Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 02:51 PM EDT

PDB ID	:	6CIZ
Title	:	Human Cytochrome P450 17A1 in complex with inhibitor: abiraterone C6 nitrile
Authors	:	Scott, E.E.; Fehl, C.
Deposited on	:	2018-02-25
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

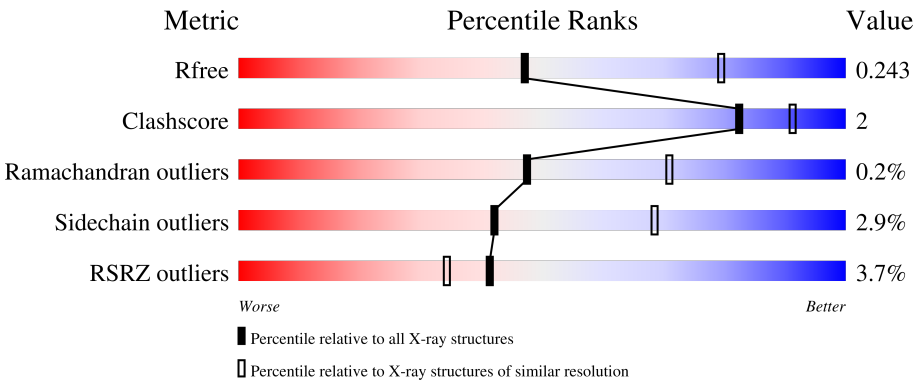
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	2% 87% 8% 5%
1	B	494	2% 87% 8% 5%
1	C	494	5% 90% 6% •
1	D	494	6% 86% 9% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30175 atoms, of which 14760 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
			Total	C	H	N	O	S			
1	A	468	7408	2391	3680	645	677	15	0	0	0
1	B	469	7377	2397	3639	646	680	15	0	0	0
1	C	477	7479	2432	3684	657	691	15	0	0	0
1	D	468	7368	2393	3637	646	677	15	0	0	0

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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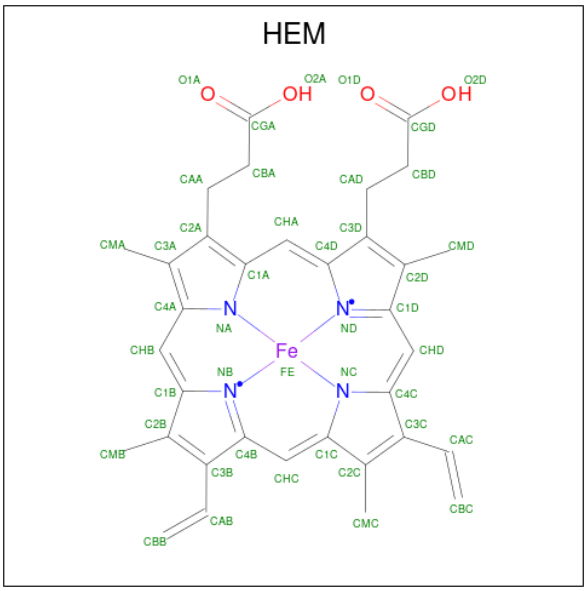
Chain	Residue	Modelled	Actual	Comment	Reference
C	22	LYS	-	expression tag	UNP P05093
C	23	THR	-	expression tag	UNP P05093
C	509	HIS	-	expression tag	UNP P05093
C	510	HIS	-	expression tag	UNP P05093
C	511	HIS	-	expression tag	UNP P05093
C	512	HIS	-	expression tag	UNP P05093
D	19	MET	-	initiating methionine	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
			Total	C	Fe	H	N	O		
2	A	1	73	34	1	30	4	4	0	0
			Total	C	Fe	H	N	O		
2	B	1	73	34	1	30	4	4	0	0
			Total	C	Fe	H	N	O		
2	C	1	73	34	1	30	4	4	0	0

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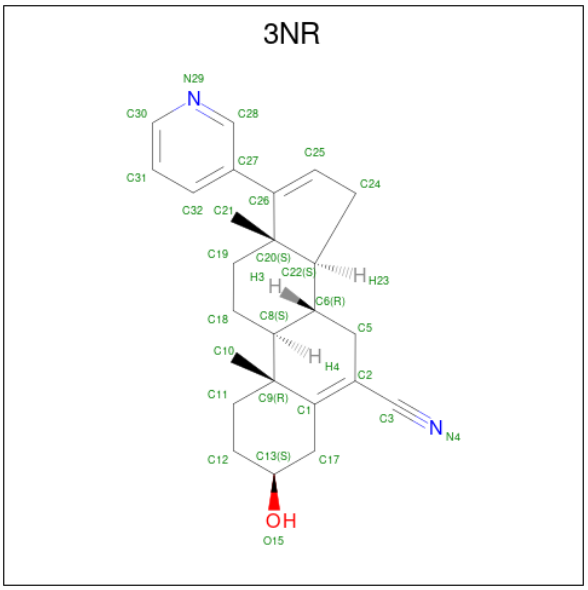
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
2	D	1	73	34	1	30	4	4	0	0

- Molecule 3 is 6-cyano-17-(3-pyridyl)-androst-5,16-dien-3-ol (three-letter code: 3NR) (formula: $C_{25}H_{30}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	28	25	2	1	0	0
3	B	1	28	25	2	1	0	0
3	C	1	28	25	2	1	0	0
3	D	1	28	25	2	1	0	0

- Molecule 4 is water.

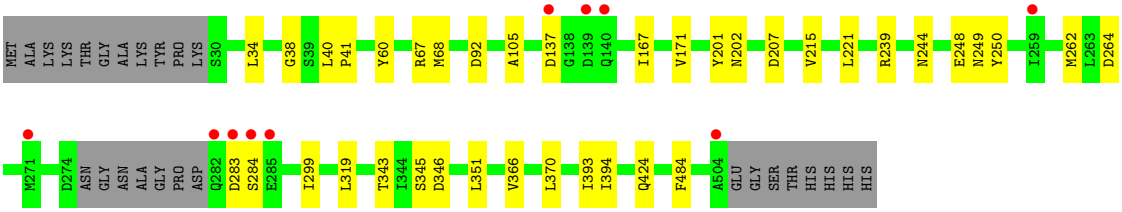
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	38	38	38	0	0
4	B	41	41	41	0	0
4	C	40	40	40	0	0
4	D	20	20	20	0	0

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.

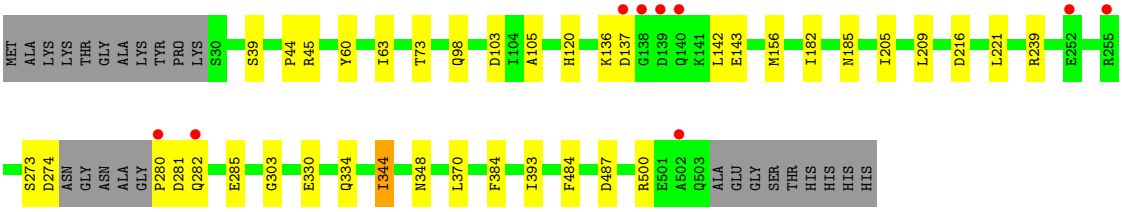
• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

Chain A:



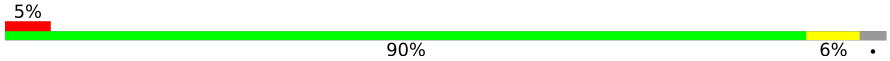
• Molecule 1: Steroid 17-alpha-hydroxylase/17,20 lyase

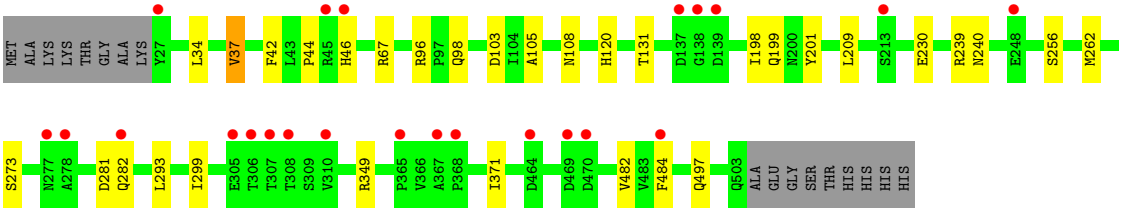
Chain B:



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

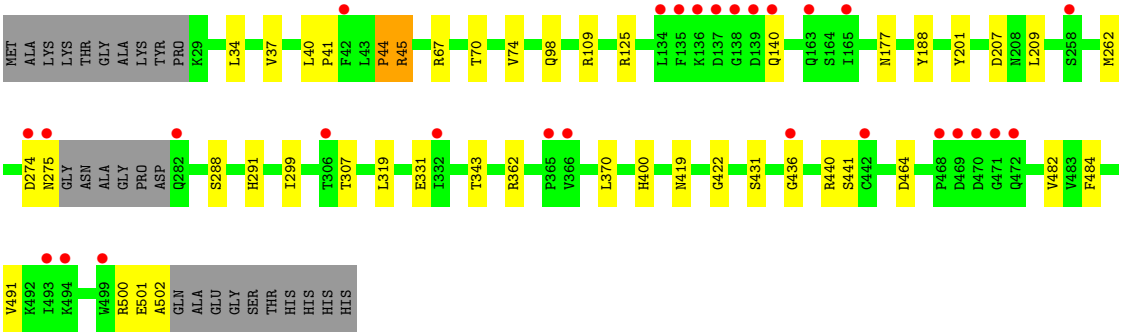
Chain C:





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

Chain D:


MET
ALA
LYS
LYS
THR
GLY
ALA
LYS
TYR
PRO
K29
L34
V37
L40
P41
F42
L43
P44
R45
R67
T70
V74
Q98
R109
R125
L134
F135
K136
D137
G138
D139
Q140
Q163
S164
I165
N177
Y188
Y201
D207
N208
L209
S258
M262
D274
N275
GLY
ASN
ALA
GLY
PRO
ASP
Q282
S288
H291
I299
T306
T307
L319
E331
I332
T343
R362
P365
V366
L370
H400
N419
G422
S431
G436
R440
S441
C442
D464
P468
D469
D470
G471
Q472
V482
V483
F484
V491
K492
I493
K494
W499
R500
E501
A502
GLN
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	89.62Å 153.35Å 169.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.34 – 2.60 39.31 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.34-2.60) 91.3 (39.31-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.185 , 0.243 0.185 , 0.243	Depositor DCC
R_{free} test set	3616 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	45.3	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 38.9	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	30175	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3NR, 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	0.24	0/3808	0.42	0/5155
1	B	0.25	0/3819	0.42	0/5170
1	C	0.25	0/3879	0.42	0/5254
1	D	0.25	0/3811	0.43	0/5158
All	All	0.25	0/15317	0.43	0/20737

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3728	3680	3797	19	0
1	B	3738	3639	3804	19	0
1	C	3795	3684	3856	17	0
1	D	3731	3637	3803	22	0
2	A	43	30	30	3	0
2	B	43	30	30	4	0
2	C	43	30	30	2	0
2	D	43	30	30	6	0
3	A	28	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	0	0	0
3	C	28	0	0	0	0
3	D	28	0	0	0	0
4	A	38	0	0	0	0
4	B	41	0	0	0	0
4	C	40	0	0	0	0
4	D	20	0	0	1	0
All	All	15415	14760	15380	75	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 2.

