



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:16 pm BST

PDB ID : 6DWM
Title : Structure of Human Cytochrome P450 1A1 with Bergamottin
Authors : Bart, A.G.; Scott, E.E.
Deposited on : 2018-06-26
Resolution : 2.85 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 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 : 2.11
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) : 2.11

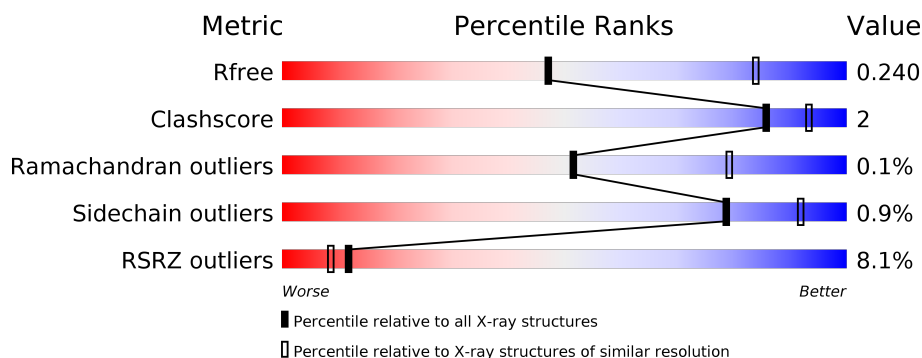
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	491	<div> <div>4%</div> <div>89%</div> <div>6%</div> <div>•</div> </div>
1	B	491	<div> <div>5%</div> <div>92%</div> <div>5%</div> <div>•</div> </div>
1	C	491	<div> <div>10%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
1	D	491	<div> <div>12%</div> <div>91%</div> <div>•</div> <div>5%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30704 atoms, of which 15307 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 Cytochrome P450 1A1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	470	Total	C	H	N	O	S	0	0	0
			7533	2412	3770	655	675	21			
1	B	476	Total	C	H	N	O	S	0	0	0
			7620	2440	3808	663	688	21			
1	C	464	Total	C	H	N	O	S	0	0	0
			7426	2381	3710	646	668	21			
1	D	464	Total	C	H	N	O	S	0	0	0
			7424	2381	3709	645	668	21			

There are 52 discrepancies between the modelled and reference sequences:

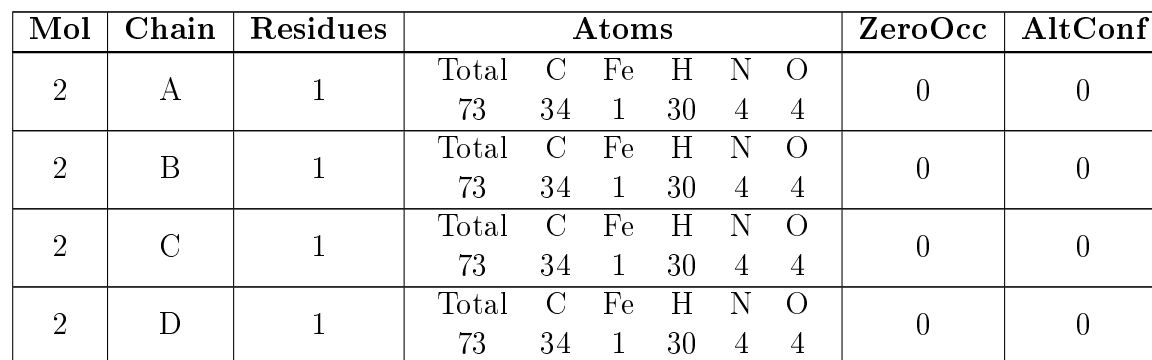
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	expression tag	UNP P04798
A	29	ALA	-	expression tag	UNP P04798
A	30	LYS	-	expression tag	UNP P04798
A	31	LYS	-	expression tag	UNP P04798
A	32	THR	-	expression tag	UNP P04798
A	33	SER	-	expression tag	UNP P04798
A	34	SER	-	expression tag	UNP P04798
A	513	HIS	-	expression tag	UNP P04798
A	514	HIS	-	expression tag	UNP P04798
A	515	HIS	-	expression tag	UNP P04798
A	516	HIS	-	expression tag	UNP P04798
A	517	HIS	-	expression tag	UNP P04798
A	518	HIS	-	expression tag	UNP P04798
B	28	MET	-	expression tag	UNP P04798
B	29	ALA	-	expression tag	UNP P04798
B	30	LYS	-	expression tag	UNP P04798
B	31	LYS	-	expression tag	UNP P04798
B	32	THR	-	expression tag	UNP P04798
B	33	SER	-	expression tag	UNP P04798
B	34	SER	-	expression tag	UNP P04798
B	513	HIS	-	expression tag	UNP P04798

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	514	HIS	-	expression tag	UNP P04798
B	515	HIS	-	expression tag	UNP P04798
B	516	HIS	-	expression tag	UNP P04798
B	517	HIS	-	expression tag	UNP P04798
B	518	HIS	-	expression tag	UNP P04798
C	28	MET	-	expression tag	UNP P04798
C	29	ALA	-	expression tag	UNP P04798
C	30	LYS	-	expression tag	UNP P04798
C	31	LYS	-	expression tag	UNP P04798
C	32	THR	-	expression tag	UNP P04798
C	33	SER	-	expression tag	UNP P04798
C	34	SER	-	expression tag	UNP P04798
C	513	HIS	-	expression tag	UNP P04798
C	514	HIS	-	expression tag	UNP P04798
C	515	HIS	-	expression tag	UNP P04798
C	516	HIS	-	expression tag	UNP P04798
C	517	HIS	-	expression tag	UNP P04798
C	518	HIS	-	expression tag	UNP P04798
D	28	MET	-	expression tag	UNP P04798
D	29	ALA	-	expression tag	UNP P04798
D	30	LYS	-	expression tag	UNP P04798
D	31	LYS	-	expression tag	UNP P04798
D	32	THR	-	expression tag	UNP P04798
D	33	SER	-	expression tag	UNP P04798
D	34	SER	-	expression tag	UNP P04798
D	513	HIS	-	expression tag	UNP P04798
D	514	HIS	-	expression tag	UNP P04798
D	515	HIS	-	expression tag	UNP P04798
D	516	HIS	-	expression tag	UNP P04798
D	517	HIS	-	expression tag	UNP P04798
D	518	HIS	-	expression tag	UNP P04798

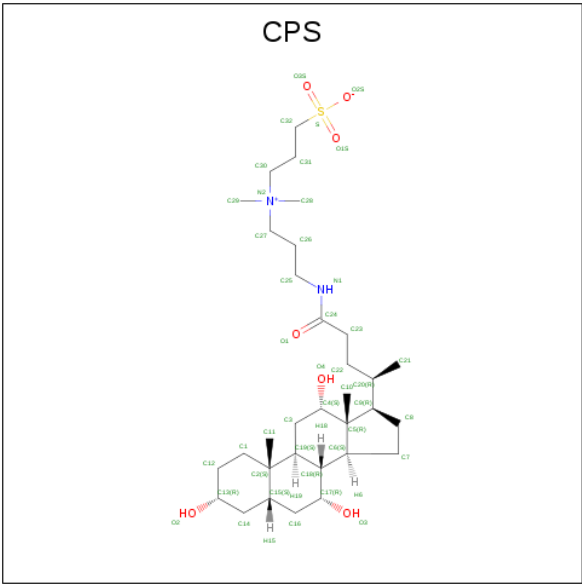
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



- # HJJ
-
- The chemical structure is a complex organic molecule, likely a derivative of a natural product. It features a central benzene ring (C11-C18) substituted with a carboxylate group (C14=O15, C17-O16), a furan ring (C19-C22, O23), and a side chain (C10-O09). The side chain consists of a methoxy group (C10-O09), a methylene group (C08), a double bond (C06=C07), a methylene group (C05), another double bond (C03=C04), and a terminal methyl group (C01). The furan ring is substituted with a methyl group (C21) and a methoxy group (C20-O09). The carboxylate group is substituted with a methyl group (C13).
- CC1=CC(OC)=C(C(=O)O)C1C2=CC(OC)=C(C)O2

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			47	21	22	4		
3	B	1	Total	C	H	O	0	0
			47	21	22	4		
3	C	1	Total	C	H	O	0	0
			47	21	22	4		
3	D	1	Total	C	H	O	0	0
			47	21	22	4		

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (three-letter code: CPS) (formula: C₃₂H₅₈N₂O₇S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0
			75	26	44	1	4	
4	D	1	Total	C	H	N	O	0
			72	25	42	1	4	

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		

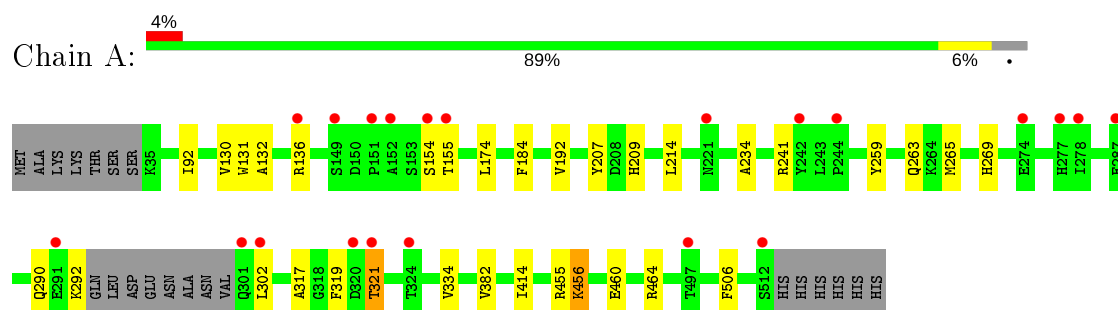
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		
6	B	27	Total	O	0	0
			27	27		

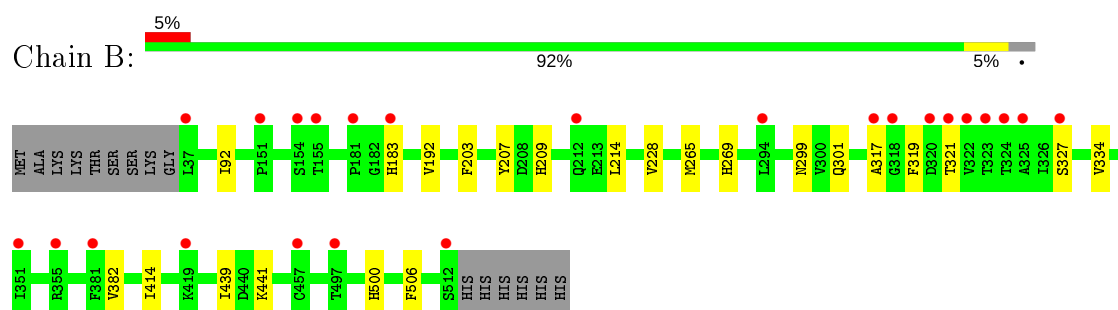
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

