.39
2	C	600	HEM	C3D-C2D	7.31	1.52	1.36
3	B	601	8QD	C14-C09	7.24	1.50	1.39
3	C	601	8QD	C17-C18	6.17	1.66	1.53
3	D	601	8QD	C14-N13	5.93	1.47	1.34
3	A	601	8QD	C17-C18	5.84	1.65	1.53
3	C	601	8QD	C14-N13	5.81	1.46	1.34
3	A	601	8QD	C14-N13	5.79	1.46	1.34
3	B	601	8QD	C17-C18	5.71	1.65	1.53
3	D	601	8QD	C17-C18	5.51	1.65	1.53
3	B	601	8QD	C14-N13	5.20	1.45	1.34
3	C	601	8QD	C04-C19	5.05	1.63	1.53
3	D	601	8QD	C04-C19	5.05	1.63	1.53
3	B	601	8QD	C04-C19	5.03	1.63	1.53
3	D	601	8QD	C10-C09	5.00	1.47	1.39
3	A	601	8QD	C04-C19	4.91	1.63	1.53
2	A	600	HEM	C3C-C2C	-4.90	1.33	1.40
3	A	601	8QD	C10-C09	4.87	1.47	1.39
3	C	601	8QD	C10-C09	4.75	1.47	1.39
3	B	601	8QD	C10-C09	4.72	1.47	1.39
2	D	600	HEM	C3C-C2C	-4.70	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	8QD	C11-C12	4.64	1.51	1.37
3	D	601	8QD	C11-C12	4.62	1.51	1.37
3	C	601	8QD	C11-C12	4.60	1.51	1.37
3	B	601	8QD	C12-N13	4.52	1.47	1.33
3	A	601	8QD	C15-C05	4.45	1.63	1.54
3	D	601	8QD	C12-N13	4.36	1.46	1.33
3	B	601	8QD	C11-C12	4.31	1.50	1.37
3	B	601	8QD	C15-C05	4.26	1.62	1.54
2	C	600	HEM	C3C-C2C	-4.25	1.34	1.40
3	A	601	8QD	C12-N13	4.23	1.46	1.33
3	C	601	8QD	C12-N13	4.21	1.46	1.33
2	B	600	HEM	C3C-C2C	-4.16	1.34	1.40
3	C	601	8QD	C26-C24	4.08	1.59	1.51
3	D	601	8QD	C15-C05	3.98	1.62	1.54
3	A	601	8QD	C11-C10	3.89	1.47	1.38
2	C	600	HEM	C3C-CAC	3.85	1.55	1.47
3	C	601	8QD	C11-C10	3.83	1.47	1.38
3	D	601	8QD	C11-C10	3.82	1.47	1.38
3	C	601	8QD	C15-C05	3.82	1.62	1.54
3	B	601	8QD	C11-C10	3.78	1.46	1.38
2	A	600	HEM	C3C-CAC	3.78	1.55	1.47
3	B	601	8QD	C26-C24	3.70	1.58	1.51
3	A	601	8QD	C26-C24	3.61	1.58	1.51
2	D	600	HEM	C3C-CAC	3.55	1.55	1.47
2	B	600	HEM	C3C-CAC	3.54	1.55	1.47
3	D	601	8QD	C26-C24	3.37	1.58	1.51
3	A	601	8QD	C09-C08	3.36	1.53	1.48
3	C	601	8QD	C09-C08	3.30	1.53	1.48
3	B	601	8QD	C03-C02	3.23	1.60	1.52
3	A	601	8QD	C03-C02	3.23	1.60	1.52
2	D	600	HEM	CAB-C3B	3.21	1.56	1.47
3	C	601	8QD	C03-C02	3.19	1.60	1.52
3	D	601	8QD	C09-C08	3.15	1.53	1.48
3	C	601	8QD	C20-C01	3.14	1.60	1.55
2	B	600	HEM	CAB-C3B	3.12	1.55	1.47
2	C	600	HEM	CAB-C3B	3.07	1.55	1.47
3	D	601	8QD	C03-C02	3.01	1.60	1.52
3	B	601	8QD	C20-C01	2.97	1.60	1.55
2	A	600	HEM	CAB-C3B	2.91	1.55	1.47
3	A	601	8QD	C20-C01	2.86	1.60	1.55
3	D	601	8QD	C20-C01	2.85	1.60	1.55
3	B	601	8QD	C09-C08	2.74	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	8QD	C22-C23	2.67	1.59	1.53
3	A	601	8QD	O25-C24	-2.57	1.35	1.43
2	D	600	HEM	FE-ND	2.36	2.08	1.96
3	D	601	8QD	C22-C23	2.27	1.58	1.53
3	A	601	8QD	C18-C19	2.26	1.57	1.53
2	C	600	HEM	CMB-C2B	2.23	1.55	1.50
3	D	601	8QD	O25-C24	-2.22	1.36	1.43
3	A	601	8QD	C20-C19	-2.19	1.52	1.56
3	C	601	8QD	O25-C24	-2.19	1.36	1.43
3	B	601	8QD	O25-C24	-2.16	1.36	1.43
2	C	600	HEM	CAA-C2A	2.15	1.55	1.52
2	B	600	HEM	CAA-C2A	2.12	1.55	1.52
3	D	601	8QD	C18-C19	2.11	1.57	1.53
2	B	600	HEM	FE-ND	2.11	2.07	1.96
3	B	601	8QD	C23-C24	2.06	1.56	1.51
3	C	601	8QD	C20-C19	-2.04	1.52	1.56
3	A	601	8QD	C22-C23	2.04	1.57	1.53
3	B	601	8QD	C18-C19	2.03	1.57	1.53
2	D	600	HEM	CMB-C2B	2.01	1.55	1.50
2	A	600	HEM	CMB-C2B	2.01	1.55	1.50
3	C	601	8QD	C22-C23	2.00	1.57	1.53