All (75) 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:D:44:PRO:O	1:D:45:ARG:HB2	1.84	0.76
1:A:40:LEU:HD21	1:A:68:MET:HE1	1.70	0.73
1:B:281:ASP:OD1	1:B:282:GLN:N	2.26	0.68
2:C:600:HEM:HHC	2:C:600:HEM:HBB2	1.75	0.67
1:D:288:SER:OG	1:D:291:HIS:ND1	2.24	0.67
1:D:125:ARG:NH1	2:D:600:HEM:O1D	2.32	0.63
1:C:239:ARG:NH1	1:C:240:ASN:OD1	2.31	0.62
1:C:98:GLN:NE2	1:C:103:ASP:OD2	2.33	0.61
1:A:40:LEU:HD21	1:A:68:MET:CE	2.30	0.61
2:C:600:HEM:HBC2	2:C:600:HEM:HHD	1.82	0.61
1:B:274:ASP:C	1:B:280:PRO:HB3	2.22	0.60
1:D:274:ASP:O	1:D:275:ASN:HB3	2.01	0.60
1:D:209:LEU:HD23	1:D:482:VAL:HG11	1.83	0.59
2:A:600:HEM:HBC2	2:A:600:HEM:HHD	1.86	0.58
2:D:600:HEM:HBC2	2:D:600:HEM:HHD	1.87	0.57
1:B:142:LEU:HD11	1:B:182:ILE:HD11	1.87	0.57
1:B:60:TYR:CD2	1:C:37:VAL:HG21	2.39	0.57
1:B:303:GLY:HA2	2:B:600:HEM:HMC2	1.85	0.57
1:B:63:ILE:HG12	1:C:34:LEU:HD22	1.86	0.56
1:C:105:ALA:O	1:C:239:ARG:NH2	2.39	0.55
1:B:60:TYR:CG	1:C:37:VAL:HG21	2.42	0.55
1:A:34:LEU:HD13	1:D:74:VAL:HG22	1.89	0.55
1:A:343:THR:N	1:A:346:ASP:OD2	2.39	0.54
1:A:60:TYR:CG	1:D:37:VAL:HG11	2.42	0.54
2:B:600:HEM:HHA	2:B:600:HEM:HBA2	1.91	0.53
1:A:202:ASN:ND2	3:A:601:3NR:O15	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PRO:HG3	1:D:37:VAL:O	2.10	0.51
1:B:143:GLU:OE2	1:B:344:ILE:N	2.41	0.51
1:B:330:GLU:O	1:B:334:GLN:HG3	2.11	0.51
2:D:600:HEM:HMB2	2:D:600:HEM:HBB2	1.92	0.50
1:A:370:LEU:HD12	1:A:394:ILE:HB	1.93	0.50
1:B:39:SER:HA	1:C:67:ARG:O	2.12	0.50
1:B:370:LEU:HD22	2:B:600:HEM:HMA1	1.94	0.49
1:B:273:SER:OG	1:B:281:ASP:HB3	2.12	0.49
1:C:105:ALA:HB2	1:C:209:LEU:HD11	1.94	0.49
1:D:98:GLN:HG3	1:D:109:ARG:HD3	1.94	0.49
2:D:600:HEM:HBA1	2:D:600:HEM:HMA1	1.95	0.48
1:B:384:PHE:CG	1:C:34:LEU:HD23	2.48	0.48
1:C:37:VAL:HG13	1:C:37:VAL:O	2.14	0.47
2:A:600:HEM:HBA2	2:A:600:HEM:HHA	1.96	0.47
1:A:351:LEU:HD13	1:A:424:GLN:HA	1.97	0.47
1:D:501:GLU:O	1:D:502:ALA:HB3	2.14	0.46
1:C:96:ARG:NH1	1:C:371:ILE:O	2.49	0.46
1:B:105:ALA:O	1:B:239:ARG:NH2	2.47	0.46
1:A:34:LEU:HD13	1:D:74:VAL:CG2	2.46	0.46
1:D:370:LEU:HD22	2:D:600:HEM:HMA1	1.98	0.46
1:A:167:ILE:O	1:A:171:VAL:HG12	2.16	0.45
1:A:250:TYR:OH	1:A:264:ASP:OD1	2.34	0.45
1:A:38:GLY:HA3	1:D:40:LEU:HD23	1.99	0.45
1:D:299:ILE:HG23	2:D:600:HEM:HBC1	1.97	0.45
1:D:262:MET:SD	1:D:299:ILE:HG13	2.58	0.44
1:A:105:ALA:O	1:A:239:ARG:NH2	2.45	0.44
1:D:362:ARG:NH1	1:D:400:HIS:O	2.50	0.44
1:D:419:ASN:OD1	1:D:422:GLY:N	2.46	0.44
1:D:319:LEU:HD21	1:D:491:VAL:HG12	1.99	0.44
1:C:230:GLU:OE1	1:C:230:GLU:N	2.43	0.43
1:B:44:PRO:O	1:B:45:ARG:HB2	2.18	0.43
1:C:209:LEU:HD23	1:C:482:VAL:HG21	2.00	0.43
1:A:343:THR:HG22	1:A:345:SER:H	1.84	0.43
1:A:262:MET:SD	1:A:299:ILE:HG13	2.59	0.42
1:C:198:ILE:HA	1:C:201:TYR:CE2	2.55	0.42
1:D:41:PRO:HD2	4:D:701:HOH:O	2.19	0.42
1:B:98:GLN:NE2	1:B:103:ASP:OD2	2.52	0.42
1:B:205:ILE:O	1:B:209:LEU:HB2	2.20	0.42
1:D:177:ASN:OD1	1:D:188:TYR:N	2.50	0.42
1:C:131:THR:HB	1:C:262:MET:HE2	2.02	0.41
1:A:366:VAL:CG2	2:A:600:HEM:HMB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:HEM:HBB2	2:B:600:HEM:HMB2	2.02	0.41
1:C:262:MET:SD	1:C:299:ILE:HG13	2.61	0.41
1:C:273:SER:HA	1:C:281:ASP:OD1	2.20	0.41
1:A:67:ARG:HH21	1:D:41:PRO:HB3	1.85	0.41
1:A:215:VAL:HG21	1:A:393:ILE:HG12	2.02	0.41
1:B:73:THR:CG2	1:B:393:ILE:HD13	2.50	0.41
1:B:136:LYS:HG2	1:B:137:ASP:N	2.35	0.41
1:D:436:GLY:HA3	1:D:441:SER:HA	2.03	0.41

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	464/494 (94%)	443 (96%)	21 (4%)	0	100	100
1	B	465/494 (94%)	444 (96%)	21 (4%)	0	100	100
1	C	475/494 (96%)	452 (95%)	22 (5%)	1 (0%)	47	71
1	D	464/494 (94%)	435 (94%)	27 (6%)	2 (0%)	34	57
All	All	1868/1976 (94%)	1774 (95%)	91 (5%)	3 (0%)	47	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	44	PRO
1	D	45	ARG
1	D	44	PRO

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	417/436 (96%)	405 (97%)	12 (3%)	42	68
1	B	419/436 (96%)	408 (97%)	11 (3%)	46	72
1	C	424/436 (97%)	412 (97%)	12 (3%)	43	69
1	D	418/436 (96%)	404 (97%)	14 (3%)	38	64
All	All	1678/1744 (96%)	1629 (97%)	49 (3%)	42	68

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ASP
1	A	137	ASP
1	A	201	TYR
1	A	207	ASP
1	A	221	LEU
1	A	244	ASN
1	A	248	GLU
1	A	249	ASN
1	A	283	ASP
1	A	284	SER
1	A	319	LEU
1	A	484	PHE
1	B	120	HIS
1	B	156	MET
1	B	185	ASN
1	B	216	ASP
1	B	221	LEU
1	B	285	GLU
1	B	344	ILE
1	B	348	ASN
1	B	484	PHE
1	B	487	ASP
1	B	500	ARG
1	C	37	VAL

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Mol	Chain	Res	Type
1	C	42	PHE
1	C	46	HIS
1	C	108	ASN
1	C	120	HIS
1	C	199	GLN
1	C	256	SER
1	C	282	GLN
1	C	293	LEU
1	C	349	ARG
1	C	484	PHE
1	C	497	GLN
1	D	34	LEU
1	D	67	ARG
1	D	70	THR
1	D	140	GLN
1	D	201	TYR
1	D	207	ASP
1	D	307	THR
1	D	331	GLU
1	D	343	THR
1	D	431	SER
1	D	440	ARG
1	D	464	ASP
1	D	484	PHE
1	D	500	ARG