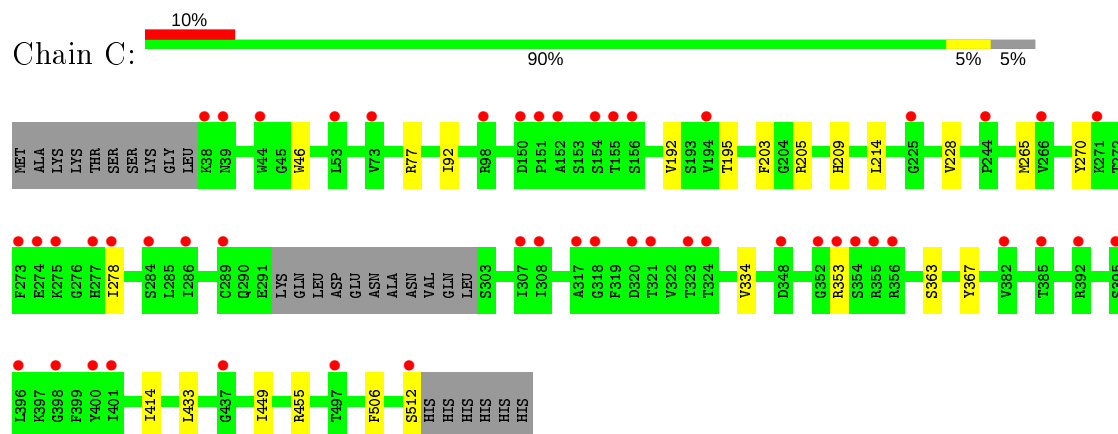
• Molecule 1: Cytochrome P450 1A1



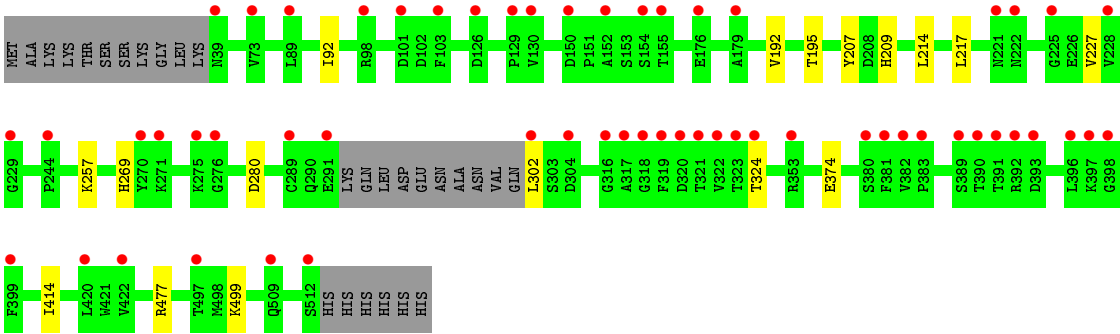
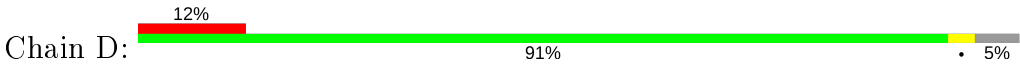
• Molecule 1: Cytochrome P450 1A1



• Molecule 1: Cytochrome P450 1A1



• Molecule 1: Cytochrome P450 1A1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.33Å 194.76Å 236.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.36 – 2.85 39.36 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.36-2.85) 93.9 (39.36-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.204 , 0.240 0.204 , 0.240	Depositor DCC
R_{free} test set	2000 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30704	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CPS, HEM, HJJ

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	0.29	0/3857	0.46	0/5223
1	B	0.30	0/3907	0.47	0/5295
1	C	0.27	0/3810	0.42	0/5162
1	D	0.27	0/3809	0.43	0/5162
All	All	0.28	0/15383	0.45	0/20842

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	3763	3770	3766	16	0
1	B	3812	3808	3806	15	0
1	C	3716	3710	3708	11	0
1	D	3715	3709	3705	8	0
2	A	43	30	30	5	0
2	B	43	30	30	7	0
2	C	43	30	30	5	0
2	D	43	30	30	4	0
3	A	25	22	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	22	0	0	0
3	C	25	22	0	0	0
3	D	25	22	0	0	0
4	A	31	44	42	0	0
4	D	30	42	40	1	0
5	B	6	8	8	0	0
5	D	6	8	8	0	0
6	A	19	0	0	0	0
6	B	27	0	0	0	0
All	All	15397	15307	15203	67	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 (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ALA:O	1:A:136:ARG:HG3	1.91	0.70
1:A:292:LYS:NZ	1:A:302:LEU:O	2.19	0.70
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.74	0.69
1:D:92:ILE:HD12	1:D:414:ILE:HD11	1.74	0.69
2:D:601:HEM:HMC2	2:D:601:HEM:HBC2	1.74	0.68
1:B:92:ILE:HD12	1:B:414:ILE:HD11	1.75	0.67
1:B:317:ALA:O	1:B:321:THR:HG22	1.95	0.66
2:C:601:HEM:HMC2	2:C:601:HEM:HBC2	1.79	0.65
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.80	0.64
1:A:456:LYS:NZ	1:A:460:GLU:OE1	2.30	0.63
1:A:460:GLU:OE2	1:A:464:ARG:NH1	2.33	0.61
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.86	0.58
1:C:92:ILE:HD12	1:C:414:ILE:HD11	1.86	0.57
2:D:601:HEM:HBB2	2:D:601:HEM:HMB2	1.86	0.57
1:B:327:SER:OG	1:B:500:HIS:NE2	2.35	0.56
1:B:321:THR:HG21	2:B:601:HEM:CHC	2.35	0.56
2:C:601:HEM:HMB2	2:C:601:HEM:HBB2	1.88	0.55
1:B:299:ASN:ND2	1:B:301:GLN:OE1	2.41	0.54
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.90	0.54
1:C:46:TRP:O	1:C:77:ARG:NH2	2.34	0.54
1:A:92:ILE:HD12	1:A:414:ILE:HD11	1.89	0.54
1:D:195:THR:HG21	1:D:214:LEU:HD11	1.89	0.54
1:A:382:VAL:HG11	2:A:601:HEM:HMA2	1.91	0.52
1:B:207:TYR:HB2	1:B:214:LEU:HD22	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD22	1:A:184:PHE:CE2	2.45	0.51
2:D:601:HEM:CMC	2:D:601:HEM:HBC2	2.40	0.50
1:B:382:VAL:HG11	2:B:601:HEM:HMA2	1.95	0.48
1:A:265:MET:O	1:A:269:HIS:ND1	2.47	0.48
2:C:601:HEM:CMC	2:C:601:HEM:HBC2	2.44	0.48
1:A:317:ALA:O	1:A:321:THR:HG23	2.13	0.47
1:D:269:HIS:NE2	1:D:280:ASP:OD2	2.44	0.47
1:B:334:VAL:HG21	1:B:506:PHE:CE2	2.49	0.47
2:B:601:HEM:HBB2	2:B:601:HEM:CMB	2.45	0.47
2:B:601:HEM:HBC2	2:B:601:HEM:CMC	2.44	0.47
2:C:601:HEM:CMB	2:C:601:HEM:HBB2	2.45	0.46
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.45	0.46
1:B:265:MET:O	1:B:269:HIS:ND1	2.49	0.46
1:C:205:ARG:HD3	1:C:265:MET:CE	2.46	0.45
2:D:601:HEM:HBB2	2:D:601:HEM:CMB	2.46	0.45
1:D:324:THR:OG1	1:D:499:LYS:NZ	2.42	0.45
1:C:455:ARG:NH1	2:C:601:HEM:O2D	2.50	0.44
1:C:353:ARG:NH1	1:C:512:SER:O	2.42	0.44
1:A:130:VAL:HG13	1:A:302:LEU:CD2	2.47	0.44
1:A:234:ALA:O	1:A:241:ARG:NH1	2.49	0.44
2:A:601:HEM:CMB	2:A:601:HEM:HBB2	2.47	0.44
1:D:207:TYR:HB2	1:D:214:LEU:HD22	1.99	0.44
1:A:334:VAL:HG21	1:A:506:PHE:CE2	2.52	0.44
1:C:195:THR:HG21	1:C:214:LEU:HD11	2.00	0.44
1:B:192:VAL:HG11	1:B:209:HIS:HA	2.00	0.44
1:B:203:PHE:HB3	1:B:265:MET:CE	2.47	0.44
1:D:217:LEU:HD12	1:D:257:LYS:HZ2	1.82	0.44
1:D:192:VAL:HG11	1:D:209:HIS:HA	2.00	0.43
1:A:207:TYR:HB2	1:A:214:LEU:HD22	2.00	0.43
4:D:603:CPS:H21A	4:D:603:CPS:H4	2.00	0.43
1:B:321:THR:HG21	2:B:601:HEM:C4B	2.54	0.42
1:C:334:VAL:HG21	1:C:506:PHE:CE2	2.54	0.42
1:A:290:GLN:O	1:A:292:LYS:N	2.50	0.42
1:C:367:TYR:CD1	1:C:433:LEU:HD11	2.55	0.42
1:C:203:PHE:CG	1:C:265:MET:HE2	2.56	0.41
1:B:439:ILE:O	1:B:441:LYS:NZ	2.43	0.41
1:A:131:TRP:CZ2	1:A:455:ARG:HD3	2.54	0.41
1:C:192:VAL:HG11	1:C:209:HIS:HA	2.03	0.41
1:B:228:VAL:O	1:B:228:VAL:HG12	2.19	0.41
1:C:228:VAL:HG12	1:C:228:VAL:O	2.20	0.41
1:D:374:GLU:OE1	1:D:374:GLU:HA	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:ILE:HG22	1:B:441:LYS:HD3	2.02	0.40
1:A:192:VAL:HG11	1:A:209:HIS:HA	2.02	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	466/491 (95%)	453 (97%)	13 (3%)	0	100	100
1	B	474/491 (96%)	462 (98%)	12 (2%)	0	100	100
1	C	460/491 (94%)	449 (98%)	10 (2%)	1 (0%)	47	75
1	D	460/491 (94%)	448 (97%)	12 (3%)	0	100	100
All	All	1860/1964 (95%)	1812 (97%)	47 (2%)	1 (0%)	51	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	449	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	420/439 (96%)	413 (98%)	7 (2%)	60	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	426/439 (97%)	424 (100%)	2 (0%)	88	96
1	C	415/439 (94%)	412 (99%)	3 (1%)	84	94
1	D	415/439 (94%)	412 (99%)	3 (1%)	84	94
All	All	1676/1756 (95%)	1661 (99%)	15 (1%)	78	92

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

Mol	Chain	Res	Type
1	A	154	SER
1	A	155	THR
1	A	259	TYR
1	A	263	GLN
1	A	319	PHE
1	A	321	THR
1	A	456	LYS
1	B	183	HIS
1	B	319	PHE
1	C	270	TYR
1	C	278	ILE
1	C	363	SER
1	D	227	VAL
1	D	302	LEU
1	D	477	ARG