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	8QD	C06-C07-C08	-11.79	103.17	112.87
3	D	601	8QD	C06-C07-C08	-11.44	103.46	112.87
3	A	601	8QD	C06-C07-C08	-11.38	103.52	112.87
3	C	601	8QD	C06-C07-C08	-10.66	104.11	112.87
3	D	601	8QD	C05-C15-C08	8.96	107.34	99.70
3	C	601	8QD	C05-C15-C08	8.01	106.54	99.70
3	A	601	8QD	C05-C15-C08	7.88	106.42	99.70
3	B	601	8QD	C05-C15-C08	7.53	106.13	99.70
3	C	601	8QD	C06-C05-C15	6.08	108.60	104.05
2	A	600	HEM	C4D-ND-C1D	5.90	111.17	105.07
2	D	600	HEM	C4D-ND-C1D	5.70	110.96	105.07
2	C	600	HEM	C4D-ND-C1D	5.53	110.78	105.07
3	D	601	8QD	C06-C05-C15	5.35	108.05	104.05
2	B	600	HEM	C4D-ND-C1D	5.21	110.46	105.07
3	C	601	8QD	C06-C05-C04	-5.18	115.35	121.57
3	B	601	8QD	C22-C23-C24	5.16	117.08	110.47
3	A	601	8QD	C06-C05-C15	5.12	107.88	104.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	8QD	C06-C05-C15	4.77	107.62	104.05
3	A	601	8QD	C06-C05-C04	-4.66	115.98	121.57
3	B	601	8QD	C09-C14-N13	-4.57	116.74	123.49
3	B	601	8QD	C06-C05-C04	-4.44	116.24	121.57
3	C	601	8QD	C03-C04-C19	4.42	115.97	110.49
3	A	601	8QD	C22-C20-C01	4.24	114.04	107.77
2	D	600	HEM	C4B-CHC-C1C	4.18	128.07	122.56
3	A	601	8QD	C09-C14-N13	-4.07	117.47	123.49
3	A	601	8QD	C22-C23-C24	3.95	115.54	110.47
2	B	600	HEM	C4B-CHC-C1C	3.82	127.60	122.56
2	C	600	HEM	C4B-CHC-C1C	3.80	127.57	122.56
3	D	601	8QD	C09-C14-N13	-3.80	117.88	123.49
3	C	601	8QD	C09-C14-N13	-3.77	117.92	123.49
3	B	601	8QD	C12-N13-C14	3.66	123.18	116.85
3	C	601	8QD	C22-C20-C01	3.59	113.08	107.77
3	A	601	8QD	C12-N13-C14	3.56	123.00	116.85
3	C	601	8QD	C16-C15-C17	-3.52	106.99	111.13
3	B	601	8QD	C10-C09-C14	3.49	121.59	117.63
2	C	600	HEM	CMA-C3A-C4A	-3.42	123.22	128.46
3	D	601	8QD	C06-C05-C04	-3.30	117.61	121.57
2	A	600	HEM	C4B-CHC-C1C	3.27	126.87	122.56
3	A	601	8QD	C03-C04-C19	3.27	114.55	110.49
3	A	601	8QD	C15-C08-C07	-3.25	105.77	109.72
3	C	601	8QD	C15-C08-C07	-3.25	105.77	109.72
3	B	601	8QD	C01-C26-C24	-3.25	107.99	112.76
3	D	601	8QD	C15-C08-C07	-3.20	105.83	109.72
3	A	601	8QD	C01-C26-C24	-3.19	108.07	112.76
2	A	600	HEM	C4C-CHD-C1D	3.14	126.70	122.56
3	D	601	8QD	C22-C20-C01	3.12	112.39	107.77
3	C	601	8QD	C12-N13-C14	3.11	122.23	116.85
3	B	601	8QD	C21-C20-C19	-3.08	106.93	111.18
3	D	601	8QD	C12-N13-C14	3.05	122.13	116.85
3	D	601	8QD	C01-C26-C24	-3.03	108.30	112.76
2	D	600	HEM	CHD-C1D-ND	2.93	127.61	124.43
3	B	601	8QD	C15-C08-C07	-2.86	106.25	109.72
3	D	601	8QD	C10-C09-C14	2.81	120.82	117.63
3	D	601	8QD	C09-C08-C07	2.81	129.04	125.19
2	B	600	HEM	CMC-C2C-C3C	2.75	129.82	124.68
3	A	601	8QD	C10-C09-C14	2.69	120.68	117.63
2	C	600	HEM	C4C-CHD-C1D	2.65	126.06	122.56
3	C	601	8QD	C10-C09-C14	2.65	120.63	117.63
3	A	601	8QD	C16-C15-C17	-2.64	108.02	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	600	HEM	CMA-C3A-C4A	-2.59	124.48	128.46
3	B	601	8QD	C23-C22-C20	2.58	117.21	112.78
3	D	601	8QD	C03-C04-C19	2.58	113.69	110.49
2	C	600	HEM	CHA-C4D-ND	2.55	127.53	124.38
2	C	600	HEM	CMD-C2D-C1D	2.54	128.90	125.04
3	C	601	8QD	C01-C26-C24	-2.52	109.06	112.76
3	C	601	8QD	C15-C05-C04	-2.51	110.43	113.12
2	B	600	HEM	O2A-CGA-CBA	2.50	122.06	114.03
2	C	600	HEM	CBA-CAA-C2A	2.46	116.81	112.62
2	D	600	HEM	CHC-C4B-NB	2.45	127.09	124.43
2	C	600	HEM	CAD-CBD-CGD	-2.44	108.35	113.60
3	B	601	8QD	C16-C15-C17	-2.37	108.33	111.13
3	B	601	8QD	C22-C20-C01	2.35	111.25	107.77
3	D	601	8QD	C16-C15-C17	-2.34	108.37	111.13
2	D	600	HEM	C4C-CHD-C1D	2.34	125.65	122.56
2	B	600	HEM	CHC-C4B-NB	2.34	126.97	124.43
2	C	600	HEM	CAA-CBA-CGA	-2.32	107.25	113.76
2	B	600	HEM	O1A-CGA-CBA	-2.32	115.62	123.08
3	A	601	8QD	C21-C20-C19	-2.28	108.05	111.18
2	B	600	HEM	CAA-CBA-CGA	-2.22	107.53	113.76
2	C	600	HEM	CHC-C4B-C3B	2.21	127.95	124.57
2	A	600	HEM	CMD-C2D-C1D	2.21	128.40	125.04
2	C	600	HEM	O2A-CGA-CBA	2.20	121.10	114.03
2	C	600	HEM	CMA-C3A-C2A	2.17	129.03	124.94
2	B	600	HEM	CMD-C2D-C1D	2.17	128.34	125.04
2	C	600	HEM	C3B-C2B-C1B	2.14	108.07	106.49
2	A	600	HEM	CHC-C4B-NB	2.11	126.72	124.43
3	D	601	8QD	C15-C05-C04	-2.09	110.89	113.12
3	D	601	8QD	C10-C09-C08	-2.09	117.67	120.99
2	C	600	HEM	O1A-CGA-CBA	-2.08	116.39	123.08
3	D	601	8QD	C21-C20-C19	-2.08	108.32	111.18
3	D	601	8QD	C16-C15-C05	-2.06	109.93	112.98
2	A	600	HEM	CAD-C3D-C4D	2.06	128.25	124.66
3	A	601	8QD	C05-C06-C07	-2.04	98.10	101.39
3	D	601	8QD	C03-C02-C01	-2.03	107.77	111.84
2	A	600	HEM	CAA-CBA-CGA	-2.02	108.09	113.76
2	D	600	HEM	C1B-NB-C4B	2.02	107.16	105.07

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	600	HEM	C4B-C3B-CAB-CBB
2	C	600	HEM	CAA-CBA-CGA-O2A
2	B	600	HEM	CAD-CBD-CGD-O1D
2	C	600	HEM	CAA-CBA-CGA-O1A
2	B	600	HEM	CAD-CBD-CGD-O2D
3	B	601	8QD	C07-C08-C09-C10
3	D	601	8QD	C07-C08-C09-C10
2	D	600	HEM	CAA-CBA-CGA-O2A

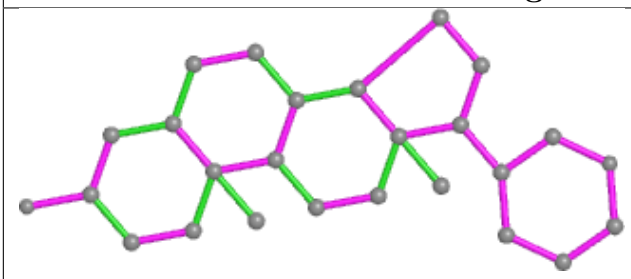
There are no ring outliers.

3 monomers are involved in 8 short contacts:

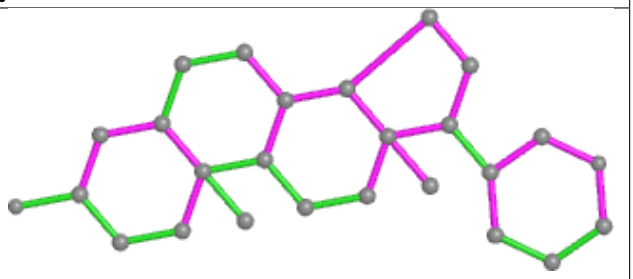
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	HEM	3	0
2	C	600	HEM	4	0
2	A	600	HEM	1	0

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.