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

Mol	Chain	Res	Type
1	A	48	HIS
1	A	50	HIS
1	B	78	HIS
1	C	50	HIS
1	C	120	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	3NR	A	601	2	32,32,32	1.36	5 (15%)	42,50,50	2.34	12 (28%)
2	HEM	D	600	1,3	41,50,50	1.49	3 (7%)	45,82,82	1.48	7 (15%)
3	3NR	D	601	2	32,32,32	1.22	3 (9%)	42,50,50	2.36	13 (30%)
2	HEM	C	600	1,3	41,50,50	1.49	4 (9%)	45,82,82	1.52	9 (20%)
2	HEM	A	600	1,3	41,50,50	1.49	5 (12%)	45,82,82	1.51	11 (24%)
2	HEM	B	600	1,3	41,50,50	1.45	4 (9%)	45,82,82	1.51	9 (20%)
3	3NR	C	601	2	32,32,32	1.23	4 (12%)	42,50,50	2.40	15 (35%)
3	3NR	B	601	2	32,32,32	1.34	5 (15%)	42,50,50	2.30	12 (28%)

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	3NR	A	601	2	-	1/4/67/67	0/5/5/5
2	HEM	D	600	1,3	-	3/12/54/54	-
3	3NR	D	601	2	-	1/4/67/67	0/5/5/5
2	HEM	C	600	1,3	-	3/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	600	1,3	-	4/12/54/54	-
2	HEM	B	600	1,3	-	6/12/54/54	-
3	3NR	C	601	2	-	0/4/67/67	0/5/5/5
3	3NR	B	601	2	-	2/4/67/67	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	3NR	C20-C26	-4.57	1.49	1.53
3	A	601	3NR	C20-C26	-4.56	1.49	1.53
3	D	601	3NR	C20-C26	-4.47	1.49	1.53
2	D	600	HEM	C3C-C2C	-4.43	1.34	1.40
2	A	600	HEM	C3C-C2C	-4.38	1.34	1.40
2	C	600	HEM	C3C-C2C	-4.38	1.34	1.40
3	B	601	3NR	C20-C26	-4.06	1.49	1.53
2	A	600	HEM	C3C-CAC	3.91	1.55	1.47
2	C	600	HEM	C3C-CAC	3.91	1.55	1.47
2	D	600	HEM	C3C-CAC	3.85	1.55	1.47
2	B	600	HEM	C3C-C2C	-3.72	1.35	1.40
2	B	600	HEM	C3C-CAC	3.72	1.55	1.47
3	B	601	3NR	C1-C2	-3.65	1.30	1.34
3	A	601	3NR	C1-C2	-3.18	1.31	1.34
2	D	600	HEM	CAB-C3B	3.13	1.55	1.47
2	B	600	HEM	CAB-C3B	3.10	1.55	1.47
2	C	600	HEM	CAB-C3B	3.04	1.55	1.47
2	A	600	HEM	CAB-C3B	2.85	1.55	1.47
3	A	601	3NR	C9-C8	-2.55	1.51	1.56
3	D	601	3NR	C1-C2	-2.53	1.32	1.34
3	C	601	3NR	C9-C1	-2.51	1.50	1.53
3	B	601	3NR	C9-C8	-2.51	1.51	1.56
3	C	601	3NR	C24-C25	2.29	1.53	1.50
3	A	601	3NR	C24-C25	2.27	1.53	1.50
3	D	601	3NR	C24-C25	2.26	1.53	1.50
3	C	601	3NR	C9-C8	-2.23	1.52	1.56
3	B	601	3NR	C9-C1	-2.22	1.50	1.53
2	B	600	HEM	CAA-C2A	2.15	1.55	1.52
2	C	600	HEM	CAA-C2A	2.15	1.55	1.52
3	A	601	3NR	C9-C1	-2.14	1.50	1.53
3	B	601	3NR	C24-C25	2.07	1.53	1.50
2	A	600	HEM	CAA-C2A	2.04	1.55	1.52
2	A	600	HEM	CMD-C2D	2.03	1.55	1.50

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	3NR	C24-C22-C20	-9.30	97.08	104.05
3	D	601	3NR	C24-C22-C20	-9.25	97.12	104.05
3	B	601	3NR	C24-C22-C20	-9.00	97.31	104.05
3	C	601	3NR	C24-C22-C20	-8.36	97.79	104.05
3	C	601	3NR	C20-C22-C6	-5.89	106.81	113.12
3	D	601	3NR	C24-C25-C26	-4.54	109.14	112.87
3	A	601	3NR	C24-C25-C26	-4.51	109.16	112.87
3	A	601	3NR	C20-C22-C6	-4.35	108.46	113.12
3	D	601	3NR	C20-C22-C6	-4.33	108.48	113.12
3	B	601	3NR	C20-C22-C6	-4.30	108.52	113.12
3	B	601	3NR	C5-C6-C22	-4.27	105.97	111.18
3	B	601	3NR	C24-C25-C26	-4.17	109.44	112.87
3	C	601	3NR	C24-C25-C26	-4.11	109.49	112.87
3	B	601	3NR	C24-C22-C6	-4.08	116.67	121.57
3	D	601	3NR	C22-C6-C8	-3.97	103.78	109.09
3	D	601	3NR	C5-C6-C22	-3.85	106.48	111.18
3	C	601	3NR	C22-C6-C8	-3.70	104.13	109.09
3	C	601	3NR	C5-C6-C22	-3.58	106.82	111.18
3	A	601	3NR	C5-C6-C22	-3.57	106.83	111.18
3	C	601	3NR	C13-C17-C1	-3.55	105.96	112.05
2	D	600	HEM	C4B-CHC-C1C	3.52	127.21	122.56
3	A	601	3NR	C24-C22-C6	-3.50	117.37	121.57
3	C	601	3NR	C24-C22-C6	-3.45	117.43	121.57
2	B	600	HEM	C4D-ND-C1D	3.32	108.50	105.07
2	A	600	HEM	C4D-ND-C1D	3.29	108.47	105.07
3	D	601	3NR	C24-C22-C6	-3.25	117.66	121.57
2	C	600	HEM	C3B-C2B-C1B	3.15	108.82	106.49
3	B	601	3NR	C22-C6-C8	-3.09	104.95	109.09
3	C	601	3NR	C21-C20-C22	-3.06	108.47	112.98
2	C	600	HEM	C1B-NB-C4B	3.02	108.19	105.07
2	A	600	HEM	C4C-CHD-C1D	2.89	126.37	122.56
2	C	600	HEM	C4B-CHC-C1C	2.83	126.30	122.56
3	A	601	3NR	C22-C6-C8	-2.80	105.34	109.09
2	C	600	HEM	C4D-ND-C1D	2.79	107.95	105.07
2	B	600	HEM	CMC-C2C-C3C	2.78	129.88	124.68
3	C	601	3NR	C30-N29-C28	2.76	121.62	116.85
3	B	601	3NR	C30-N29-C28	2.75	121.61	116.85
2	D	600	HEM	CMA-C3A-C4A	-2.75	124.24	128.46
3	A	601	3NR	C30-N29-C28	2.75	121.60	116.85
3	D	601	3NR	C13-C17-C1	-2.74	107.35	112.05
2	B	600	HEM	C4A-C3A-C2A	2.74	108.90	107.00
3	C	601	3NR	C22-C20-C26	2.73	102.02	99.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	HEM	CAA-CBA-CGA	-2.70	106.19	113.76
2	B	600	HEM	C3D-C4D-ND	-2.65	107.22	110.17
3	A	601	3NR	C13-C17-C1	-2.64	107.52	112.05
2	D	600	HEM	CAA-CBA-CGA	-2.59	106.49	113.76
3	C	601	3NR	C10-C9-C8	-2.57	108.62	111.68
2	D	600	HEM	C4D-ND-C1D	2.55	107.71	105.07
2	A	600	HEM	C4B-CHC-C1C	2.54	125.91	122.56
2	A	600	HEM	C3D-C4D-ND	-2.54	107.34	110.17
3	A	601	3NR	C18-C19-C20	-2.53	107.27	112.74
2	C	600	HEM	C4C-CHD-C1D	2.50	125.86	122.56
3	C	601	3NR	C8-C9-C1	2.50	112.86	109.27
3	A	601	3NR	C10-C9-C8	-2.49	108.71	111.68
3	D	601	3NR	C30-N29-C28	2.49	121.15	116.85
3	B	601	3NR	C21-C20-C22	-2.47	109.33	112.98
3	B	601	3NR	C10-C9-C8	-2.39	108.83	111.68
3	B	601	3NR	C8-C9-C1	2.38	112.70	109.27
2	B	600	HEM	CHD-C1D-ND	2.37	127.01	124.43
3	D	601	3NR	C21-C20-C22	-2.36	109.50	112.98
2	B	600	HEM	C4C-CHD-C1D	2.36	125.67	122.56
2	A	600	HEM	C4A-C3A-C2A	2.36	108.64	107.00
3	B	601	3NR	C18-C19-C20	-2.35	107.65	112.74
2	D	600	HEM	CHA-C4D-ND	2.31	127.23	124.38
3	A	601	3NR	C5-C6-C8	-2.29	108.31	110.91
2	C	600	HEM	CMA-C3A-C4A	-2.29	124.94	128.46
3	D	601	3NR	C18-C19-C20	-2.29	107.78	112.74
3	A	601	3NR	C12-C13-C17	-2.28	107.18	110.31
3	D	601	3NR	C10-C9-C8	-2.28	108.97	111.68
2	A	600	HEM	CHD-C1D-ND	2.25	126.88	124.43
2	C	600	HEM	CHC-C4B-C3B	2.25	128.01	124.57
3	B	601	3NR	C13-C17-C1	-2.24	108.20	112.05
3	C	601	3NR	C18-C8-C9	-2.23	110.14	113.08
3	D	601	3NR	C8-C9-C1	2.22	112.46	109.27
2	B	600	HEM	CAA-C2A-C3A	-2.18	120.97	127.25
2	A	600	HEM	CMA-C3A-C4A	-2.17	125.13	128.46
3	C	601	3NR	C18-C19-C20	-2.16	108.06	112.74
2	C	600	HEM	CHA-C4D-ND	2.16	127.05	124.38
3	D	601	3NR	C31-C32-C27	-2.15	117.80	120.34
3	C	601	3NR	C12-C13-C17	-2.13	107.39	110.31
2	A	600	HEM	C1B-NB-C4B	2.12	107.27	105.07
2	A	600	HEM	CHA-C4D-ND	2.11	126.99	124.38
2	D	600	HEM	C1B-NB-C4B	2.11	107.25	105.07
2	B	600	HEM	C4B-CHC-C1C	2.11	125.34	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	600	HEM	C2D-C1D-ND	-2.10	107.37	109.88
2	B	600	HEM	CMA-C3A-C4A	-2.09	125.25	128.46
2	A	600	HEM	C2D-C1D-ND	-2.08	107.39	109.88
2	C	600	HEM	C2D-C1D-ND	-2.07	107.40	109.88