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

Mol	Chain	Res	Type
1	A	255	ASN
1	B	255	ASN
1	C	255	ASN
1	D	99	GLN
1	D	255	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
5	GOL	D	604	-	5,5,5	0.82	0	5,5,5	0.97	0
2	HEM	D	601	-	27,50,50	1.87	5 (18%)	17,82,82	1.40	3 (17%)
3	HJJ	D	602	-	21,27,27	2.64	10 (47%)	27,37,37	1.91	6 (22%)
5	GOL	B	603	-	5,5,5	0.95	0	5,5,5	1.08	0
3	HJJ	B	602	-	21,27,27	2.24	7 (33%)	27,37,37	1.94	8 (29%)
3	HJJ	C	602	-	21,27,27	2.65	10 (47%)	27,37,37	1.89	7 (25%)
3	HJJ	A	602	-	21,27,27	2.56	7 (33%)	27,37,37	2.00	8 (29%)
4	CPS	A	603	-	34,34,45	1.05	3 (8%)	52,53,70	2.02	16 (30%)
2	HEM	C	601	-	27,50,50	1.85	4 (14%)	17,82,82	1.63	3 (17%)
2	HEM	A	601	1	27,50,50	1.87	4 (14%)	17,82,82	1.56	5 (29%)
4	CPS	D	603	-	33,33,45	1.11	3 (9%)	52,52,70	2.16	17 (32%)
2	HEM	B	601	1	27,50,50	1.85	4 (14%)	17,82,82	1.49	4 (23%)

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
5	GOL	D	604	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	601	-	-	0/6/54/54	-
3	HJJ	D	602	-	-	6/12/12/12	0/3/3/3
5	GOL	B	603	-	-	1/4/4/4	-
3	HJJ	B	602	-	-	5/12/12/12	0/3/3/3
3	HJJ	C	602	-	-	2/12/12/12	0/3/3/3
3	HJJ	A	602	-	-	2/12/12/12	0/3/3/3
4	CPS	A	603	-	-	2/12/77/90	0/4/4/4
2	HEM	C	601	-	-	0/6/54/54	-
2	HEM	A	601	1	-	0/6/54/54	-
4	CPS	D	603	-	-	2/11/76/90	0/4/4/4
2	HEM	B	601	1	-	0/6/54/54	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	HJJ	C12-C11	5.09	1.52	1.42
3	A	602	HJJ	C12-C11	4.90	1.52	1.42
3	A	602	HJJ	O16-C17	4.86	1.44	1.36
3	A	602	HJJ	C18-C17	4.68	1.46	1.37
3	C	602	HJJ	C18-C17	4.67	1.46	1.37
3	D	602	HJJ	C12-C11	4.66	1.51	1.42
3	D	602	HJJ	O16-C17	4.50	1.44	1.36
3	C	602	HJJ	O16-C17	4.49	1.44	1.36
3	A	602	HJJ	C18-C19	4.48	1.46	1.37
3	D	602	HJJ	C18-C17	4.48	1.46	1.37
3	C	602	HJJ	C18-C19	4.41	1.46	1.37
3	A	602	HJJ	C13-C14	4.35	1.46	1.37
3	C	602	HJJ	C13-C14	4.31	1.46	1.37
3	D	602	HJJ	C18-C19	4.28	1.46	1.37
2	A	601	HEM	C3B-C2B	-4.25	1.34	1.40
2	B	601	HEM	C3B-C2B	-4.18	1.34	1.40
2	D	601	HEM	C3C-C2C	-4.17	1.34	1.40
3	B	602	HJJ	C13-C14	4.16	1.45	1.37
3	B	602	HJJ	C18-C17	4.10	1.45	1.37
3	B	602	HJJ	C12-C11	4.04	1.50	1.42
2	D	601	HEM	C3B-C2B	-4.02	1.34	1.40
2	B	601	HEM	C3C-C2C	-4.00	1.34	1.40
2	A	601	HEM	C3C-C2C	-3.99	1.34	1.40
3	B	602	HJJ	C18-C19	3.98	1.45	1.37
3	D	602	HJJ	C13-C14	3.98	1.45	1.37
2	C	601	HEM	C3B-C2B	-3.93	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	C3C-C2C	-3.92	1.34	1.40
2	C	601	HEM	C3C-CAC	3.80	1.55	1.47
2	C	601	HEM	C3B-CAB	3.77	1.55	1.47
2	A	601	HEM	C3C-CAC	3.76	1.55	1.47
2	B	601	HEM	C3C-CAC	3.69	1.55	1.47
2	A	601	HEM	C3B-CAB	3.68	1.55	1.47
2	B	601	HEM	C3B-CAB	3.64	1.55	1.47
2	D	601	HEM	C3B-CAB	3.62	1.55	1.47
2	D	601	HEM	C3C-CAC	3.61	1.55	1.47
3	B	602	HJJ	O16-C17	3.49	1.42	1.36
3	D	602	HJJ	C05-C06	3.26	1.58	1.51
4	D	603	CPS	C5-C6	-3.09	1.50	1.55
4	A	603	CPS	C5-C6	-2.74	1.50	1.55
4	A	603	CPS	C11-C2	-2.50	1.50	1.54
3	D	602	HJJ	C08-C07	2.38	1.56	1.49
3	D	602	HJJ	C12-C13	2.35	1.41	1.36
3	C	602	HJJ	C12-C13	2.34	1.41	1.36
3	D	602	HJJ	C07-C06	2.33	1.38	1.33
3	A	602	HJJ	C12-C13	2.30	1.41	1.36
3	C	602	HJJ	C08-C07	2.26	1.55	1.49
3	D	602	HJJ	C04-C03	2.25	1.57	1.50
2	D	601	HEM	CAA-C2A	2.24	1.55	1.52
3	B	602	HJJ	C12-C13	2.24	1.41	1.36
3	C	602	HJJ	C11-C17	2.21	1.44	1.41
4	A	603	CPS	C24-N1	2.17	1.38	1.33
3	C	602	HJJ	C04-C03	2.13	1.57	1.50
4	D	603	CPS	C16-C17	2.11	1.56	1.52
3	A	602	HJJ	C08-C07	2.09	1.55	1.49
3	C	602	HJJ	C07-C06	2.09	1.38	1.33
3	B	602	HJJ	C07-C06	2.07	1.38	1.33
4	D	603	CPS	C11-C2	-2.06	1.50	1.54

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	CPS	C5-C9-C20	-5.96	112.38	119.50
4	D	603	CPS	C5-C9-C20	-5.93	112.42	119.50
3	A	602	HJJ	O16-C17-C18	5.49	122.54	116.03
3	C	602	HJJ	O16-C17-C18	5.14	122.13	116.03
4	D	603	CPS	C7-C6-C18	-5.10	111.20	118.33
3	D	602	HJJ	O16-C17-C18	5.05	122.02	116.03
3	B	602	HJJ	O16-C17-C18	4.95	121.91	116.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	603	CPS	C14-C13-C12	-4.53	105.14	110.55
4	A	603	CPS	C7-C6-C18	-4.37	112.22	118.33
4	D	603	CPS	C22-C23-C24	-4.37	103.28	113.04
3	D	602	HJJ	O09-C08-C07	4.09	116.41	107.97
3	A	602	HJJ	C18-C17-C11	-4.03	118.58	123.05
4	A	603	CPS	C22-C23-C24	-4.02	104.05	113.04
4	D	603	CPS	C19-C18-C6	-3.96	104.27	109.71
3	B	602	HJJ	O09-C08-C07	3.95	116.11	107.97
3	B	602	HJJ	C18-C17-C11	-3.81	118.83	123.05
3	D	602	HJJ	C18-C17-C11	-3.78	118.86	123.05
3	C	602	HJJ	C18-C17-C11	-3.78	118.87	123.05
4	A	603	CPS	C19-C18-C6	-3.73	104.59	109.71
4	A	603	CPS	C16-C15-C2	-3.52	108.92	112.66
3	C	602	HJJ	O09-C08-C07	3.49	115.17	107.97
4	D	603	CPS	C9-C5-C4	-3.40	114.56	117.67
4	A	603	CPS	C23-C24-N1	-3.18	111.06	116.42
4	A	603	CPS	C15-C14-C13	-3.14	108.15	112.76
4	D	603	CPS	C16-C15-C2	-3.14	109.33	112.66
2	C	601	HEM	CMD-C2D-C1D	-3.12	123.66	128.46
4	D	603	CPS	C10-C5-C6	3.10	116.06	111.21
4	D	603	CPS	C1-C12-C13	-3.08	106.51	110.47
4	D	603	CPS	C23-C24-N1	-3.08	112.01	116.29
3	A	602	HJJ	C08-O09-C10	3.00	122.39	114.73
4	D	603	CPS	C15-C14-C13	-2.92	108.47	112.76
4	A	603	CPS	C9-C5-C6	-2.88	97.19	100.09
2	C	601	HEM	CAA-CBA-CGA	-2.83	107.92	112.67
4	A	603	CPS	C5-C6-C18	-2.80	111.16	114.74
4	A	603	CPS	C1-C12-C13	-2.78	106.90	110.47
4	A	603	CPS	C10-C5-C6	2.77	115.55	111.21
2	B	601	HEM	CAD-CBD-CGD	-2.77	108.02	112.67
2	A	601	HEM	CAD-CBD-CGD	-2.75	108.05	112.67
3	A	602	HJJ	C24-C06-C05	2.69	119.80	115.27
3	B	602	HJJ	C24-C06-C05	2.61	119.66	115.27
3	A	602	HJJ	C21-C20-C19	-2.59	105.95	109.97
2	A	601	HEM	CAA-CBA-CGA	-2.58	108.33	112.67
3	B	602	HJJ	C25-C02-C01	2.57	120.28	114.60
4	D	603	CPS	C5-C6-C18	-2.53	111.51	114.74
4	A	603	CPS	C9-C5-C4	-2.52	115.36	117.67
4	D	603	CPS	C3-C4-C5	-2.49	108.69	111.24
3	D	602	HJJ	C21-C20-C19	-2.45	106.17	109.97
2	A	601	HEM	CMD-C2D-C1D	-2.42	124.75	128.46
3	A	602	HJJ	O09-C08-C07	2.42	112.95	107.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	CPS	C2-C19-C18	-2.42	109.22	111.82
3	A	602	HJJ	O16-C17-C11	-2.41	118.87	121.20
3	C	602	HJJ	C21-C20-C19	-2.39	106.25	109.97
3	D	602	HJJ	C24-C06-C05	2.34	119.21	115.27
4	D	603	CPS	C2-C19-C18	-2.34	109.31	111.82
3	C	602	HJJ	C08-O09-C10	2.33	120.69	114.73
2	D	601	HEM	CMD-C2D-C1D	-2.33	124.89	128.46
3	C	602	HJJ	O16-C17-C11	-2.28	119.00	121.20
3	B	602	HJJ	C08-C07-C06	-2.27	122.11	126.04
2	B	601	HEM	CMA-C3A-C4A	-2.27	124.97	128.46
4	A	603	CPS	C19-C2-C15	2.26	111.75	108.58
2	C	601	HEM	CMA-C3A-C4A	-2.25	125.01	128.46
2	A	601	HEM	CMA-C3A-C4A	-2.23	125.03	128.46
3	C	602	HJJ	C25-C02-C01	2.22	119.51	114.60
3	D	602	HJJ	O16-C17-C11	-2.16	119.12	121.20
4	A	603	CPS	O1-C24-C23	2.16	125.96	122.02
4	D	603	CPS	C19-C2-C15	2.14	111.59	108.58
4	D	603	CPS	C6-C5-C4	-2.13	105.42	107.40
3	A	602	HJJ	C25-C02-C01	2.12	119.29	114.60
2	B	601	HEM	CMD-C2D-C1D	-2.12	125.20	128.46
4	A	603	CPS	C22-C20-C9	-2.10	105.95	110.28
2	A	601	HEM	CMC-C2C-C3C	2.09	128.59	124.68
2	D	601	HEM	CMA-C3A-C4A	-2.07	125.28	128.46
2	B	601	HEM	CAA-CBA-CGA	-2.03	109.26	112.67
4	D	603	CPS	C8-C7-C6	-2.03	101.10	105.13
3	B	602	HJJ	C08-O09-C10	2.02	119.90	114.73
2	D	601	HEM	C1D-C2D-C3D	2.01	108.39	107.00
3	B	602	HJJ	O16-C17-C11	-2.01	119.27	121.20