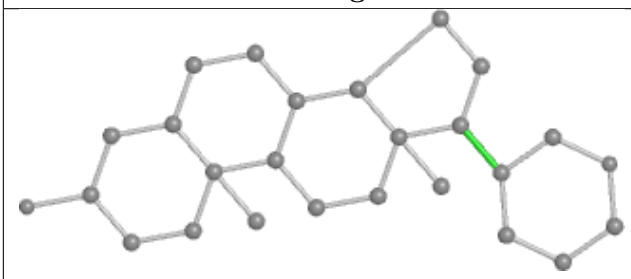
Ligand 8QD C 601



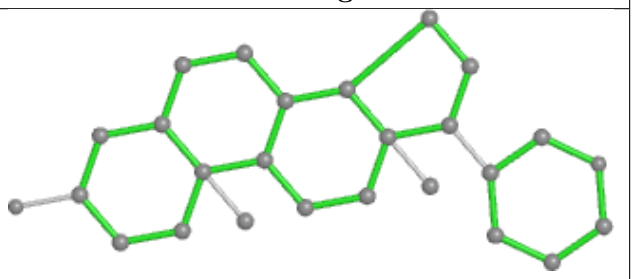
Bond lengths



Bond angles

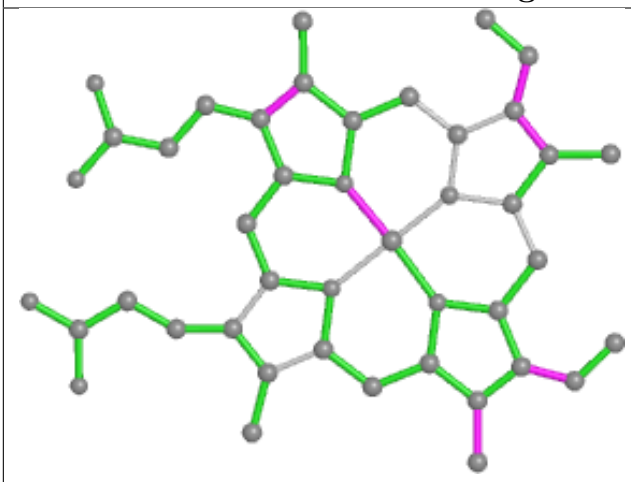


Torsions

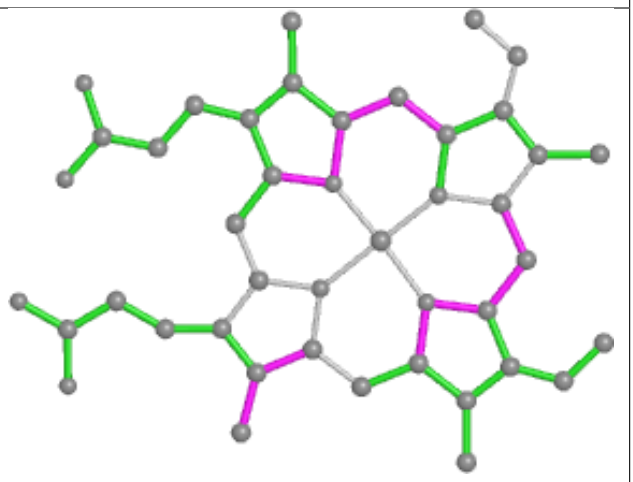


Rings

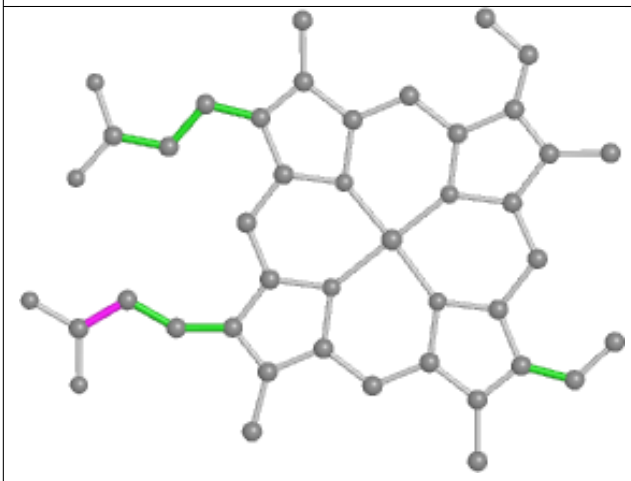
Ligand HEM D 600



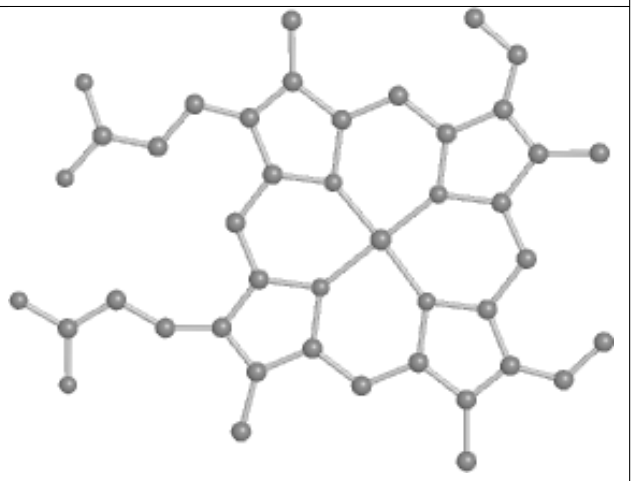
Bond lengths



Bond angles

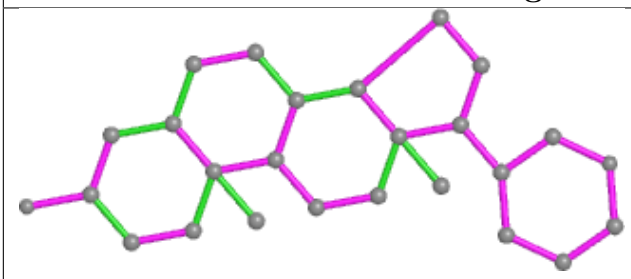


Torsions

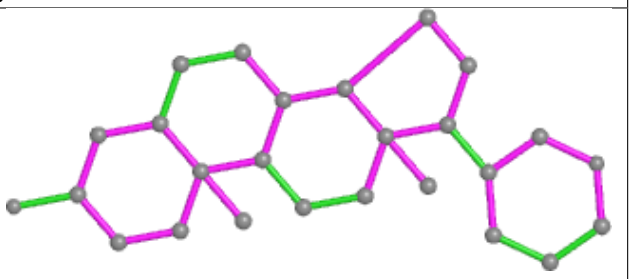


Rings

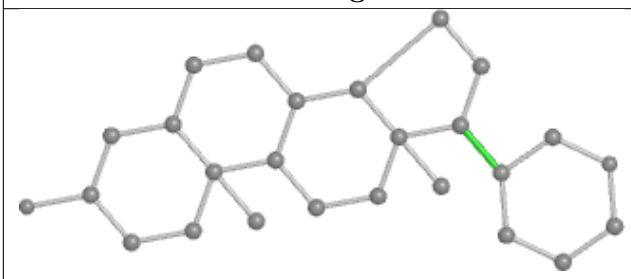
Ligand 8QD A 601