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	HEM	C1A-C2A-CAA-CBA
2	A	600	HEM	C3A-C2A-CAA-CBA
2	B	600	HEM	C1A-C2A-CAA-CBA
2	B	600	HEM	C3A-C2A-CAA-CBA
2	D	600	HEM	C1A-C2A-CAA-CBA
2	D	600	HEM	C3A-C2A-CAA-CBA
2	C	600	HEM	C4B-C3B-CAB-CBB
3	B	601	3NR	C25-C26-C27-C28
3	B	601	3NR	C25-C26-C27-C32
2	B	600	HEM	CAA-CBA-CGA-O1A
2	A	600	HEM	CAA-CBA-CGA-O2A
2	A	600	HEM	CAA-CBA-CGA-O1A
2	B	600	HEM	CAA-CBA-CGA-O2A
2	B	600	HEM	CAD-CBD-CGD-O1D
2	C	600	HEM	CAD-CBD-CGD-O2D
3	A	601	3NR	C25-C26-C27-C32
3	D	601	3NR	C25-C26-C27-C32
2	C	600	HEM	CAD-CBD-CGD-O1D
2	B	600	HEM	CAD-CBD-CGD-O2D
2	D	600	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

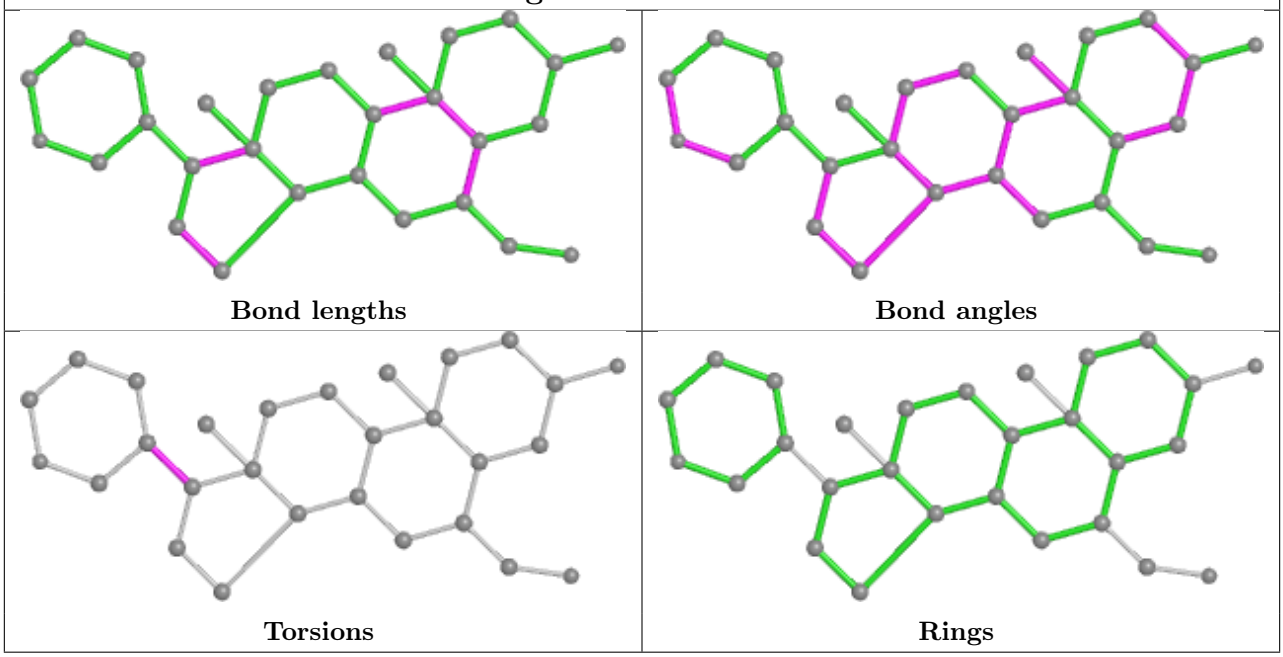
5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	3NR	1	0
2	D	600	HEM	6	0
2	C	600	HEM	2	0
2	A	600	HEM	3	0
2	B	600	HEM	4	0

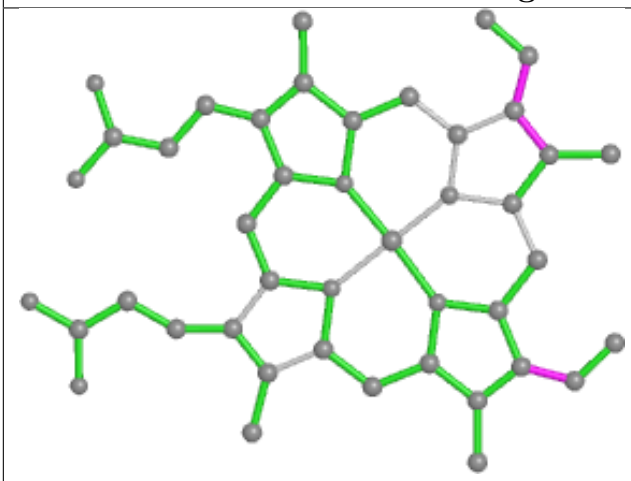
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