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	HJJ	C20-C10-O09-C08
3	A	602	HJJ	C11-C10-O09-C08
4	D	603	CPS	C21-C20-C22-C23
4	D	603	CPS	C9-C20-C22-C23
3	D	602	HJJ	C04-C05-C06-C24
3	B	602	HJJ	C04-C05-C06-C24
3	D	602	HJJ	C04-C05-C06-C07
3	B	602	HJJ	C04-C05-C06-C07
3	C	602	HJJ	C03-C04-C05-C06

Continued on next page...

Continued from previous page...

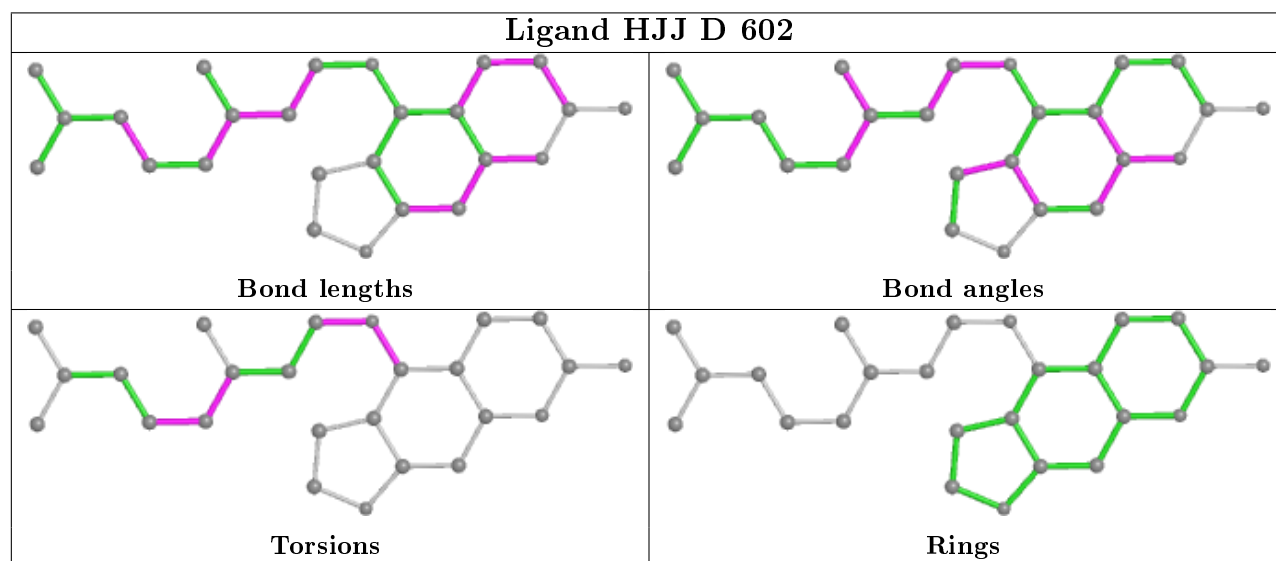
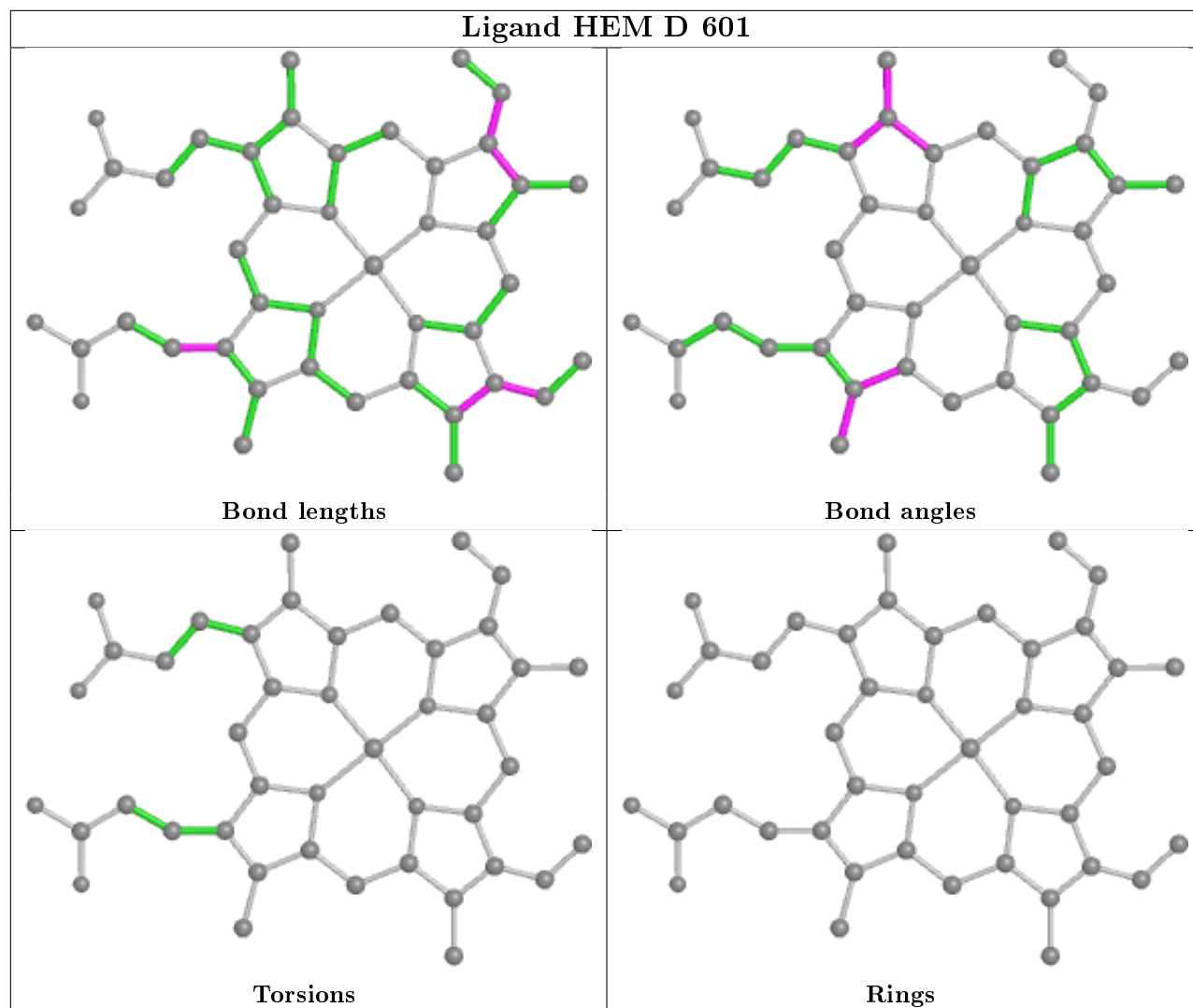
Mol	Chain	Res	Type	Atoms
3	D	602	HJJ	C20-C10-O09-C08
3	B	602	HJJ	C20-C10-O09-C08
4	A	603	CPS	C21-C20-C22-C23
3	B	602	HJJ	C07-C08-O09-C10
3	C	602	HJJ	C07-C08-O09-C10
3	B	602	HJJ	C11-C10-O09-C08
4	A	603	CPS	C21-C20-C9-C5
3	D	602	HJJ	C07-C08-O09-C10
3	D	602	HJJ	C11-C10-O09-C08
3	D	602	HJJ	C03-C04-C05-C06
5	B	603	GOL	O1-C1-C2-C3
5	D	604	GOL	O2-C2-C3-O3

