



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 03:01 PM BST

PDB ID : 4I8V
Title : Human Cytochrome P450 1A1 in complex with alpha-naphthoflavone
Authors : Walsh, A.A.; Scott, E.E.
Deposited on : 2012-12-04
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.13.1
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) : 2.13.1

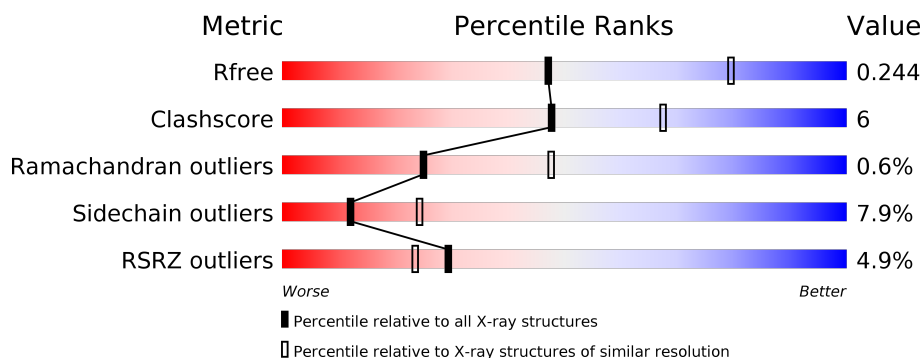
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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 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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 85%, yellow 85%, yellow 96%, orange 96%, orange 99%, grey 99%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 85% 11% • • </div> </div>
1	B	491	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, green 2%, green 78%, yellow 78%, yellow 94%, orange 94%, orange 97%, grey 97%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 78% 16% • • </div> </div>
1	C	491	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 8%, green 8%, green 69%, yellow 69%, yellow 92%, orange 92%, orange 97%, grey 97%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 8% 69% 23% • 5% </div> </div>
1	D	491	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 8%, green 8%, green 77%, yellow 77%, yellow 93%, orange 93%, orange 97%, grey 97%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 8% 77% 16% • 5% </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15532 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome P450 1A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3816	2442	664	689	21			
1	B	472	Total	C	N	O	S	0	0	0
			3776	2420	657	678	21			
1	C	468	Total	C	N	O	S	0	0	0
			3750	2404	652	673	21			
1	D	467	Total	C	N	O	S	0	0	0
			3741	2398	650	672	21			

There are 52 discrepancies between the modelled and reference sequences:

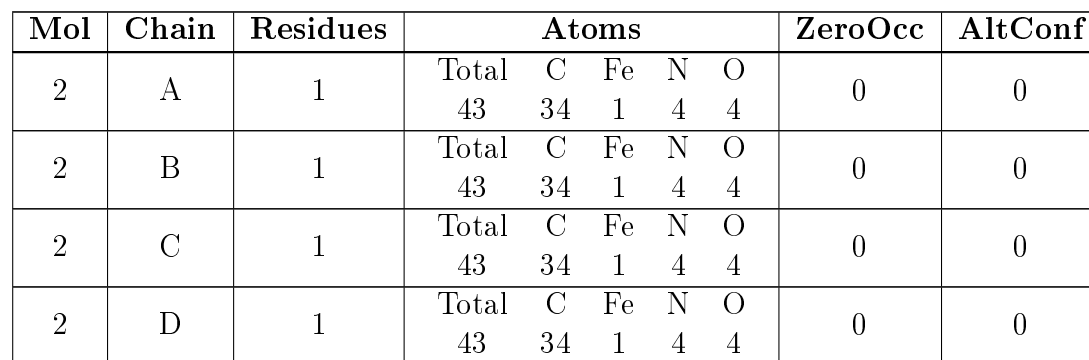
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	EXPRESSION TAG	UNP P04798
A	29	ALA	-	EXPRESSION TAG	UNP P04798
A	30	LYS	-	EXPRESSION TAG	UNP P04798
A	31	LYS	-	EXPRESSION TAG	UNP P04798
A	32	THR	-	EXPRESSION TAG	UNP P04798
A	33	SER	-	EXPRESSION TAG	UNP P04798
A	34	SER	-	EXPRESSION TAG	UNP P04798
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