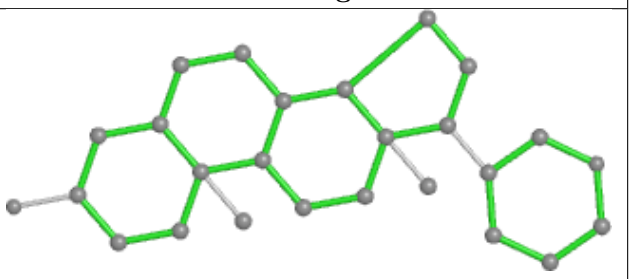
Bond lengths



Bond angles

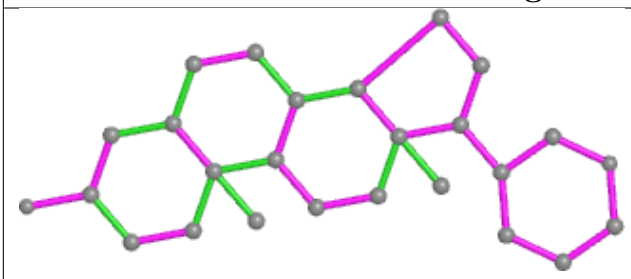


Torsions

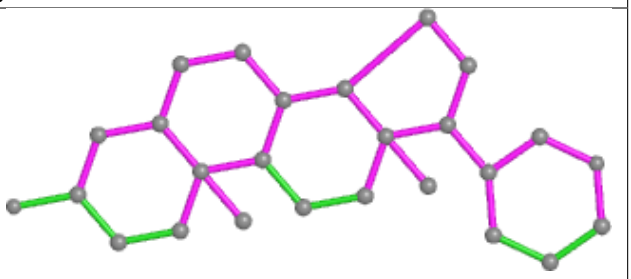


Rings

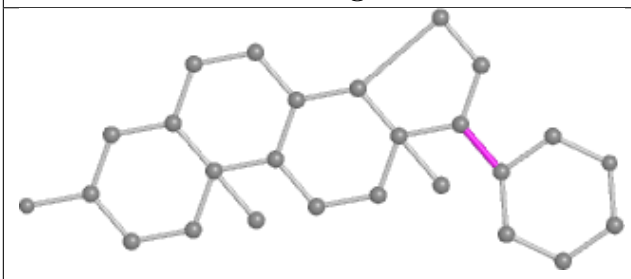
Ligand 8QD D 601



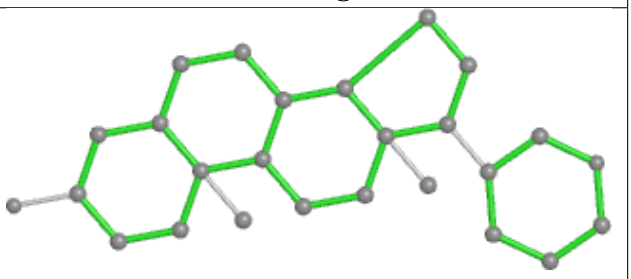
Bond lengths



Bond angles

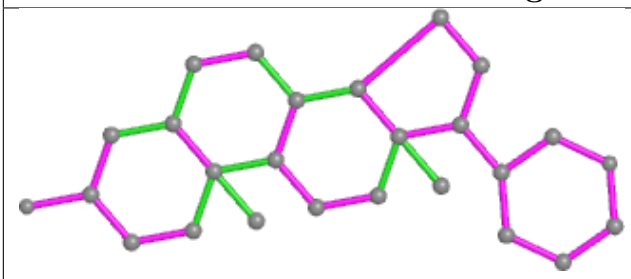


Torsions

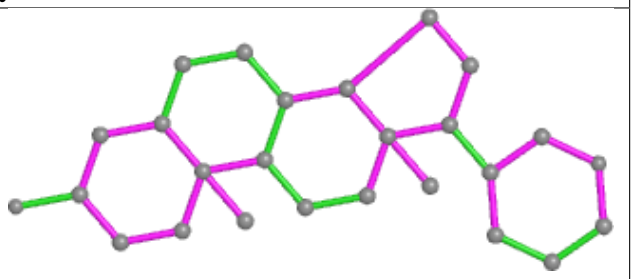


Rings

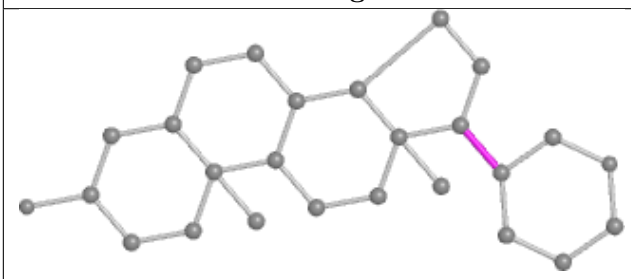
Ligand 8QD B 601



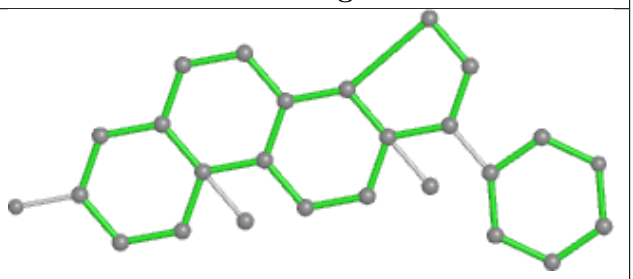
Bond lengths



Bond angles

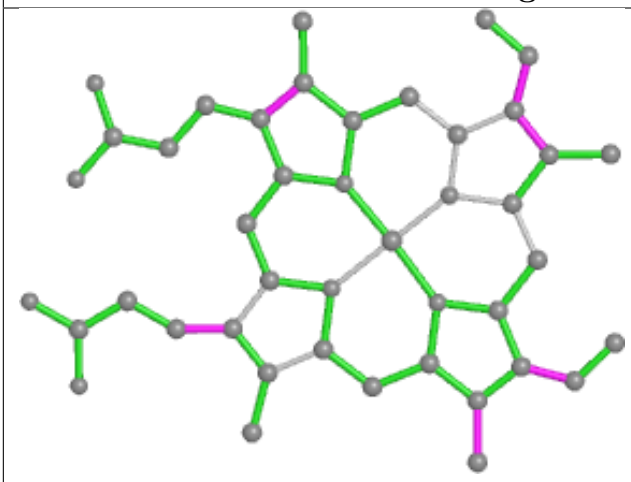