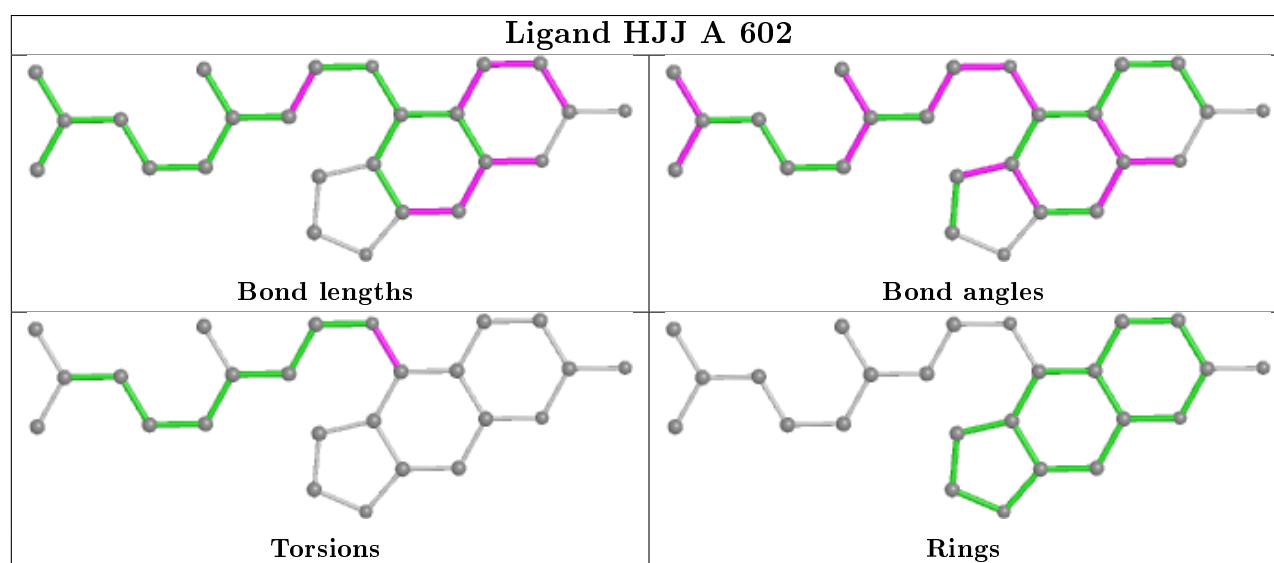
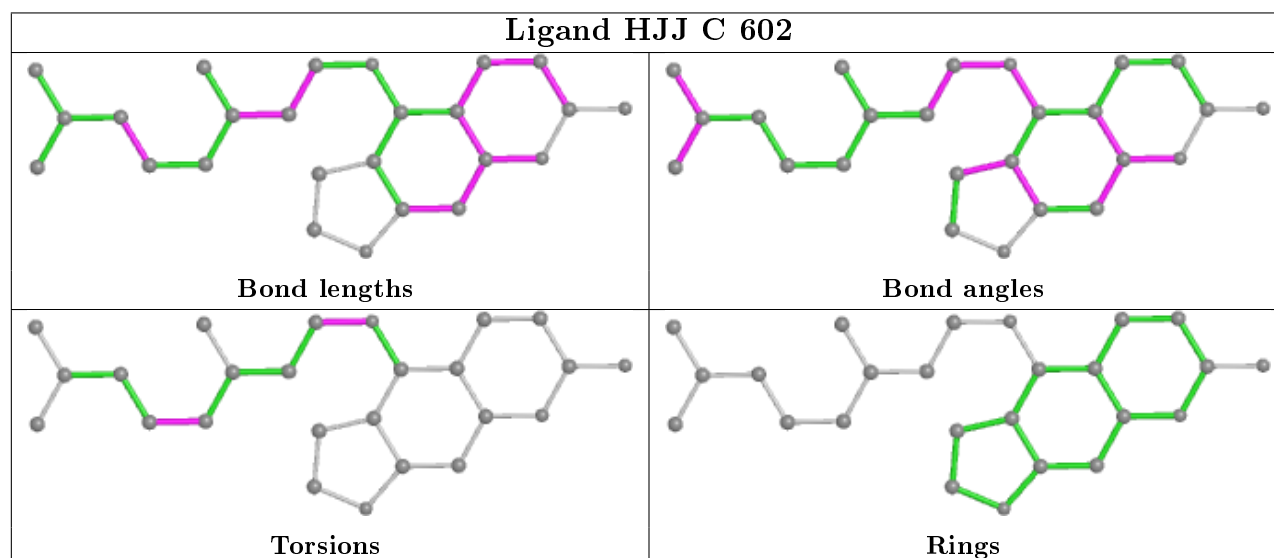
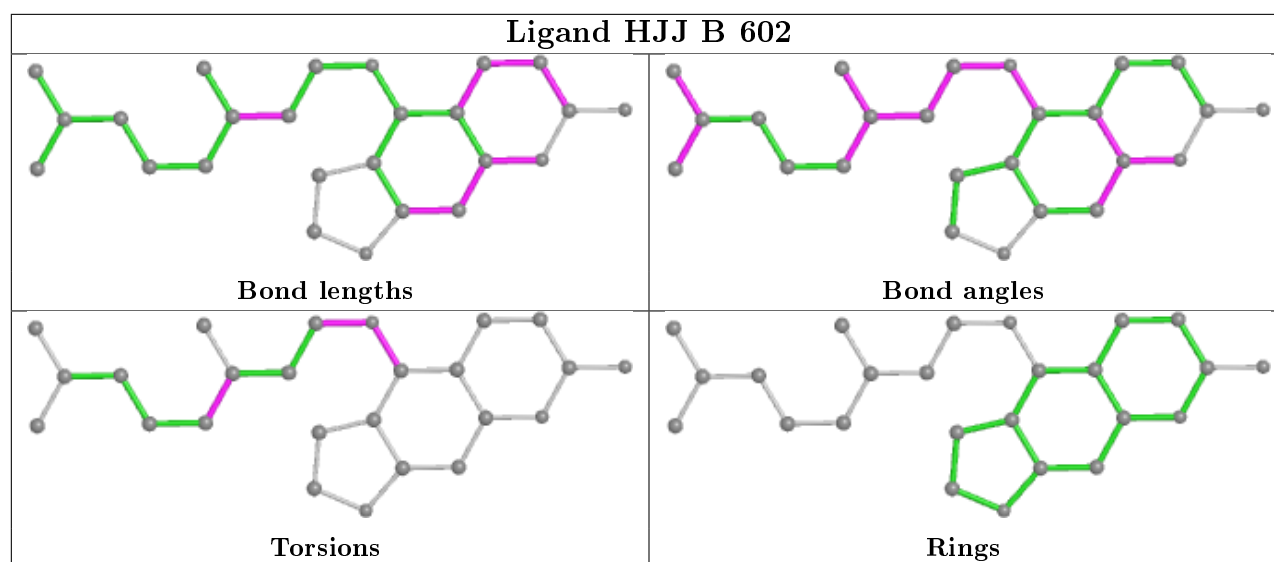
There are no ring outliers.

5 monomers are involved in 22 short contacts:

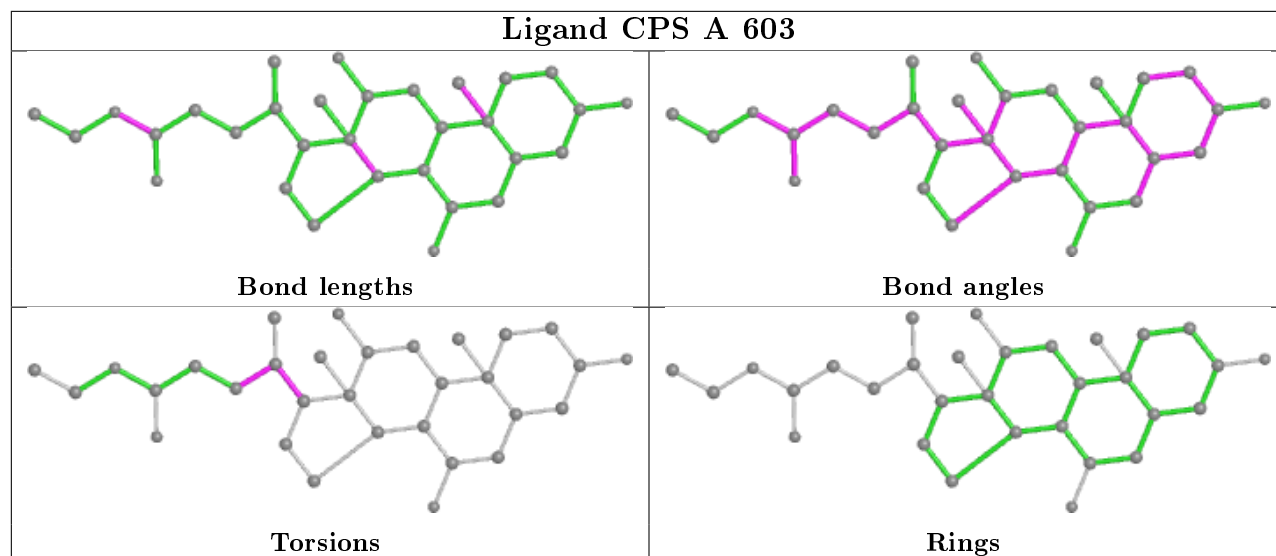
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	HEM	4	0
2	C	601	HEM	5	0
2	A	601	HEM	5	0
4	D	603	CPS	1	0
2	B	601	HEM	7	0