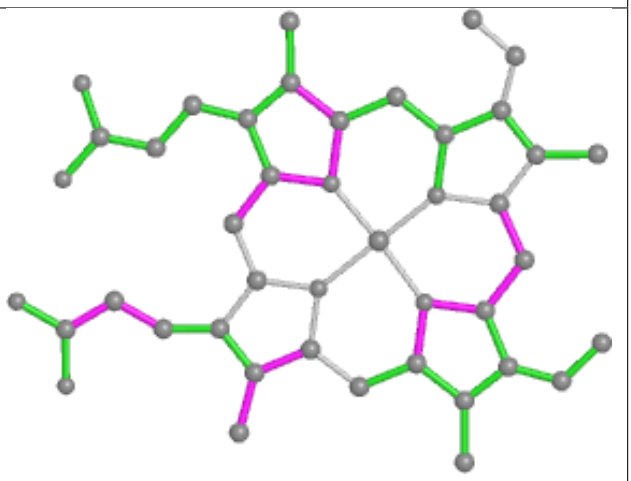
Ligand 3NR A 601



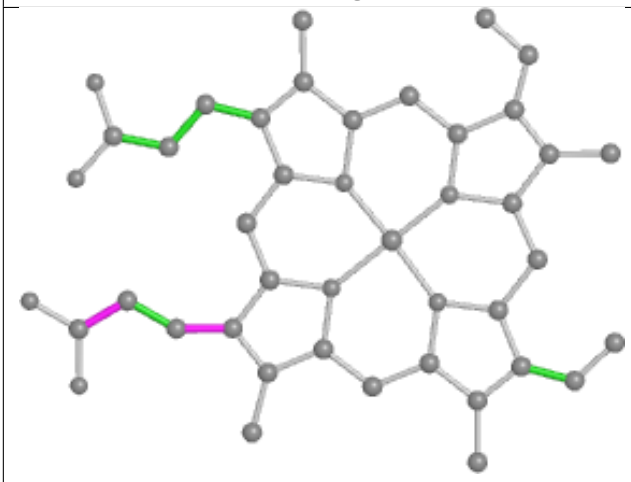
Ligand HEM D 600



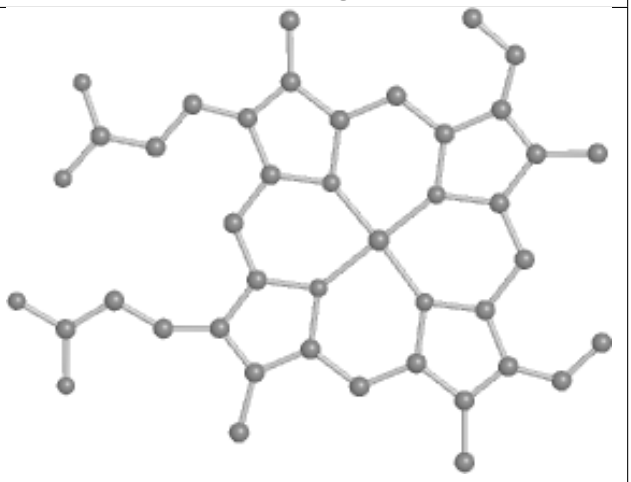
Bond lengths



Bond angles

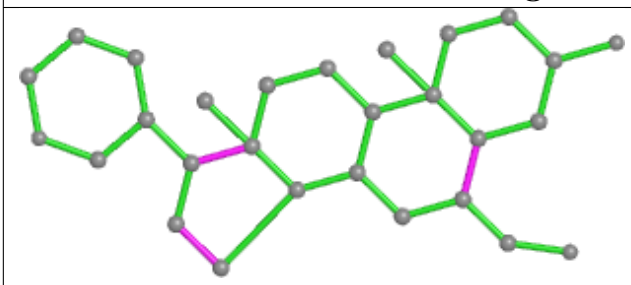


Torsions

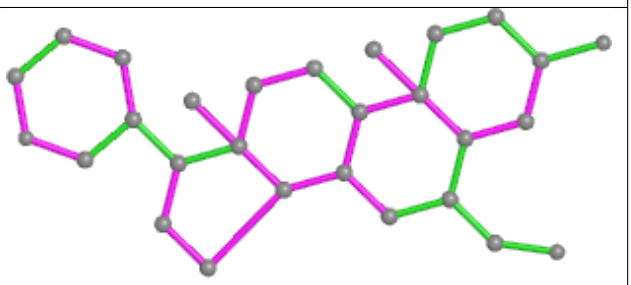


Rings

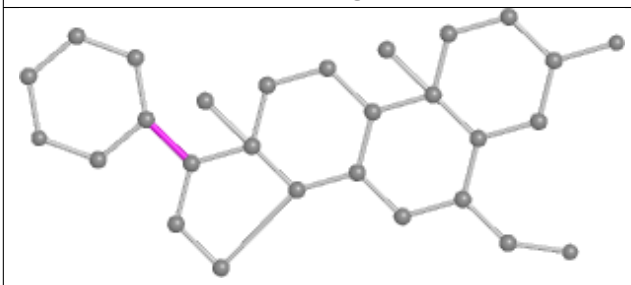
Ligand 3NR D 601



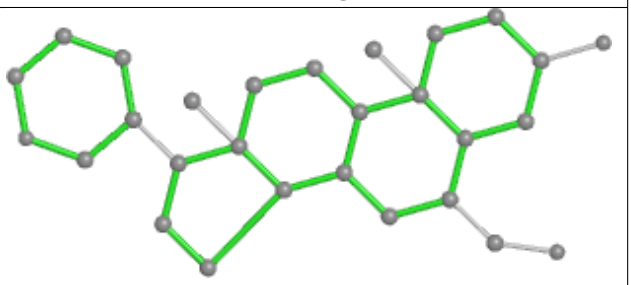
Bond lengths



Bond angles

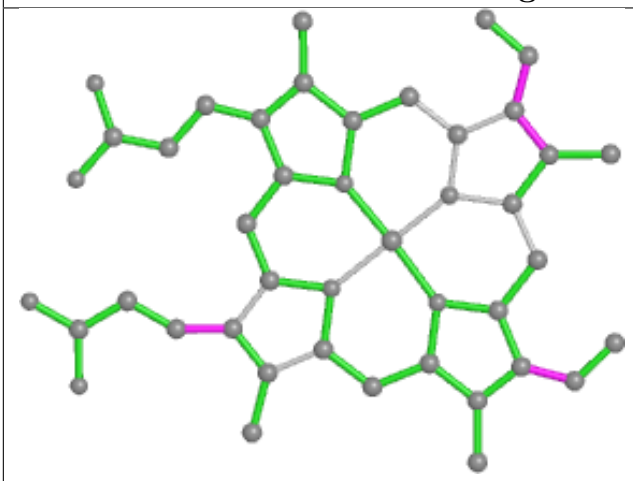


Torsions

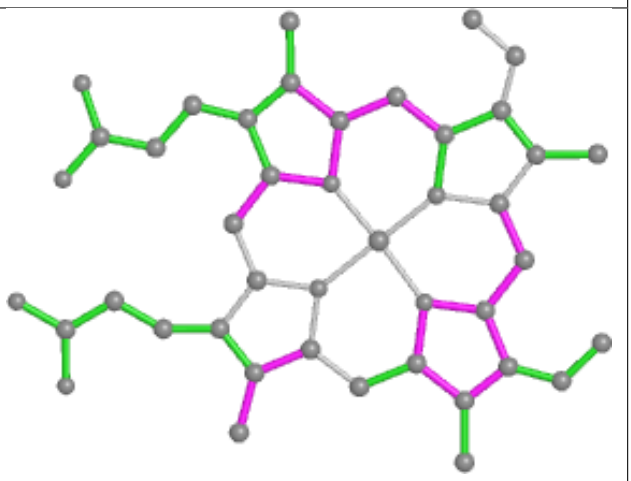


Rings

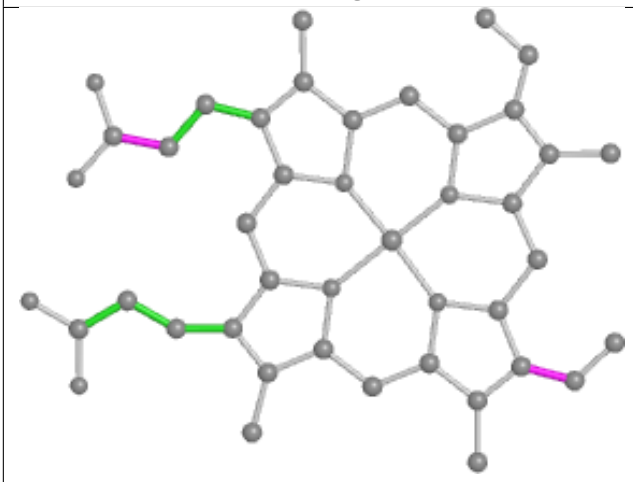
Ligand HEM C 600



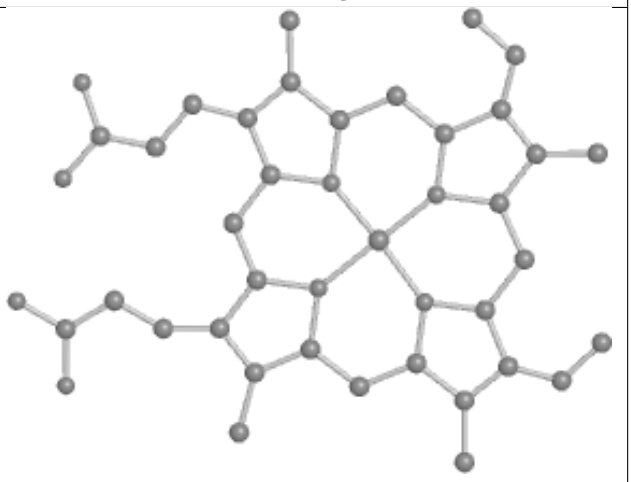
Bond lengths



Bond angles

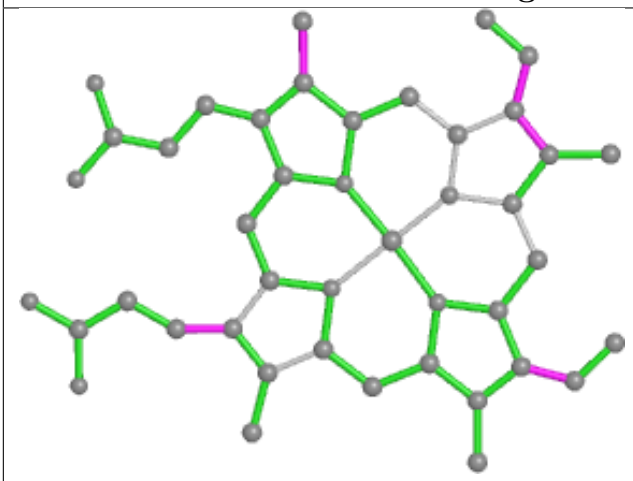


Torsions

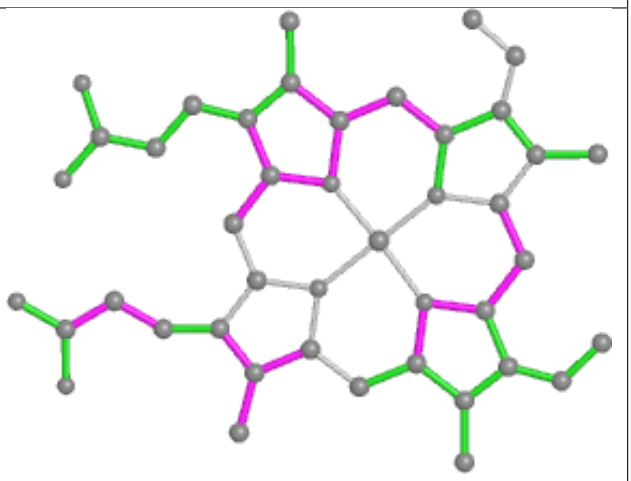


Rings

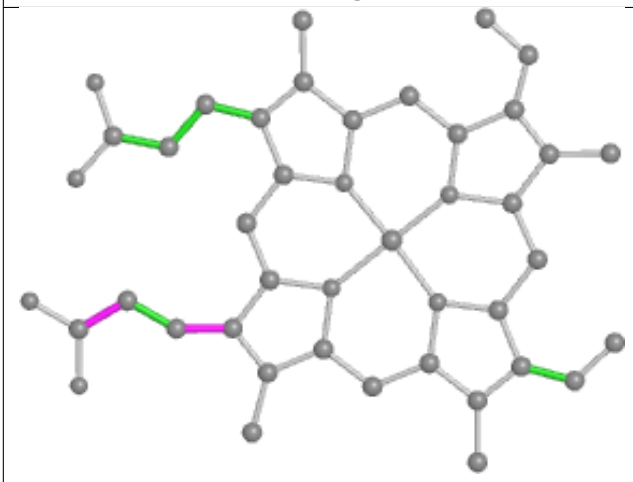
Ligand HEM A 600



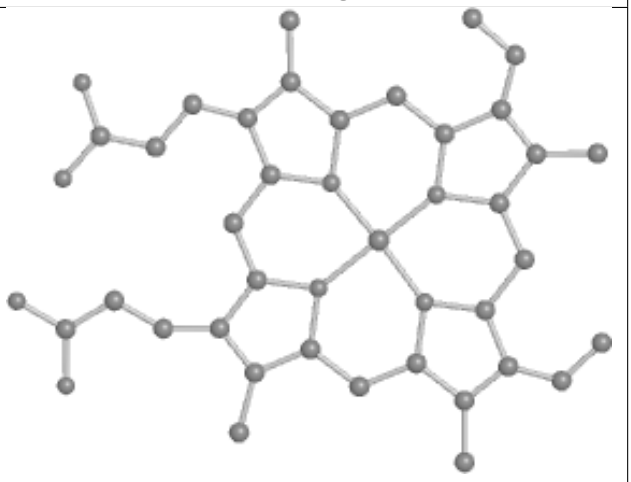
Bond lengths



Bond angles

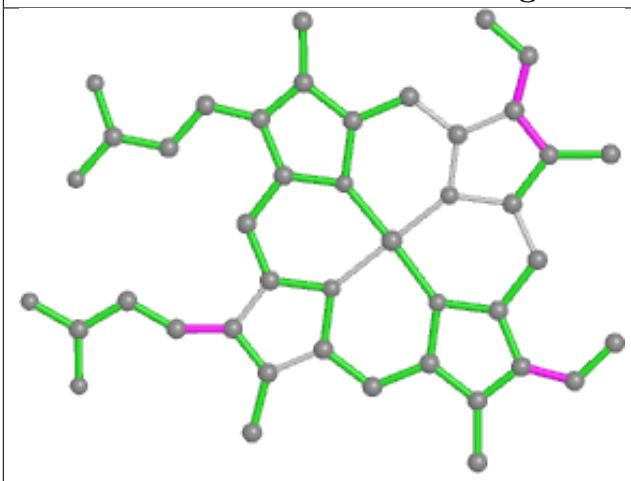


Torsions

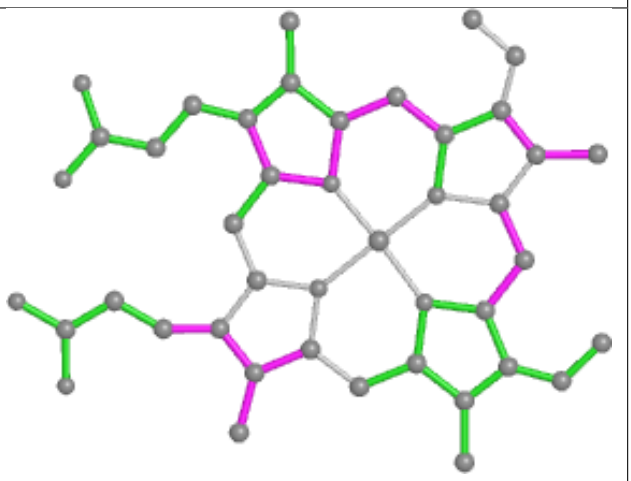


Rings

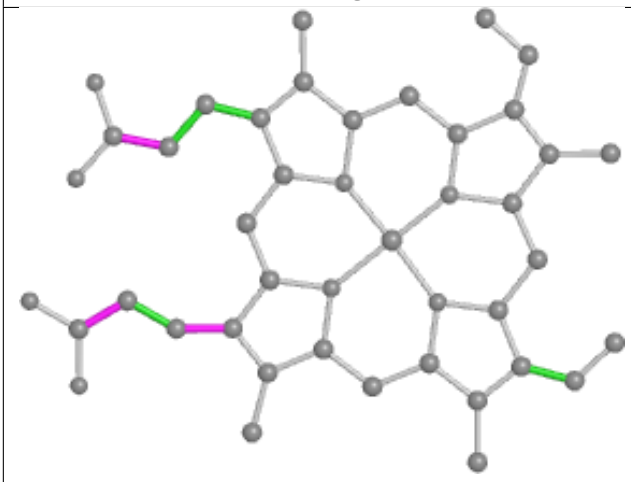
Ligand HEM B 600



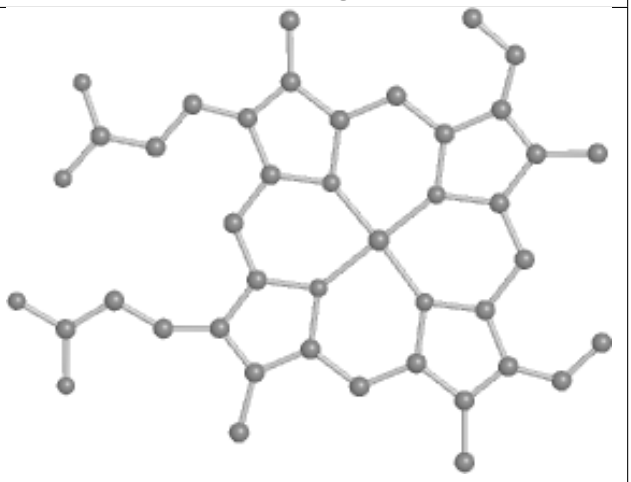
Bond lengths



Bond angles

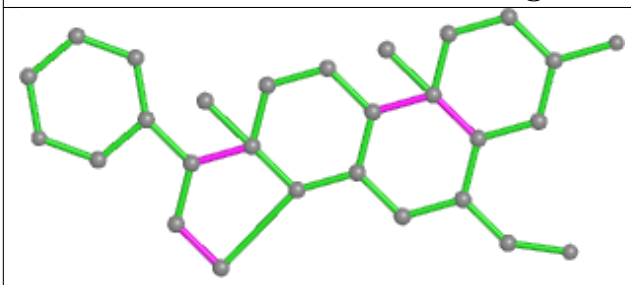


Torsions

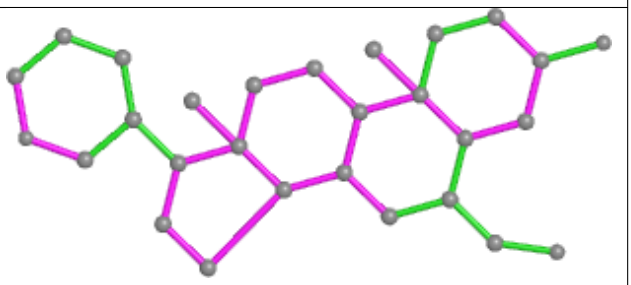


Rings

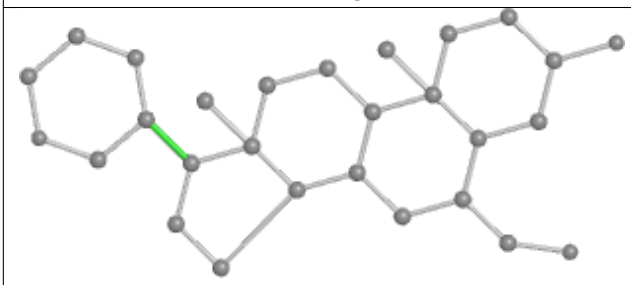
Ligand 3NR C 601



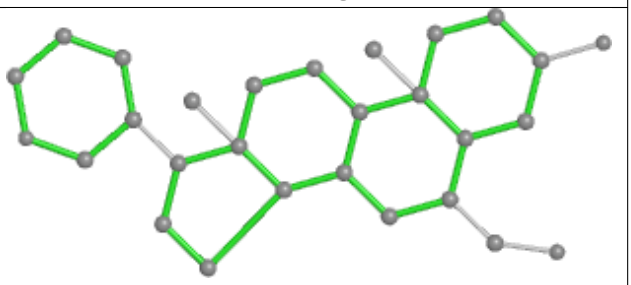