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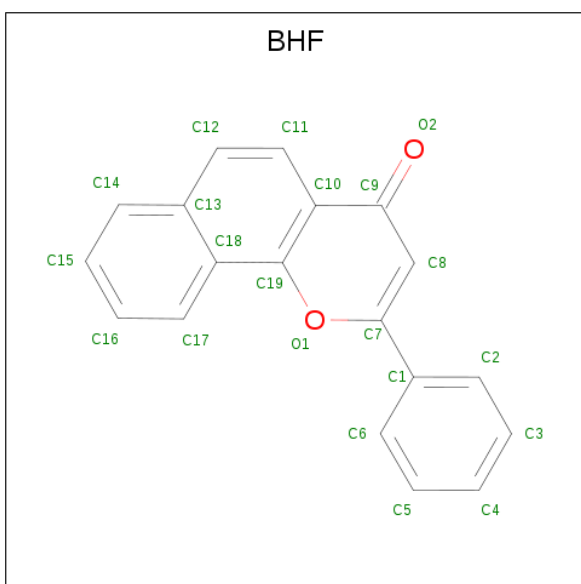
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Chain	Residue	Modelled	Actual	Comment	Reference
B	514	HIS	-	EXPRESSION TAG	UNP P04798
B	515	HIS	-	EXPRESSION TAG	UNP P04798
B	516	HIS	-	EXPRESSION TAG	UNP P04798
B	517	HIS	-	EXPRESSION TAG	UNP P04798
B	518	HIS	-	EXPRESSION TAG	UNP P04798
C	28	MET	-	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: $C_{34}H_{32}FeN_4O_4$).

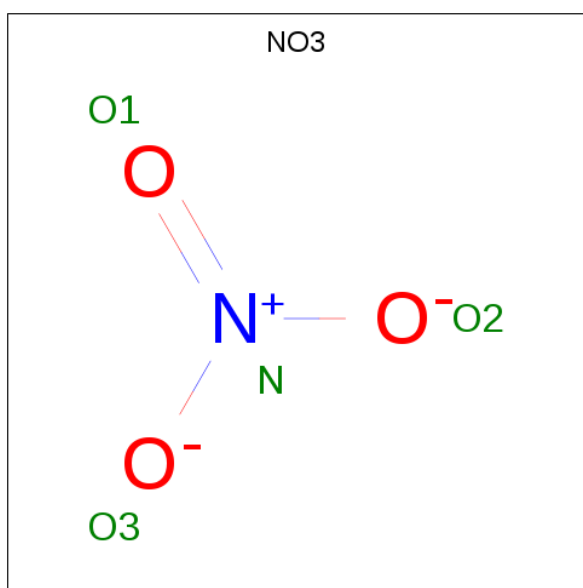


- Molecule 3 is 2-PHENYL-4H-BENZO[H]CHROMEN-4-ONE (three-letter code: BHF) (formula: C₁₉H₁₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	19	2		
3	B	1	Total	C	O	0	0
			21	19	2		
3	C	1	Total	C	O	0	0
			21	19	2		
3	D	1	Total	C	O	0	0
			21	19	2		

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		
4	A	1	Total	N	O	0	0
			4	1	3		
4	B	1	Total	N	O	0	0
			4	1	3		

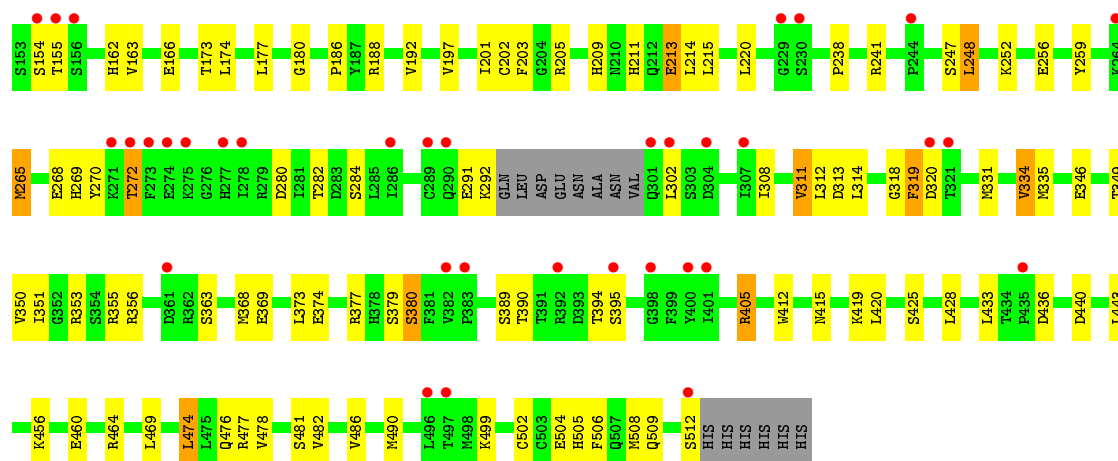
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total	O	0	0
			87	87		
5	B	76	Total	O	0	0
			76	76		
5	C	10	Total	O	0	0
			10	10		