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

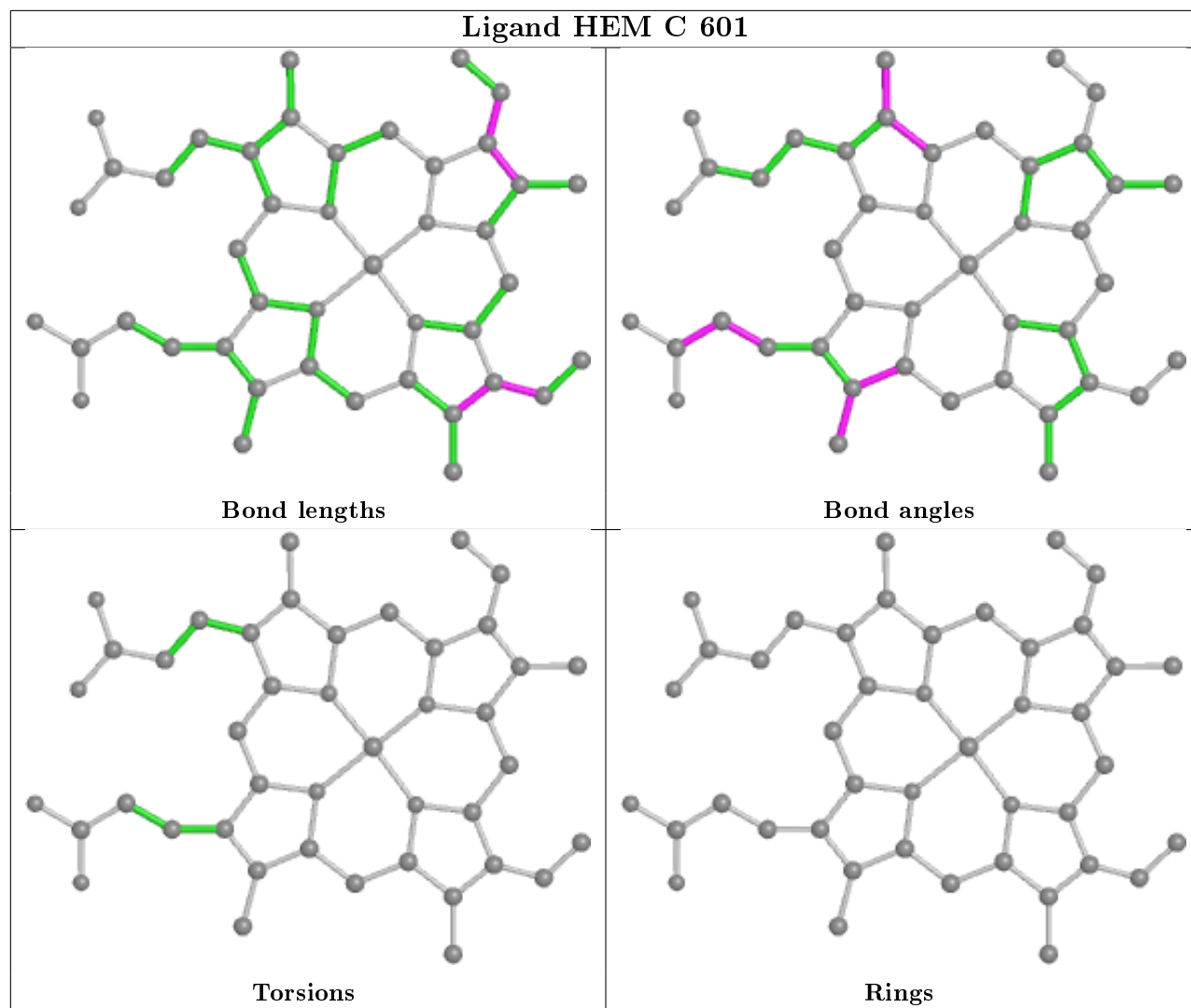


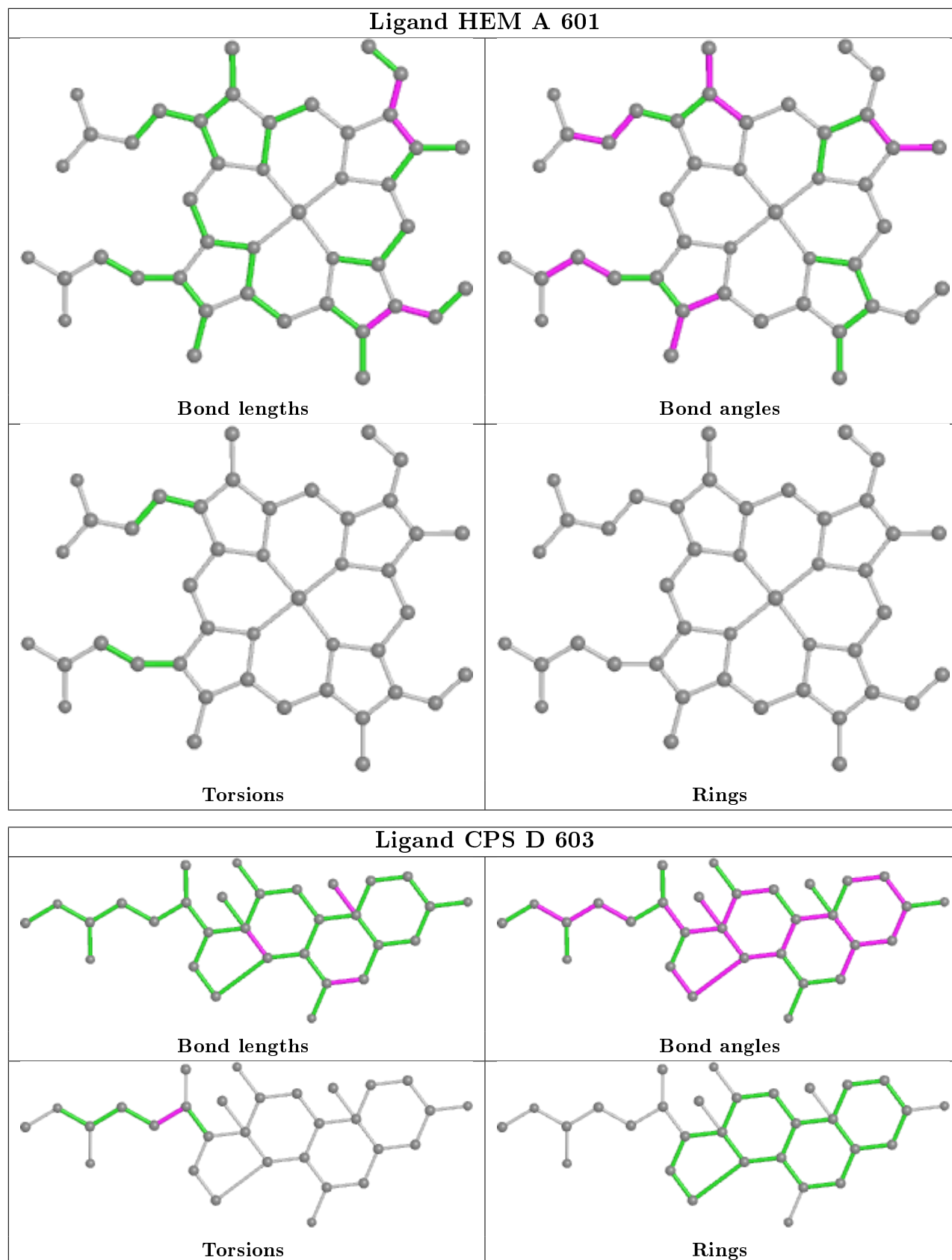


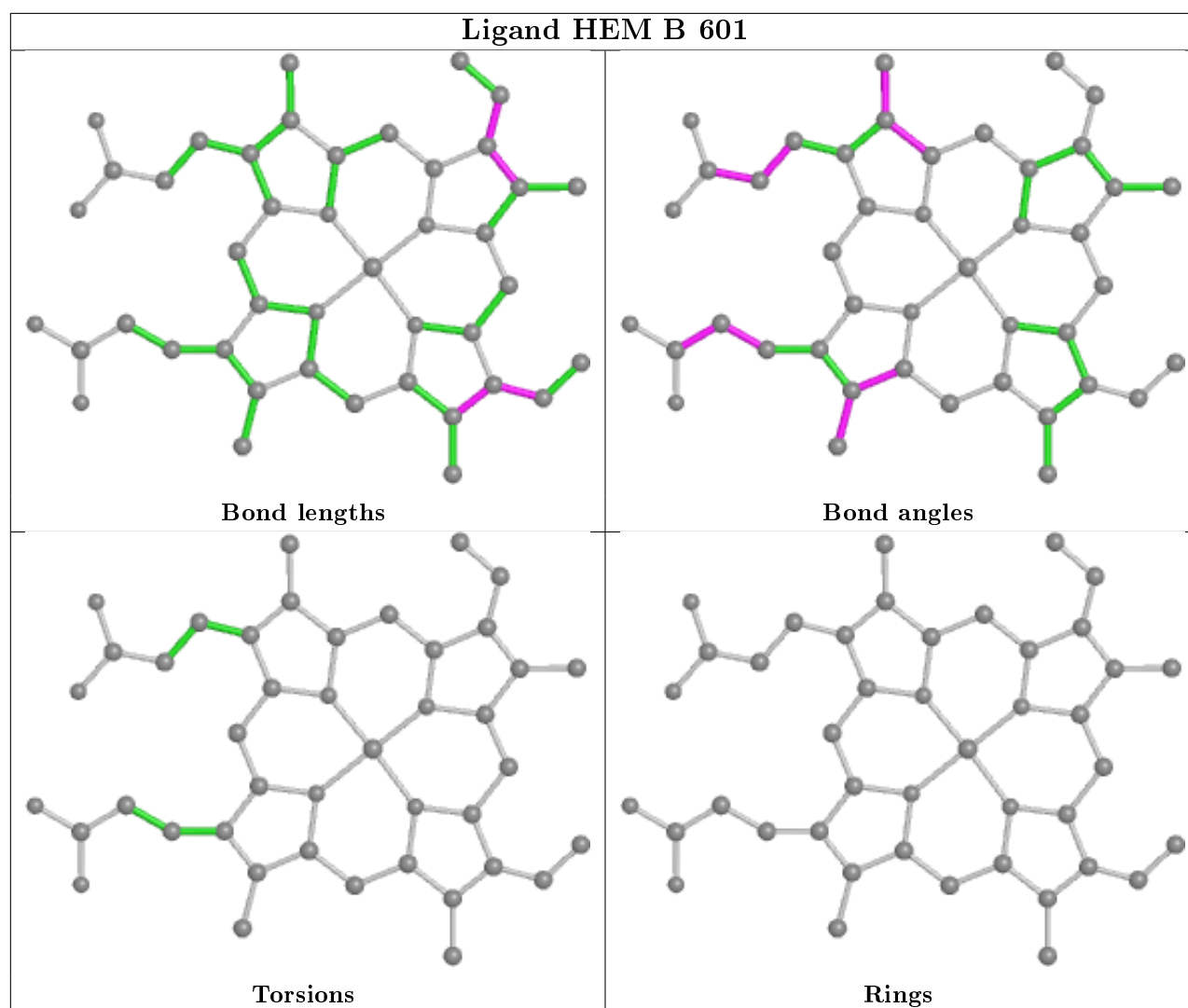
Ligand CPS A 603



Ligand HEM C 601







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	470/491 (95%)	0.30	21 (4%) 33 28	36, 62, 96, 126	0
1	B	476/491 (96%)	0.40	24 (5%) 28 24	37, 57, 92, 125	0
1	C	464/491 (94%)	0.84	50 (10%) 5 4	62, 91, 112, 135	0
1	D	464/491 (94%)	0.78	57 (12%) 4 2	56, 84, 111, 130	0
All	All	1874/1964 (95%)	0.58	152 (8%) 12 8	36, 75, 107, 135	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	277	HIS	5.1
1	D	244	PRO	4.9
1	A	155	THR	4.6
1	B	320	ASP	4.6
1	C	152	ALA	4.5
1	D	320	ASP	4.4
1	C	321	THR	4.3
1	C	154	SER	4.3
1	C	320	ASP	4.1
1	C	155	THR	4.0
1	C	398	GLY	4.0
1	C	274	GLU	4.0
1	C	396	LEU	4.0
1	D	497	THR	4.0
1	D	152	ALA	3.8
1	D	291	GLU	3.8
1	D	150	ASP	3.8
1	C	353	ARG	3.8
1	D	324	THR	3.8
1	D	225	GLY	3.7
1	B	155	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	321	THR	3.7
1	C	352	GLY	3.6
1	D	317	ALA	3.6
1	D	289	CYS	3.6
1	C	39	ASN	3.5
1	B	324	THR	3.5
1	D	391	THR	3.5
1	B	321	THR	3.5
1	C	395	SER	3.4
1	C	38	LYS	3.4
1	C	324	THR	3.4
1	D	390	THR	3.4
1	D	155	THR	3.4
1	D	302	LEU	3.3
1	D	323	THR	3.3
1	C	497	THR	3.3
1	B	497	THR	3.3
1	C	44	TRP	3.3
1	B	154	SER	3.2
1	A	291	GLU	3.2
1	C	275	LYS	3.2
1	B	151	PRO	3.2
1	A	154	SER	3.1
1	C	151	PRO	3.1
1	D	39	ASN	3.1
1	D	318	GLY	3.1
1	A	151	PRO	3.1
1	D	129	PRO	3.0
1	B	323	THR	3.0
1	B	457	CYS	3.0
1	D	509	GLN	3.0
1	A	152	ALA	3.0
1	C	273	PHE	3.0
1	D	103	PHE	2.9
1	B	318	GLY	2.9
1	C	284	SER	2.9
1	D	398	GLY	2.9
1	D	98	ARG	2.9
1	C	278	ILE	2.9
1	A	136	ARG	2.9
1	D	73	VAL	2.9
1	A	497	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	322	VAL	2.8
1	C	244	PRO	2.8
1	D	512	SER	2.8
1	D	382	VAL	2.8
1	B	37	LEU	2.8
1	D	389	SER	2.8
1	B	181	PRO	2.7
1	B	317	ALA	2.7
1	A	278	ILE	2.7
1	A	149	SER	2.7
1	D	270	TYR	2.7
1	C	318	GLY	2.7
1	A	320	ASP	2.6
1	D	393	ASP	2.6
1	A	301	GLN	2.6
1	D	383	PRO	2.6
1	B	322	VAL	2.5
1	A	512	SER	2.5
1	C	156	SER	2.5
1	A	302	LEU	2.5
1	B	325	ALA	2.5
1	C	400	TYR	2.5
1	D	221	ASN	2.5
1	C	307	ILE	2.5
1	B	183	HIS	2.5
1	A	221	ASN	2.5
1	C	308	ILE	2.5
1	D	399	PHE	2.5
1	C	53	LEU	2.5
1	D	422	VAL	2.5
1	C	271	LYS	2.4
1	C	73	VAL	2.4
1	C	266	VAL	2.4
1	D	396	LEU	2.4
1	C	317	ALA	2.4
1	D	420	LEU	2.4
1	A	324	THR	2.4
1	C	348	ASP	2.4
1	D	276	GLY	2.3
1	C	323	THR	2.3
1	D	179	ALA	2.3
1	B	294	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	385	THR	2.3
1	D	316	GLY	2.3
1	C	355	ARG	2.3
1	A	274	GLU	2.3
1	C	382	VAL	2.3
1	C	512	SER	2.3
1	D	229	GLY	2.3
1	D	275	LYS	2.3
1	D	222	ASN	2.2
1	D	392	ARG	2.2
1	D	381	PHE	2.2
1	A	277	HIS	2.2
1	D	176	GLU	2.2
1	D	319	PHE	2.2
1	C	289	CYS	2.2
1	C	354	SER	2.2
1	C	401	ILE	2.2
1	B	327	SER	2.2
1	C	286	ILE	2.2
1	A	242	TYR	2.2
1	B	355	ARG	2.2
1	D	126	ASP	2.1
1	B	419	LYS	2.1
1	D	101	ASP	2.1
1	D	397	LYS	2.1
1	D	130	VAL	2.1
1	C	437	GLY	2.1
1	A	287	GLU	2.1
1	B	351	ILE	2.1
1	D	89	LEU	2.0
1	D	380	SER	2.0
1	C	392	ARG	2.0
1	D	271	LYS	2.0
1	C	194	VAL	2.0
1	B	512	SER	2.0
1	C	356	ARG	2.0
1	C	150	ASP	2.0
1	D	304	ASP	2.0
1	C	225	GLY	2.0
1	A	321	THR	2.0
1	D	228	VAL	2.0
1	A	244	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	381	PHE	2.0
1	D	154	SER	2.0
1	C	98	ARG	2.0
1	D	353	ARG	2.0
1	B	212	GLN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