Torsions

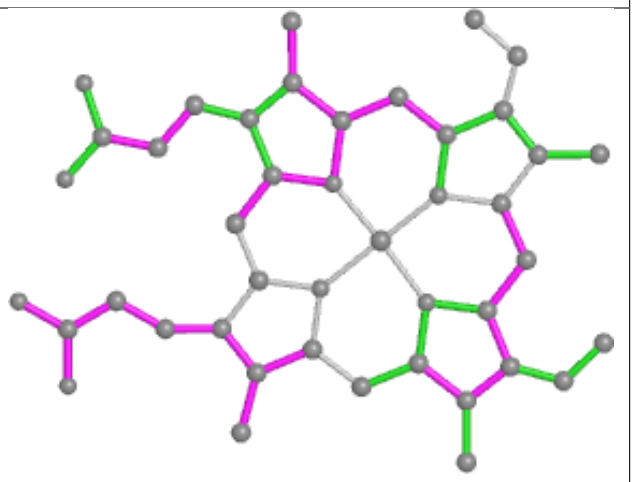


Rings

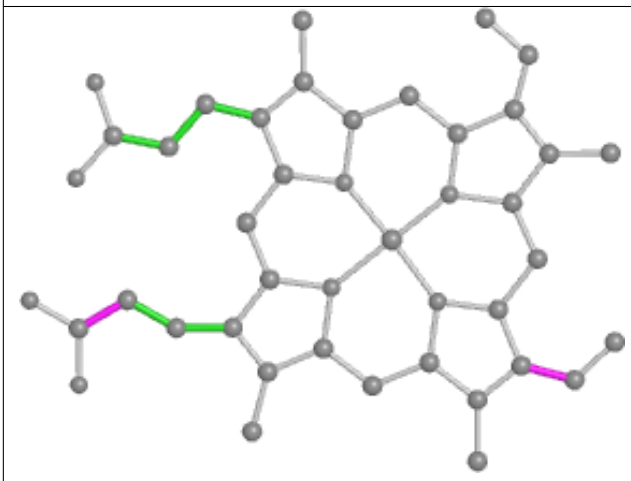
Ligand HEM C 600



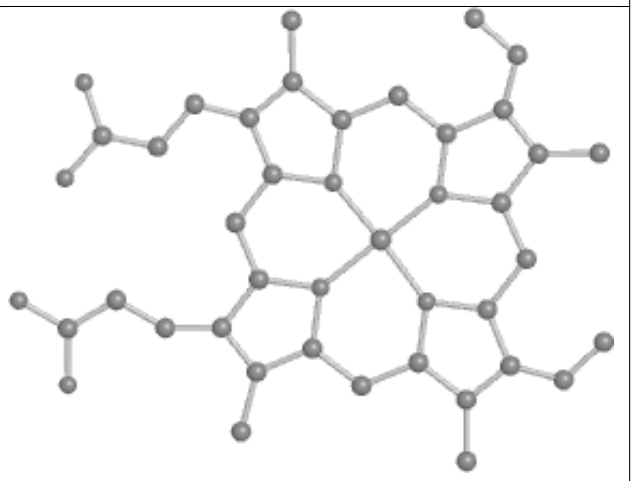
Bond lengths



Bond angles

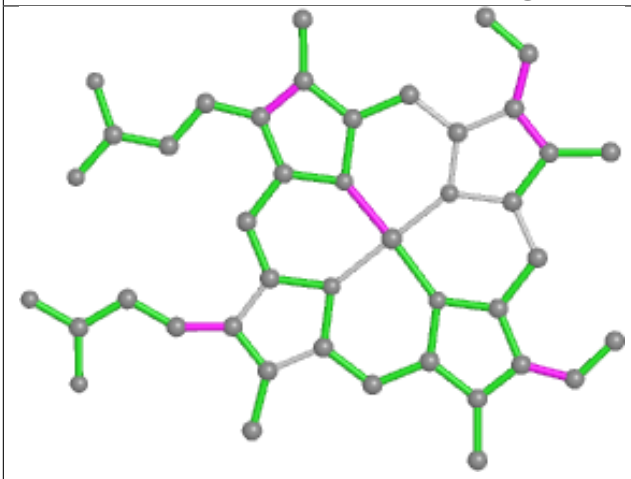


Torsions

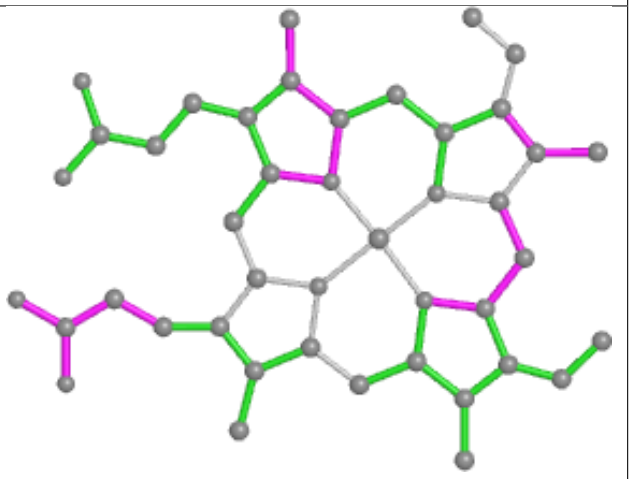


Rings

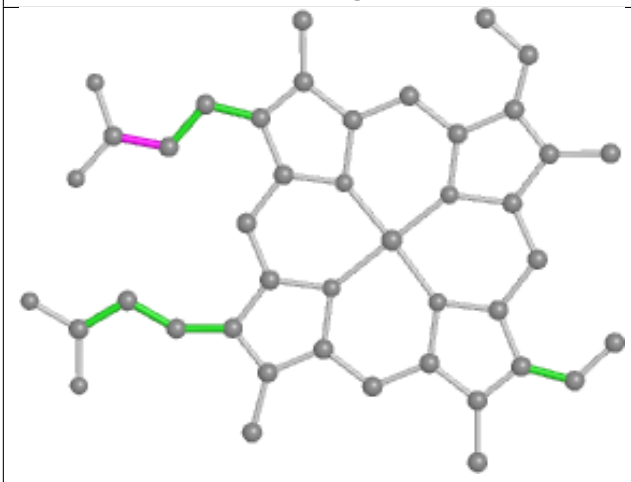
Ligand HEM B 600



Bond lengths



Bond angles



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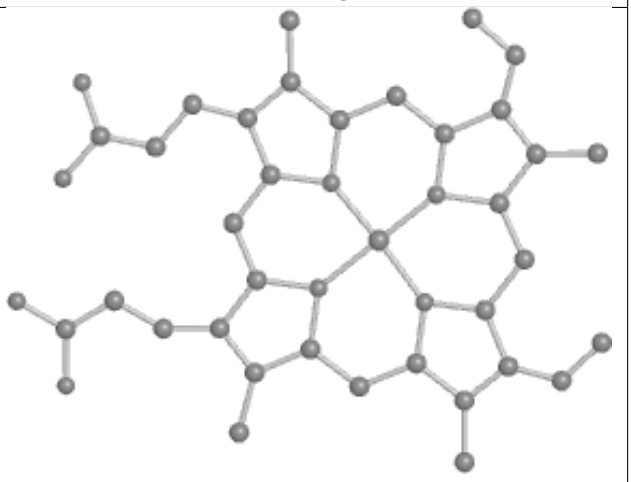
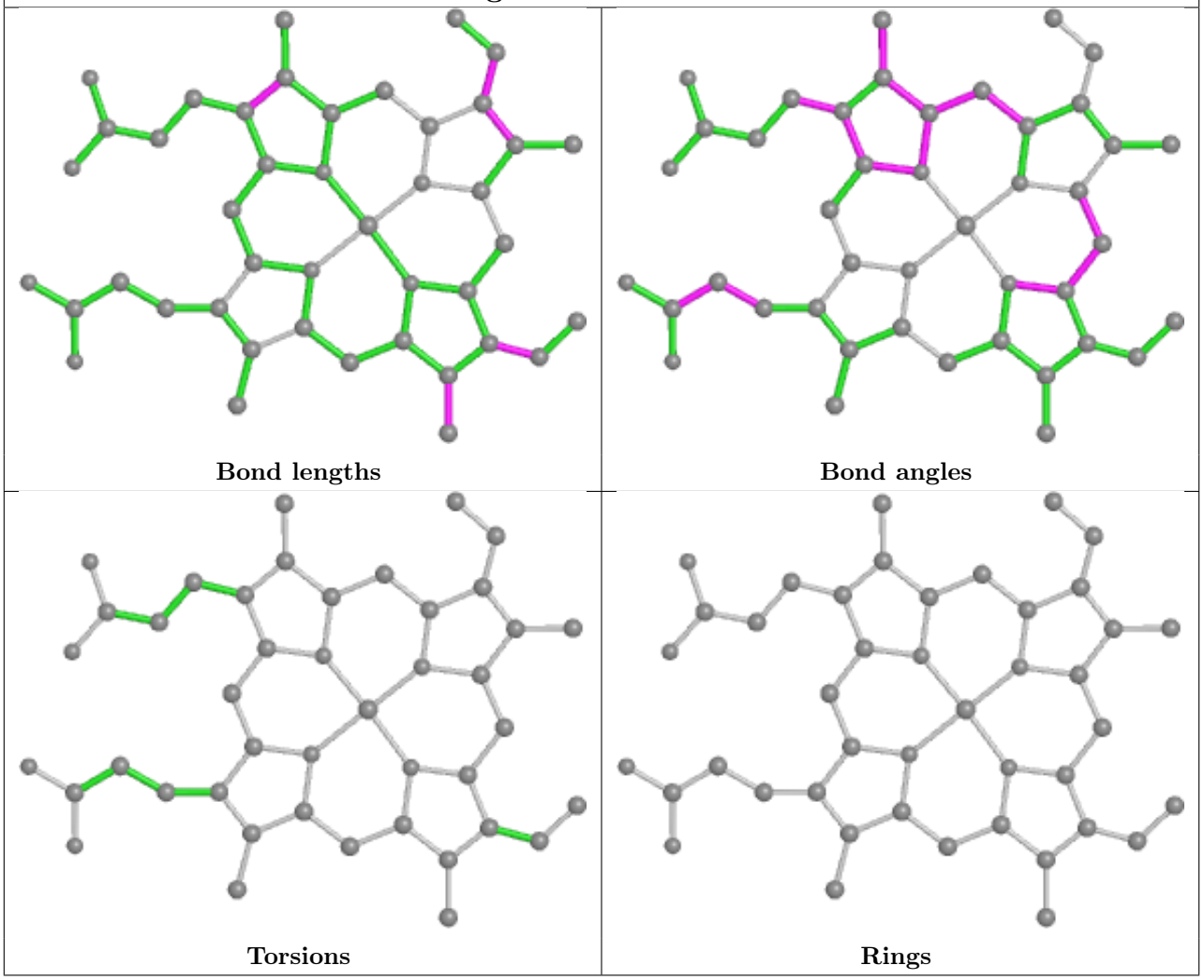