Bond lengths



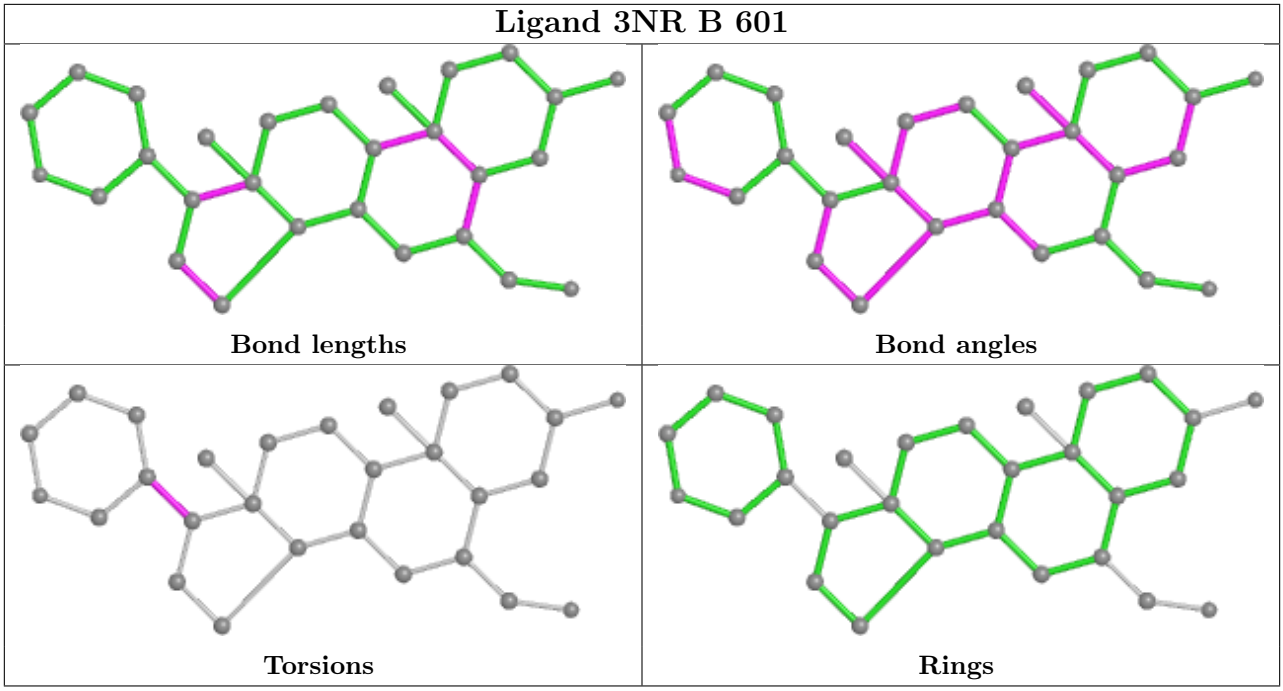
Bond angles



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	468/494 (94%)	0.04	10 (2%)	63	58	36, 52, 82, 147	0
1	B	469/494 (94%)	0.02	9 (1%)	66	62	34, 51, 84, 122	0
1	C	477/494 (96%)	0.20	23 (4%)	30	24	33, 52, 87, 119	0
1	D	468/494 (94%)	0.38	28 (5%)	21	16	37, 60, 97, 127	0
All	All	1882/1976 (95%)	0.16	70 (3%)	41	34	33, 53, 91, 147	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	ASP	6.1
1	D	139	ASP	6.1
1	A	140	GLN	5.8
1	D	471	GLY	5.5
1	D	138	GLY	5.2
1	B	140	GLN	5.1
1	D	140	GLN	5.1
1	C	27	TYR	5.1
1	D	137	ASP	5.1
1	D	468	PRO	4.8
1	B	139	ASP	4.8
1	C	139	ASP	4.7
1	D	274	ASP	4.6
1	D	42	PHE	4.6
1	D	275	ASN	4.5
1	C	277	ASN	4.5
1	C	45	ARG	4.0
1	D	469	ASP	3.9
1	C	138	GLY	3.8
1	B	138	GLY	3.6
1	C	137	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	282	GLN	3.4
1	C	46	HIS	3.4
1	C	306	THR	3.0
1	C	469	ASP	2.9
1	A	283	ASP	2.9
1	A	282	GLN	2.9
1	D	332	ILE	2.9
1	C	367	ALA	2.8
1	D	470	ASP	2.8
1	A	137	ASP	2.7
1	C	248	GLU	2.7
1	A	259	ILE	2.6
1	D	493	ILE	2.6
1	C	310	VAL	2.6
1	D	436	GLY	2.6
1	D	442	CYS	2.6
1	D	306	THR	2.5
1	B	255	ARG	2.5
1	C	282	GLN	2.5
1	B	252	GLU	2.4
1	A	285	GLU	2.4
1	D	165	ILE	2.3
1	C	464	ASP	2.3
1	A	504	ALA	2.3
1	B	137	ASP	2.3
1	C	368	PRO	2.2
1	A	271	MET	2.2
1	D	365	PRO	2.2
1	C	308	THR	2.2
1	D	135	PHE	2.2
1	D	258	SER	2.2