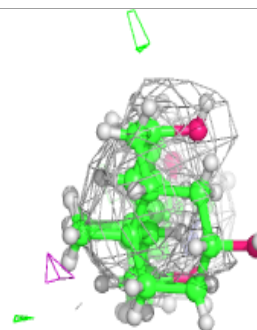
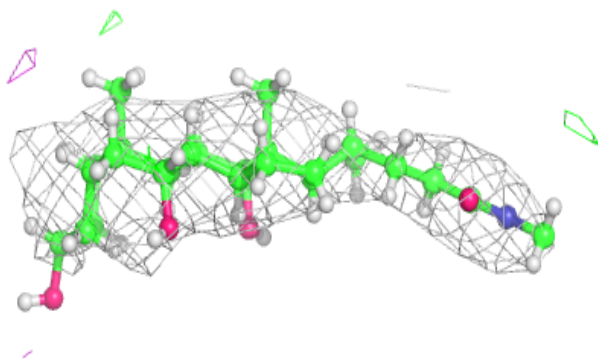
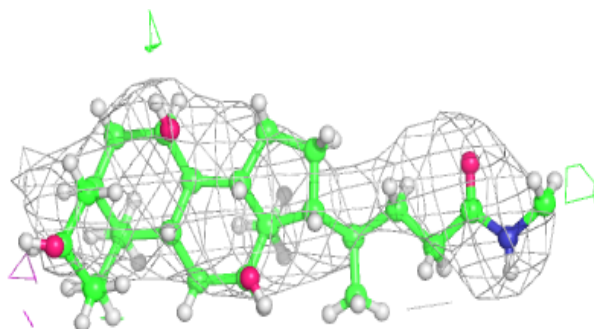
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	B	603	6/6	0.74	0.23	75,96,115,127	0
4	CPS	D	603	30/42	0.86	0.31	93,124,144,149	0
4	CPS	A	603	31/42	0.91	0.35	75,98,117,121	0
3	HJJ	D	602	25/25	0.92	0.38	64,82,101,113	0
3	HJJ	C	602	25/25	0.92	0.27	70,85,98,104	0
5	GOL	D	604	6/6	0.93	0.22	71,86,100,100	0
3	HJJ	A	602	25/25	0.93	0.29	45,61,69,76	0
2	HEM	D	601	43/43	0.94	0.39	50,65,81,86	0
3	HJJ	B	602	25/25	0.94	0.29	36,52,79,82	0
2	HEM	C	601	43/43	0.96	0.36	56,69,92,95	0
2	HEM	B	601	43/43	0.96	0.36	35,46,56,62	0
2	HEM	A	601	43/43	0.97	0.30	37,50,62,65	0

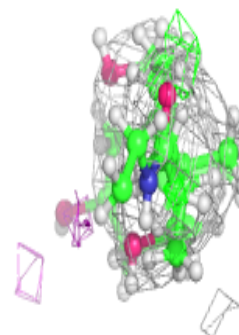
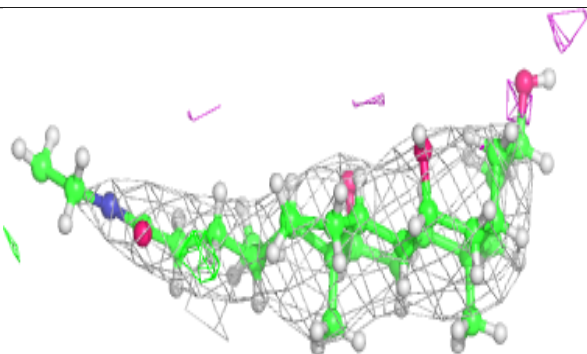
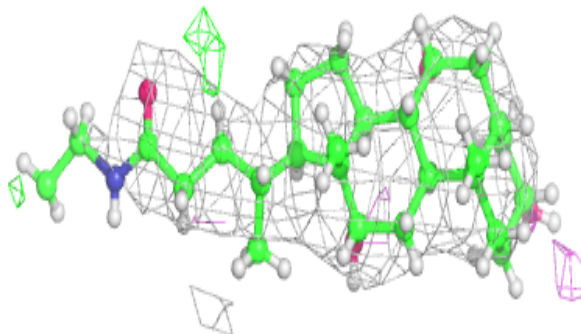
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CPS D 603:

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

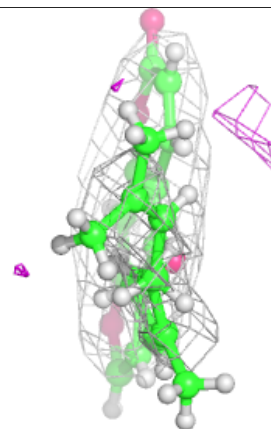
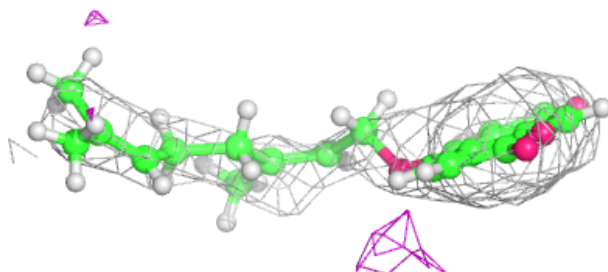
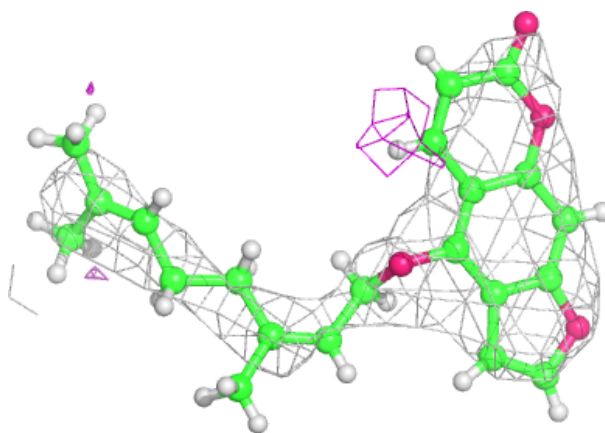
**Electron density around CPS A 603:**

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

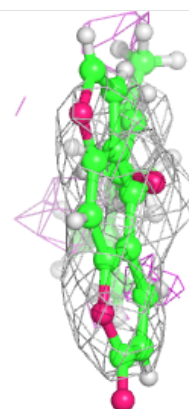
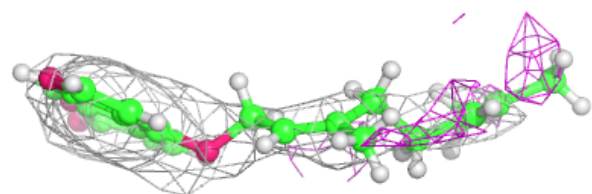
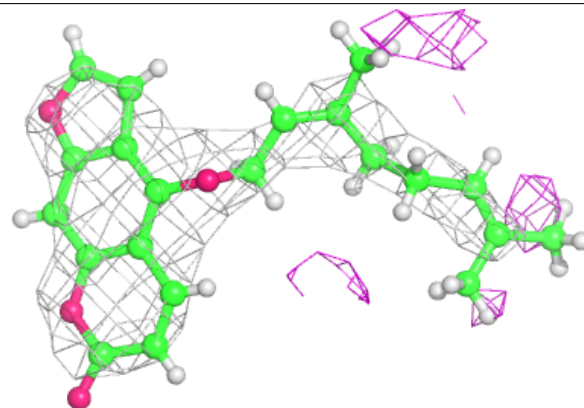


Electron density around HJJ D 602:

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

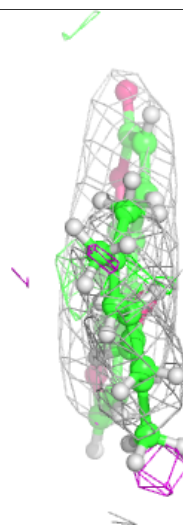
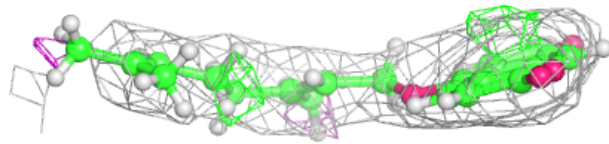
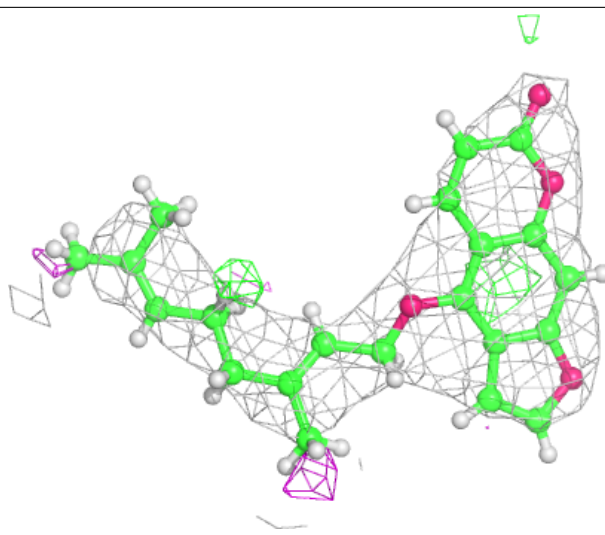
**Electron density around HJJ C 602:**