Rings

Ligand HEM A 600



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	471/494 (95%)	0.35	27 (5%)	23 22	25, 37, 65, 100	0
1	B	470/494 (95%)	0.35	31 (6%)	18 17	23, 35, 64, 92	0
1	C	473/494 (95%)	0.44	36 (7%)	13 12	24, 36, 66, 100	0
1	D	473/494 (95%)	0.75	63 (13%)	3 3	24, 44, 95, 125	0
All	All	1887/1976 (95%)	0.47	157 (8%)	11 10	23, 38, 77, 125	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	277	ASN	7.5
1	B	276	GLY	7.4
1	A	139	ASP	7.3
1	D	471	GLY	6.9
1	D	279	GLY	6.8
1	D	278	ALA	6.4
1	A	280	PRO	6.4
1	C	139	ASP	5.9
1	D	139	ASP	5.9
1	A	140	GLN	5.9
1	C	277	ASN	5.5
1	A	504	ALA	5.4
1	D	332	ILE	5.4
1	D	140	GLN	5.3
1	D	280	PRO	5.3
1	B	275	ASN	5.2
1	C	140	GLN	4.9
1	D	276	GLY	4.9
1	D	137	ASP	4.9
1	B	140	GLN	4.7
1	D	282	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	139	ASP	4.4
1	C	138	GLY	4.4
1	B	280	PRO	4.3
1	C	137	ASP	4.3
1	D	134	LEU	4.2
1	D	469	ASP	4.2
1	D	499	TRP	4.2
1	D	281	ASP	4.1
1	D	163	GLN	4.1
1	C	45	ARG	4.0
1	A	137	ASP	3.9
1	D	470	ASP	3.9
1	D	45	ARG	3.8
1	D	367	ALA	3.8
1	D	503	GLN	3.7
1	B	282	GLN	3.6
1	A	135	PHE	3.6
1	A	138	GLY	3.6
1	D	135	PHE	3.5
1	A	282	GLN	3.5
1	A	281	ASP	3.5
1	C	366	VAL	3.4
1	A	274	ASP	3.4
1	C	484	PHE	3.4
1	D	138	GLY	3.4
1	C	42	PHE	3.3
1	C	469	ASP	3.3
1	D	468	PRO	3.3
1	C	309	SER	3.2
1	D	157	LEU	3.1
1	C	470	ASP	3.1
1	A	302	ALA	3.1
1	A	279	GLY	3.1
1	A	271	MET	3.1
1	B	253	LYS	3.1
1	D	42	PHE	3.1
1	C	482	VAL	3.0
1	D	271	MET	3.0
1	B	252	GLU	3.0
1	C	367	ALA	3.0
1	D	502	ALA	3.0
1	D	306	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	459	LEU	3.0
1	B	273	SER	3.0
1	B	499	TRP	3.0
1	C	278	ALA	3.0
1	D	337	GLY	3.0
1	C	365	PRO	2.9
1	D	462	ARG	2.9
1	D	494	LYS	2.9
1	D	161	ASN	2.9
1	B	274	ASP	2.9
1	C	308	THR	2.9
1	D	275	ASN	2.9
1	C	313	TRP	2.8
1	A	136	LYS	2.8
1	D	335	ASN	2.8
1	B	255	ARG	2.8
1	B	254	PHE	2.8
1	C	133	ALA	2.8
1	C	46	HIS	2.8
1	B	500	ARG	2.8
1	D	493	ILE	2.7
1	D	448	ALA	2.7
1	C	306	THR	2.7
1	C	485	LEU	2.6
1	C	310	VAL	2.6
1	D	472	GLN	2.6
1	D	497	GLN	2.6
1	D	273	SER	2.6
1	A	134	LEU	2.6
1	C	368	PRO	2.6
1	B	306	THR	2.5
1	D	340	ARG	2.5
1	D	165	ILE	2.5
1	C	304	VAL	2.5
1	B	304	VAL	2.5
1	B	283	ASP	2.5
1	C	307	THR	2.5
1	D	46	HIS	2.5
1	A	503	GLN	2.5
1	D	274	ASP	2.5
1	C	134	LEU	2.5
1	C	483	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	366	VAL	2.4
1	B	120	HIS	2.4
1	B	301	GLY	2.4
1	D	258	SER	2.4
1	B	366	VAL	2.4
1	B	138	GLY	2.4
1	D	442	CYS	2.4
1	B	299	ILE	2.4
1	C	305	GLU	2.4
1	B	272	ASN	2.4
1	B	302	ALA	2.3
1	D	307	THR	2.3
1	D	434	PRO	2.3
1	A	251	LYS	2.3
1	C	424	GLN	2.3
1	A	497	GLN	2.3
1	D	361	LEU	2.3
1	D	349	ARG	2.3
1	D	272	ASN	2.3
1	C	136	LYS	2.3
1	A	483	VAL	2.2
1	D	311	VAL	2.2
1	D	338	PHE	2.2
1	D	334	GLN	2.2
1	A	247	LEU	2.2
1	D	136	LYS	2.2
1	D	351	LEU	2.2
1	B	271	MET	2.2
1	A	285	GLU	2.2
1	C	41	PRO	2.2
1	A	283	ASP	2.2
1	A	303	GLY	2.2
1	A	348	ASN	2.2
1	C	163	GLN	2.2
1	B	257	ASP	2.2
1	B	424	GLN	2.2
1	D	460	LEU	2.1
1	D	495	VAL	2.1
1	C	494	LYS	2.1
1	B	442	CYS	2.1
1	D	421	ALA	2.1
1	C	213	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	286	LEU	2.1
1	C	467	VAL	2.1
1	B	365	PRO	2.1
1	D	483	VAL	2.0
1	A	32	LEU	2.0
1	D	371	ILE	2.0
1	A	275	ASN	2.0
1	B	249	ASN	2.0
1	B	307	THR	2.0
1	D	164	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

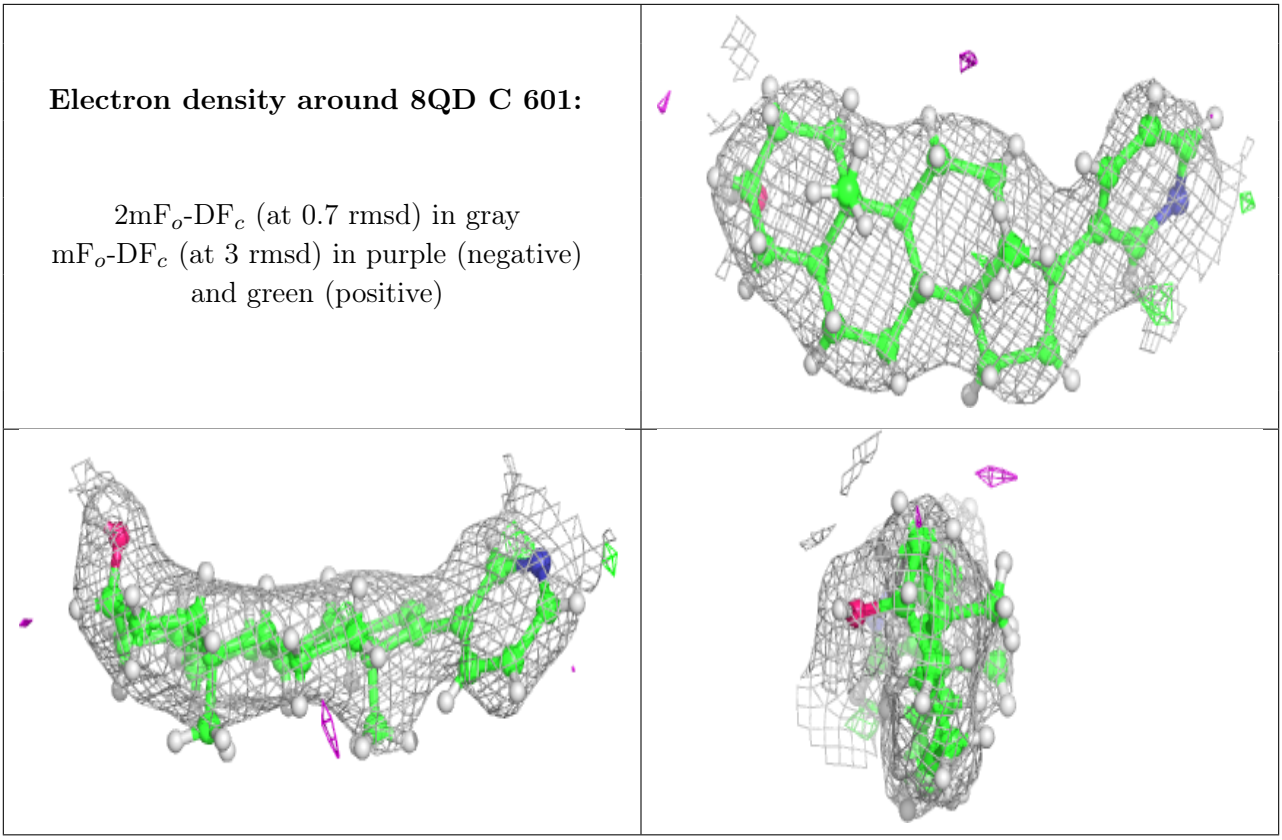
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	8QD	C	601	26/26	0.92	0.30	18,29,38,40	0
3	8QD	D	601	26/26	0.92	0.25	22,36,45,47	0
3	8QD	B	601	26/26	0.94	0.26	23,32,42,47	0
3	8QD	A	601	26/26	0.95	0.27	25,34,42,43	0
2	HEM	B	600	43/43	0.97	0.25	17,28,41,49	0
2	HEM	C	600	43/43	0.97	0.27	18,29,41,47	0
2	HEM	A	600	43/43	0.98	0.28	21,30,43,52	0
2	HEM	D	600	43/43	0.98	0.25	23,34,48,57	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.