1	C	365	PRO	2.2
1	C	307	THR	2.2
1	D	163	GLN	2.2
1	B	282	GLN	2.2
1	D	134	LEU	2.2
1	C	278	ALA	2.1
1	C	470	ASP	2.1
1	A	284	SER	2.1
1	C	305	GLU	2.1
1	C	484	PHE	2.1
1	D	499	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	494	LYS	2.0
1	B	280	PRO	2.0
1	D	366	VAL	2.0
1	D	472	GLN	2.0
1	B	502	ALA	2.0
1	C	213	SER	2.0
1	D	136	LYS	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)

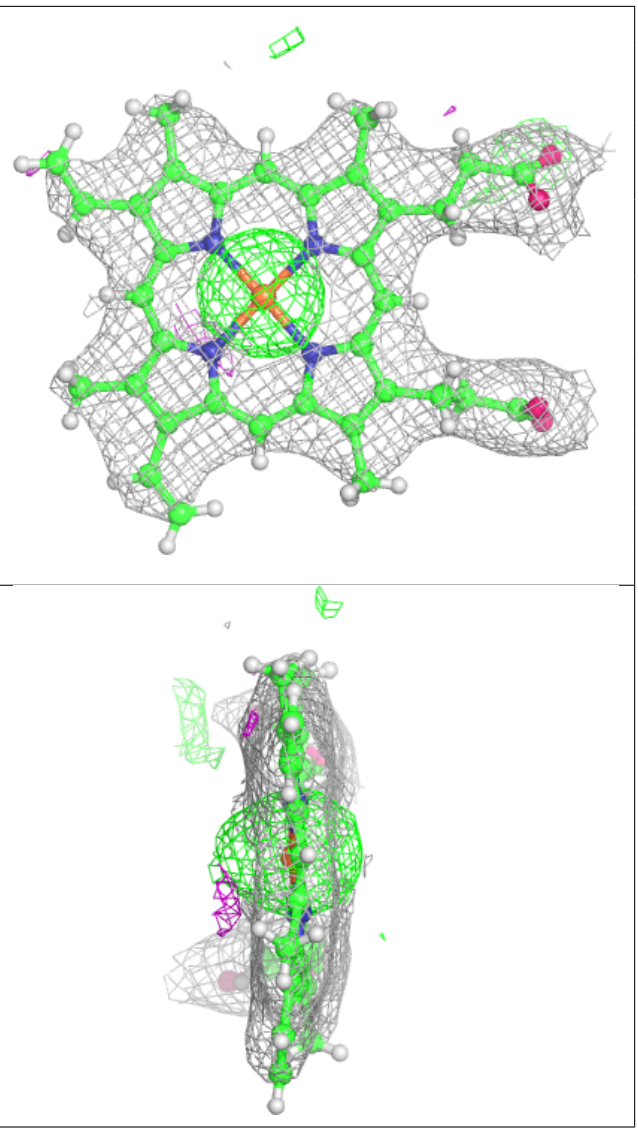
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	D	600	43/43	0.82	0.33	34,49,70,156	0
3	3NR	D	601	28/28	0.92	0.28	33,43,54,55	0
3	3NR	B	601	28/28	0.94	0.31	34,43,51,61	0
3	3NR	C	601	28/28	0.95	0.34	34,42,48,53	0
3	3NR	A	601	28/28	0.95	0.31	29,41,52,63	0
2	HEM	C	600	43/43	0.97	0.30	30,43,54,60	0
2	HEM	A	600	43/43	0.97	0.30	34,44,57,69	0
2	HEM	B	600	43/43	0.97	0.29	27,41,59,63	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.

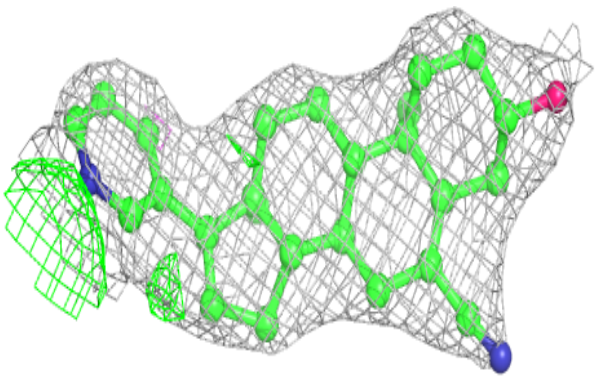
Electron density around HEM D 600:

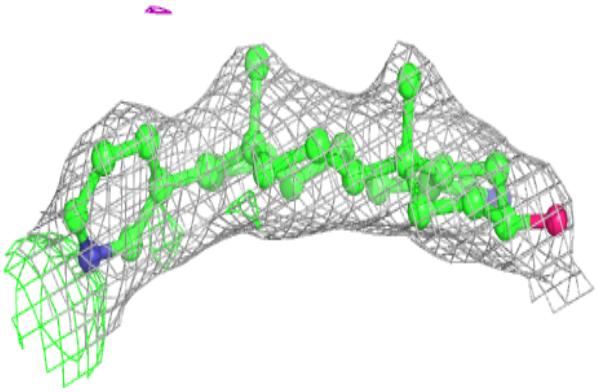
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

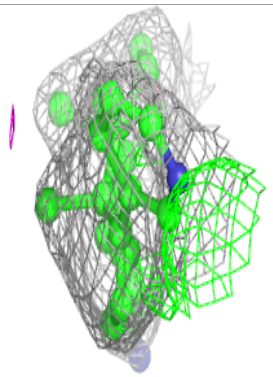


Electron density around 3NR D 601:

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

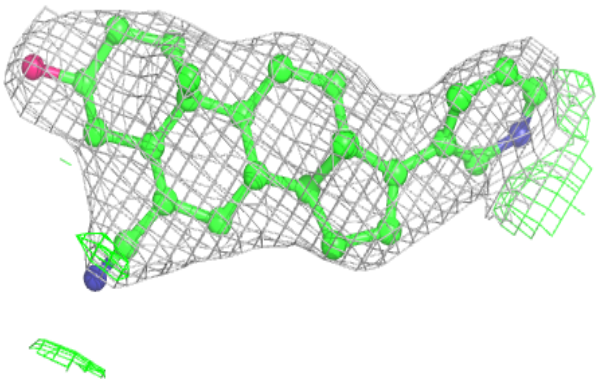


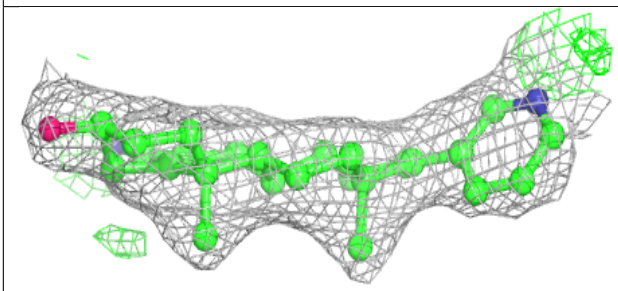


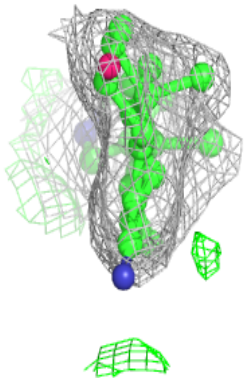


Electron density around 3NR B 601:

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

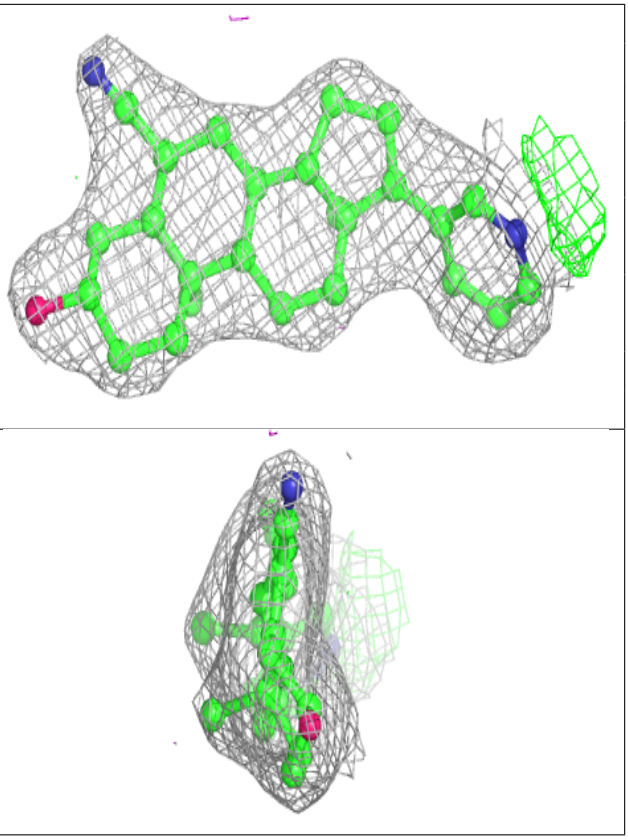






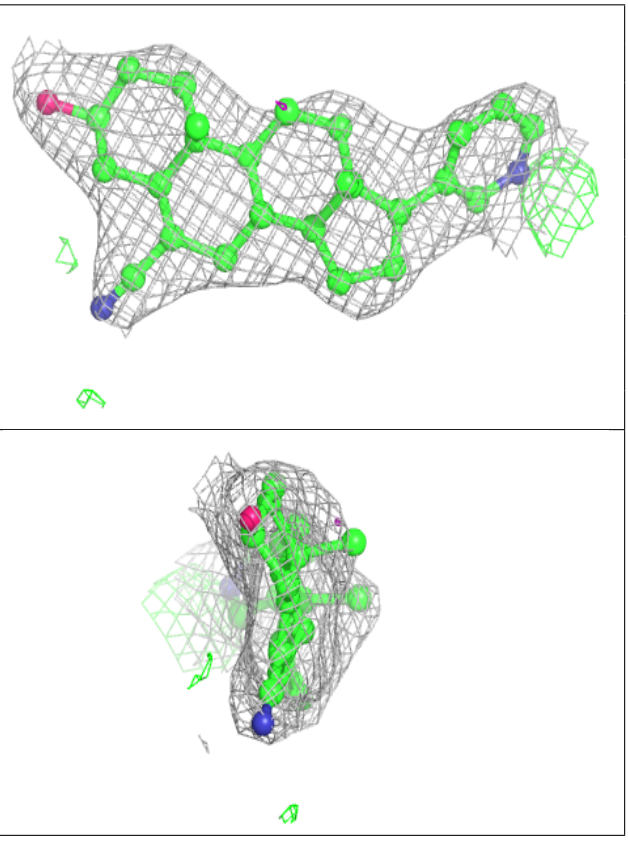
Electron density around 3NR C 601:

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



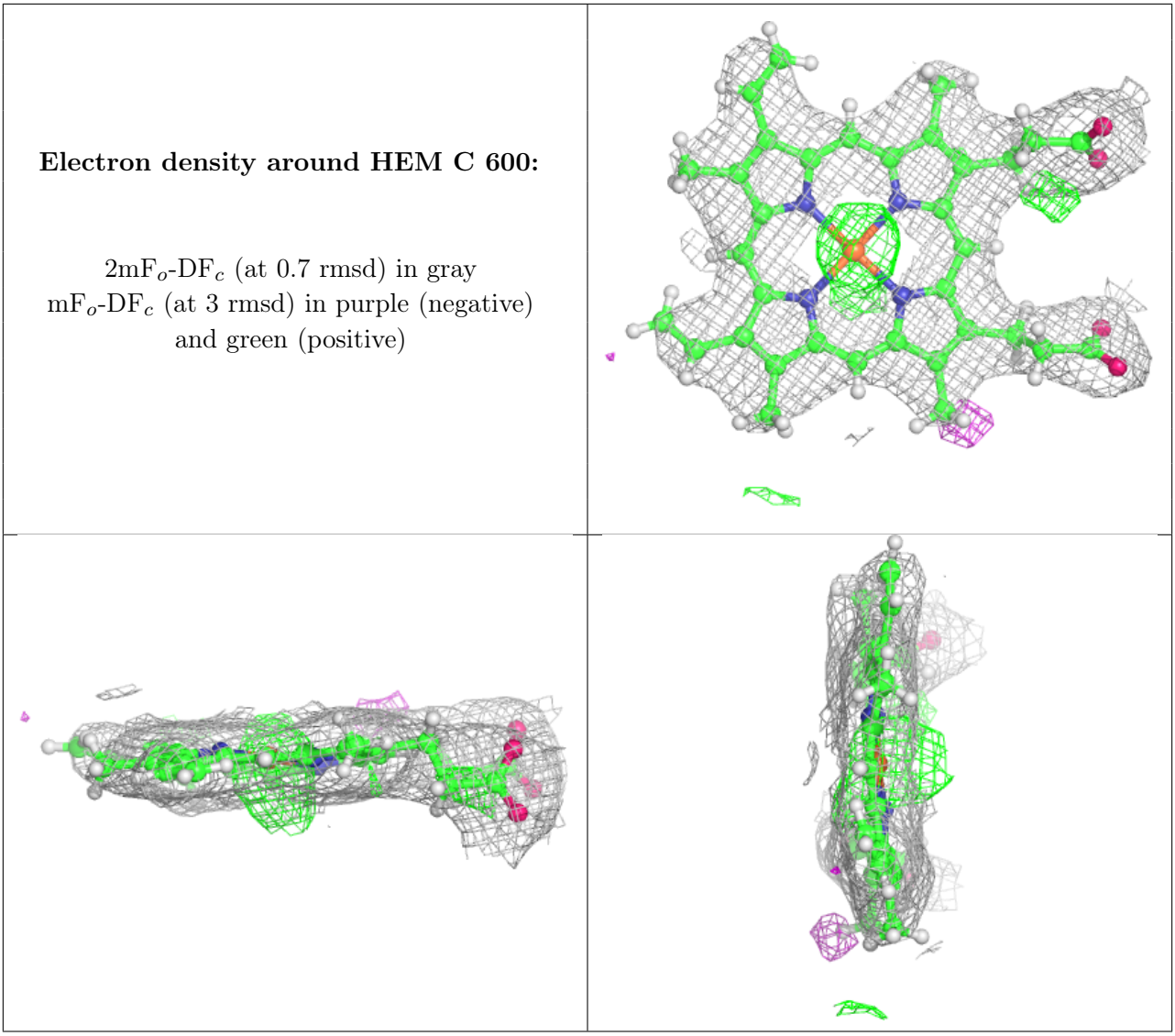
Electron density around 3NR A 601:

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



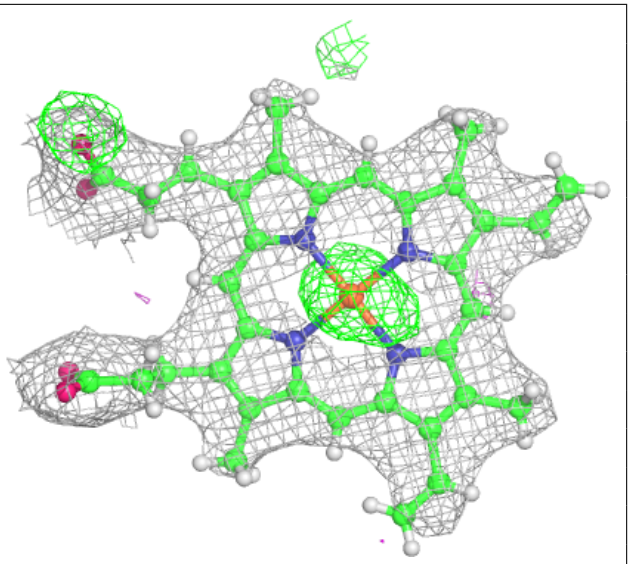
Electron density around HEM C 600:

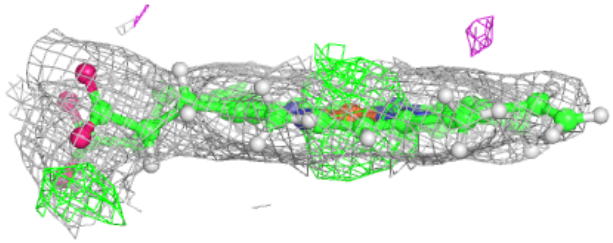
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

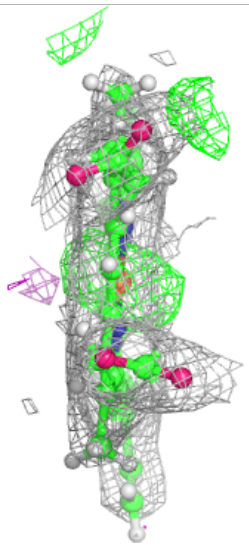


Electron density around HEM A 600:

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

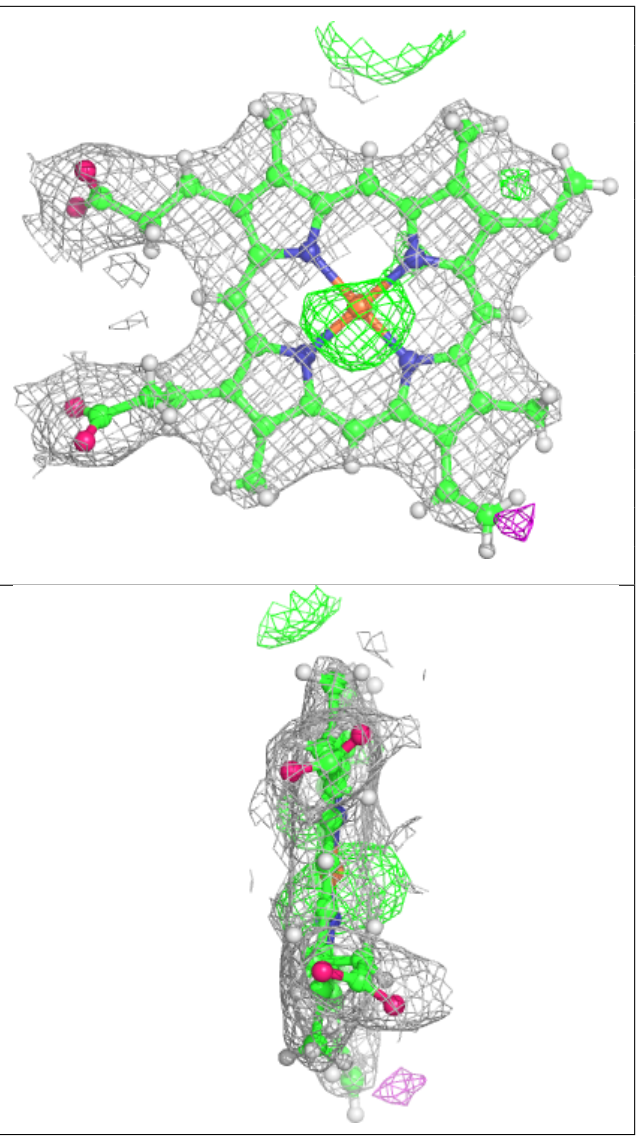






Electron density around HEM B 600:

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



6.5 Other polymers (i)

There are no such residues in this entry.