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



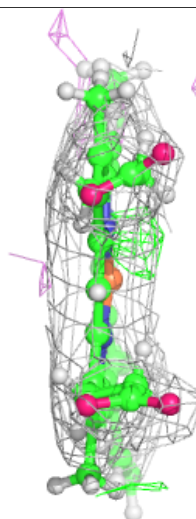
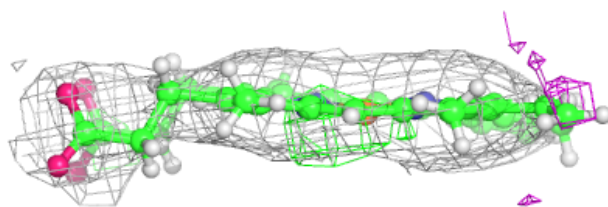
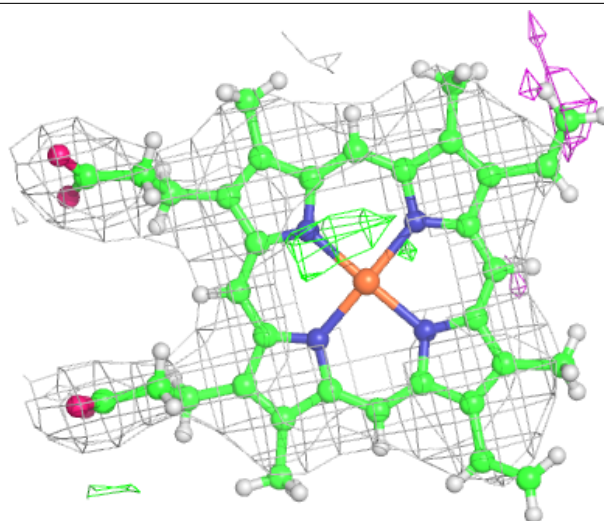
Electron density around HJJ A 602:

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



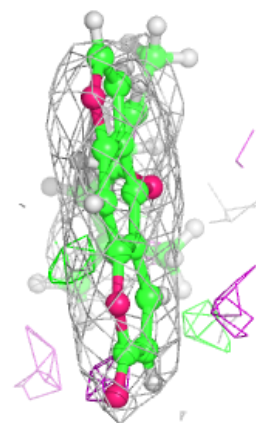
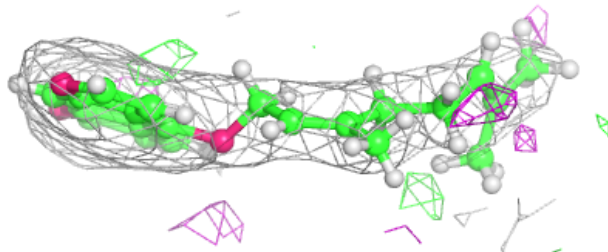
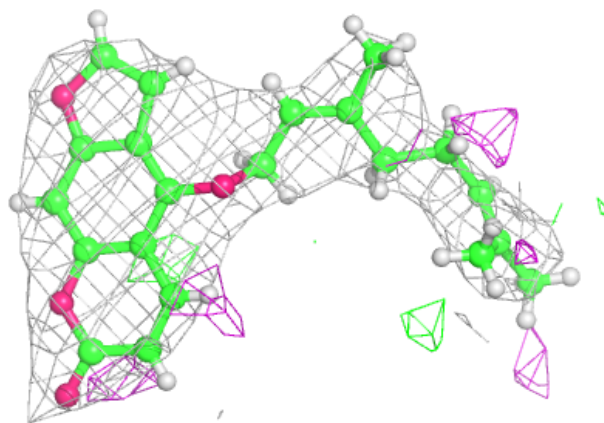
Electron density around HEM D 601:

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



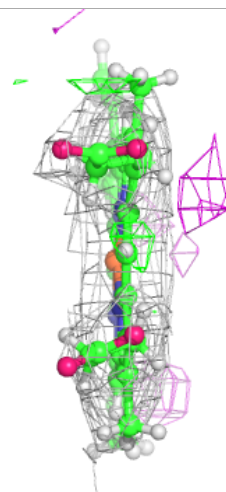
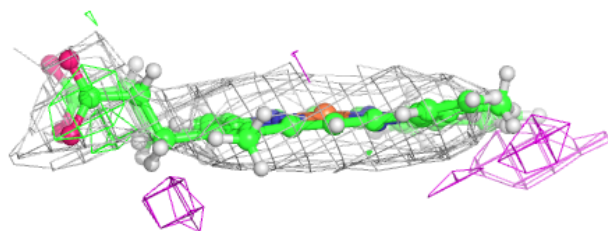
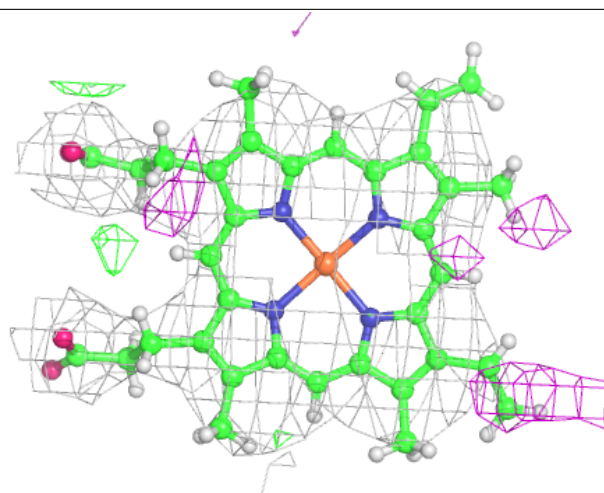
Electron density around HJJ B 602:

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



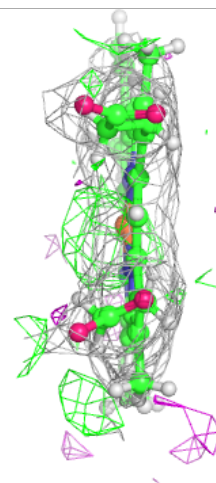
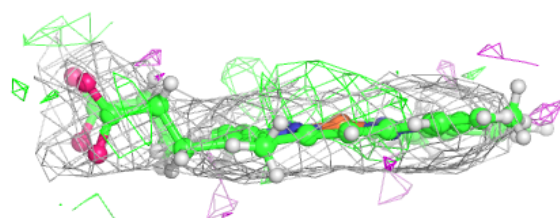
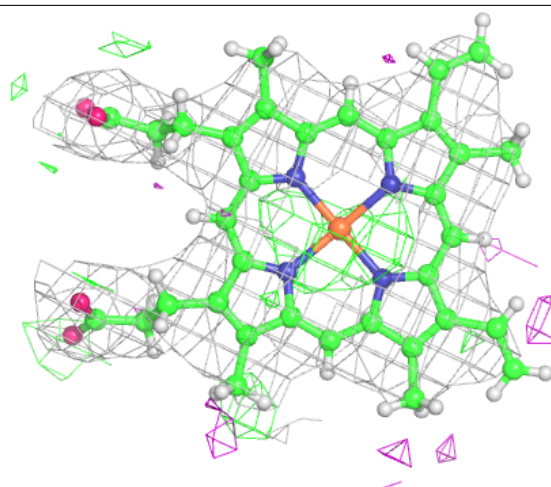
Electron density around HEM C 601:

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



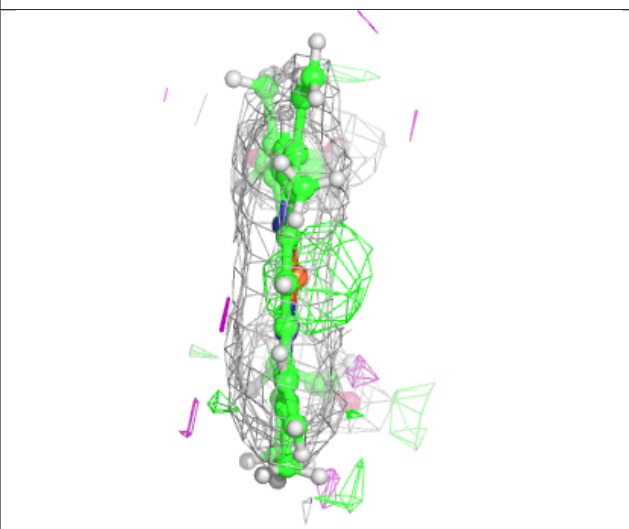
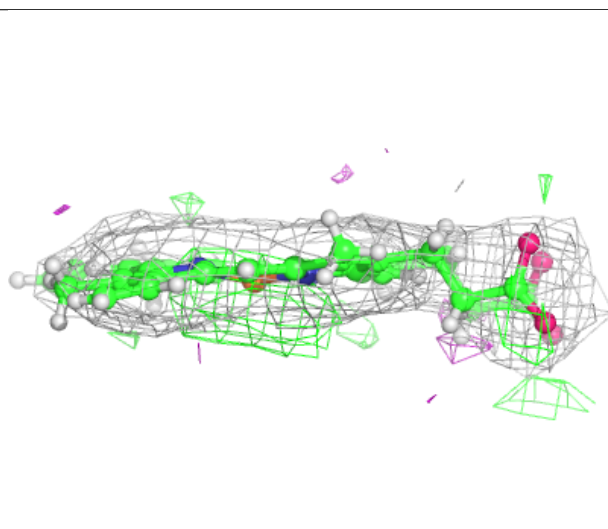
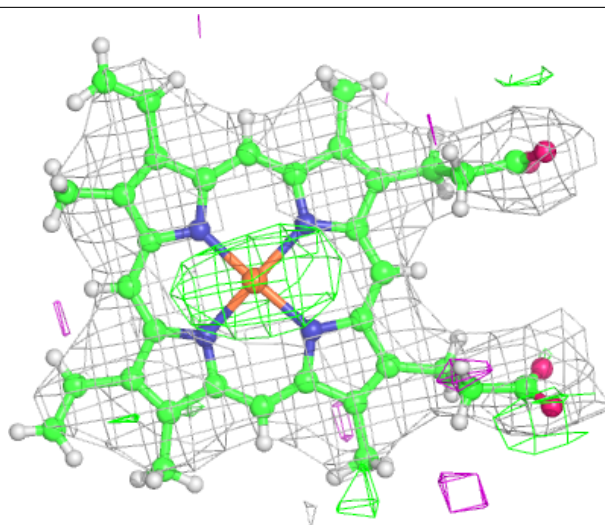
Electron density around HEM B 601:

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



Electron density around HEM A 601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.