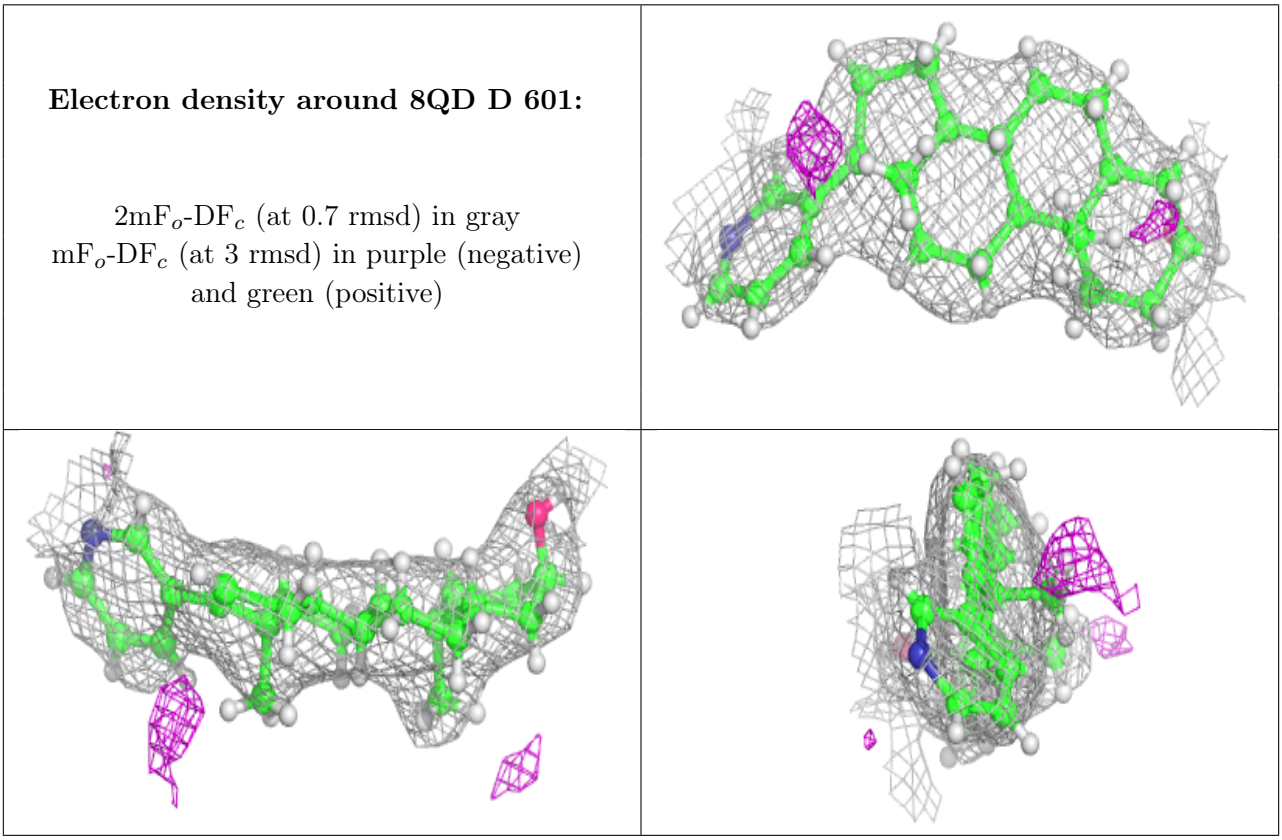
Electron density around 8QD C 601:

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



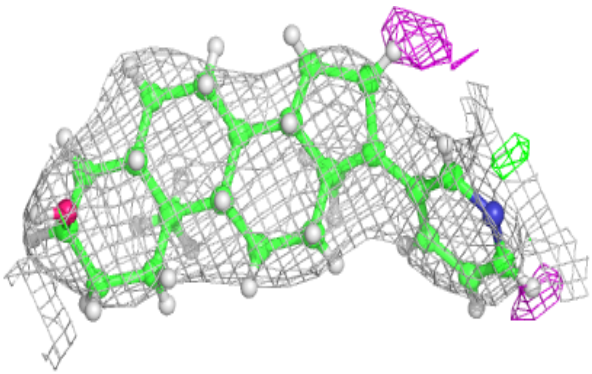
Electron density around 8QD D 601:

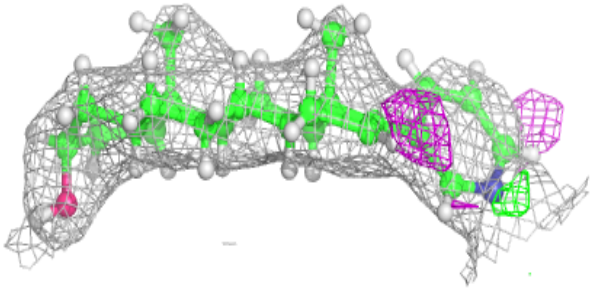
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

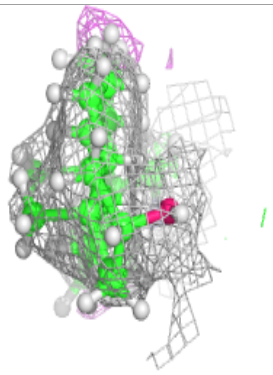


Electron density around 8QD B 601:

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

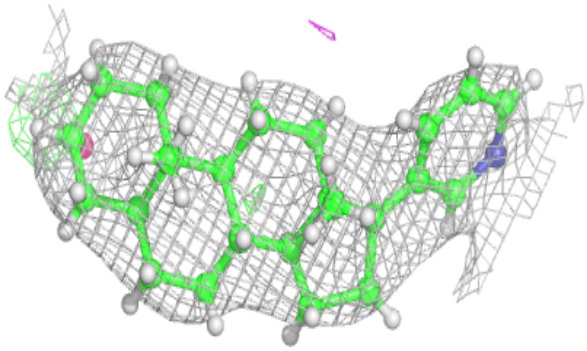


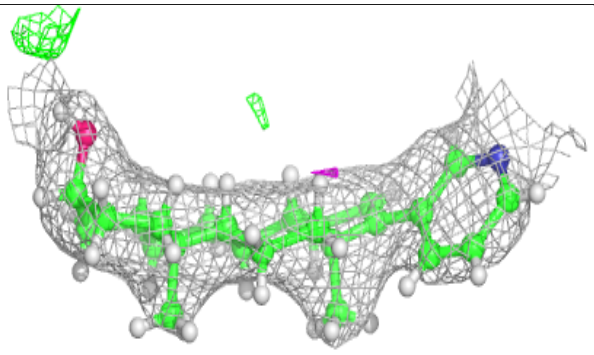


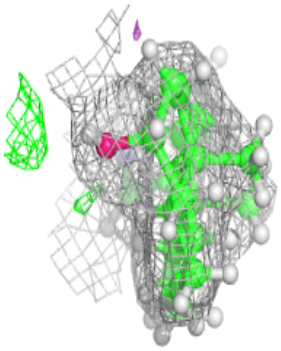


Electron density around 8QD A 601:

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

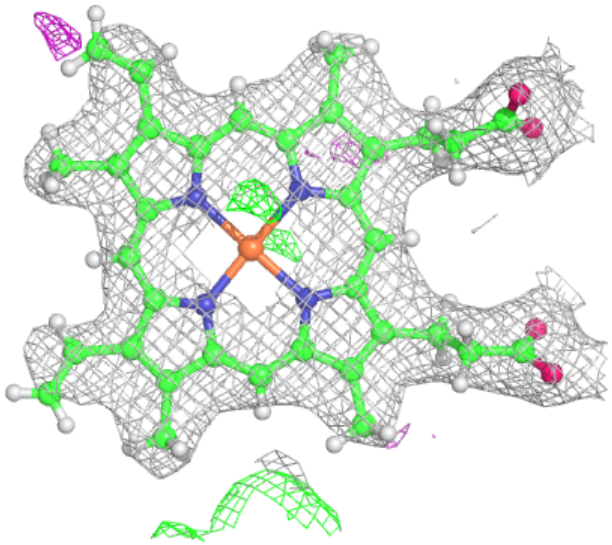


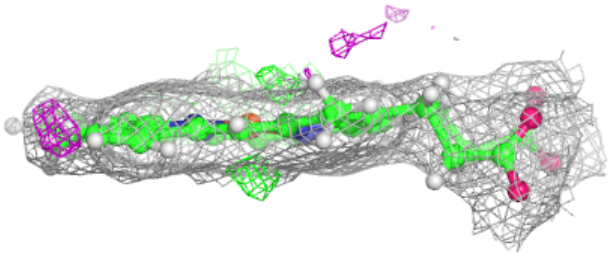


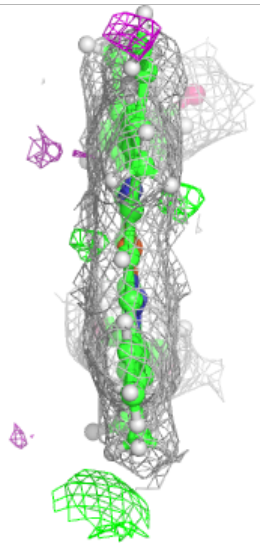


Electron density around HEM B 600:

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

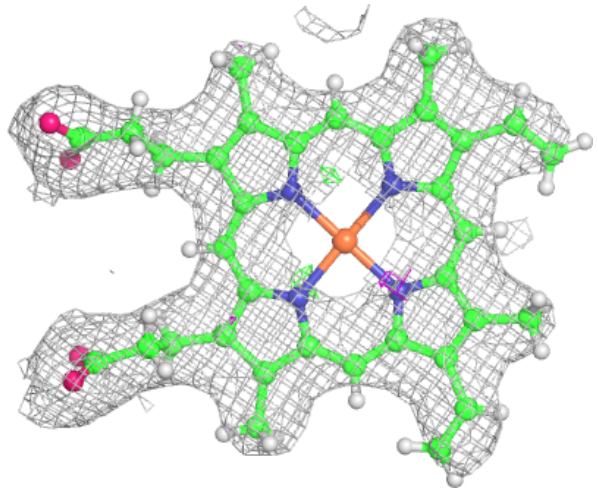


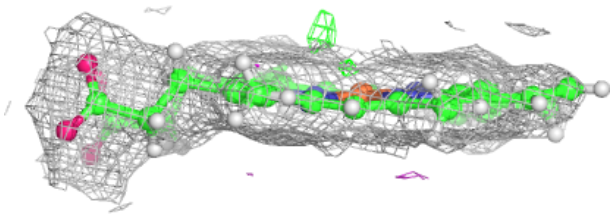


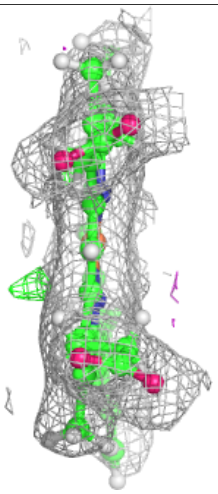


Electron density around HEM C 600:

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

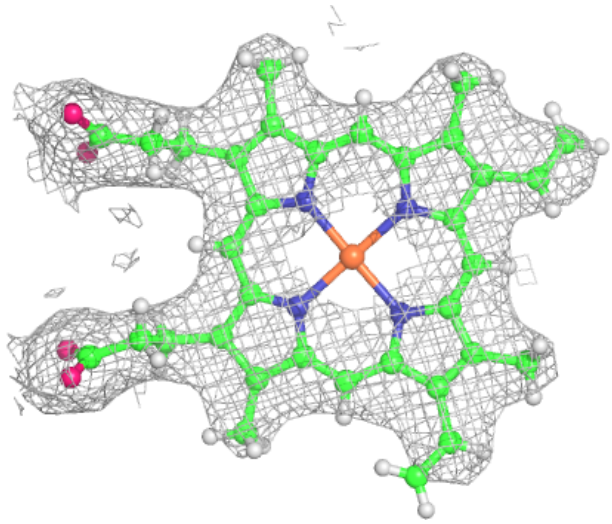


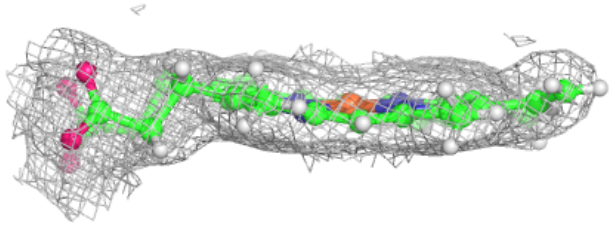


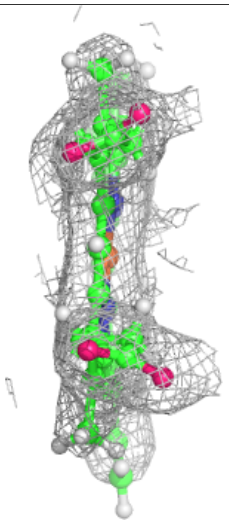


Electron density around HEM A 600:

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

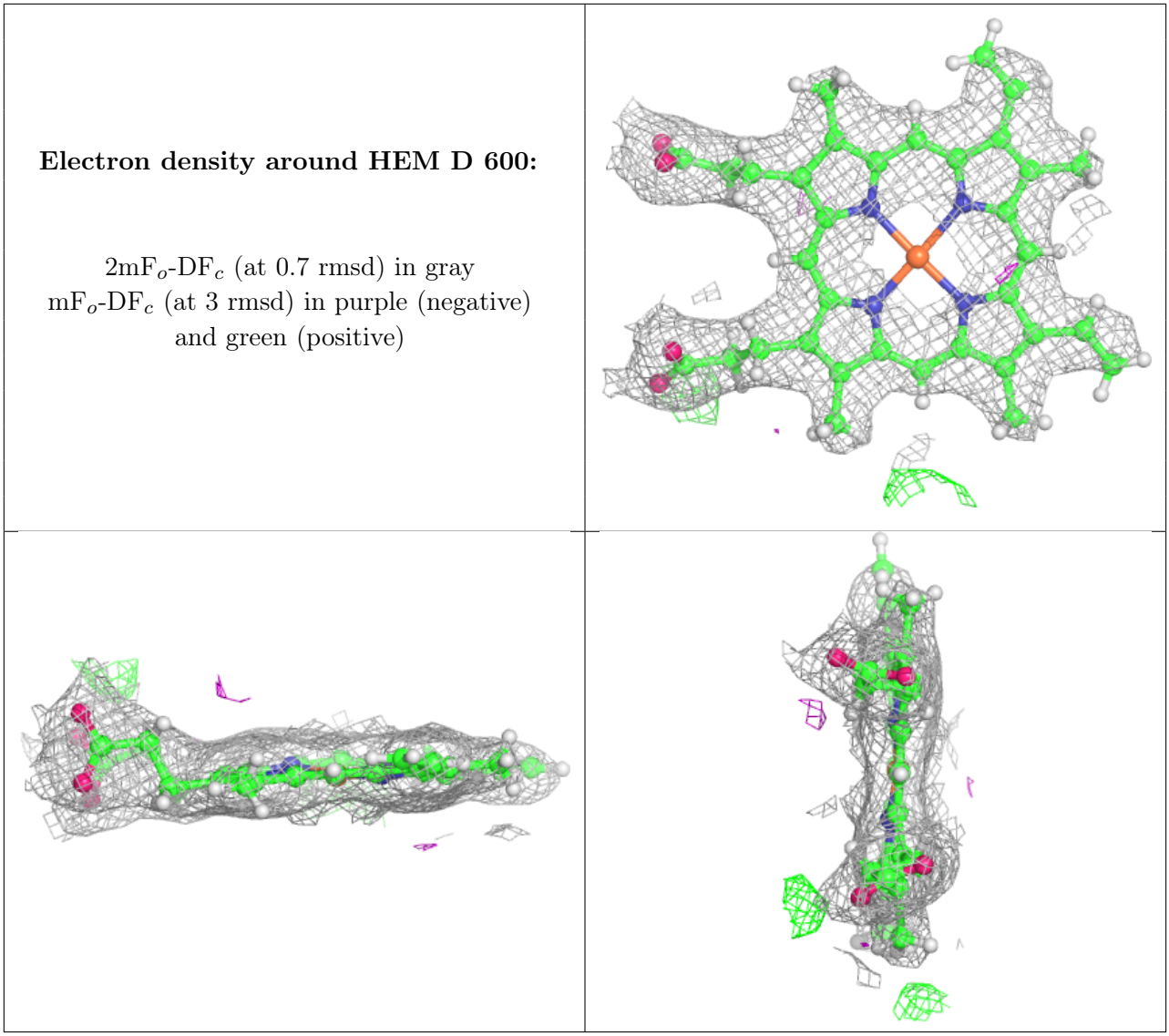






Electron density around HEM D 600:

$2mF_o$-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.