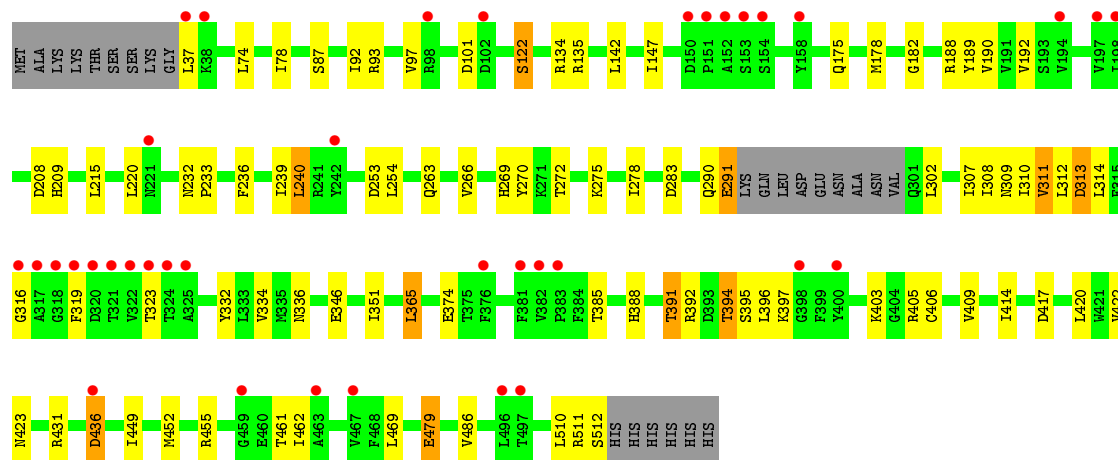
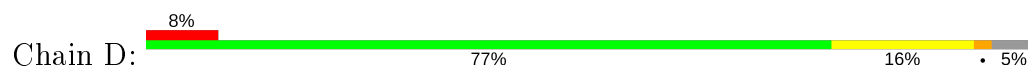
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	8	Total	O	0	0
			8	8		



• 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	65.00Å 195.49Å 235.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.24 – 2.60 38.21 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.24-2.60) 99.9 (38.21-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7	Depositor
R, R_{free}	0.188 , 0.244 0.193 , 0.244	Depositor DCC
R_{free} test set	4687 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15532	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: HEM, NO3, BHF

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	0.83	0/3911	0.91	5/5300 (0.1%)
1	B	0.77	1/3870 (0.0%)	0.86	5/5241 (0.1%)
1	C	0.57	1/3844 (0.0%)	0.72	0/5207
1	D	0.58	0/3835	0.76	1/5196 (0.0%)
All	All	0.70	2/15460 (0.0%)	0.81	11/20944 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	44	TRP	CB-CG	5.97	1.60	1.50
1	B	42	GLY	C-O	-5.28	1.15	1.23

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	313	ASP	CB-CG-OD2	5.85	123.57	118.30
1	B	431	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	93	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	77	ARG	NE-CZ-NH2	-5.46	117.57	120.30

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	3816	0	3809	28	0
1	B	3776	0	3780	43	0
1	C	3750	0	3750	64	0
1	D	3741	0	3737	43	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0
2	C	43	0	30	3	0
2	D	43	0	30	5	0
3	A	21	0	12	0	0
3	B	21	0	12	0	0
3	C	21	0	12	0	0
3	D	21	0	12	1	0
4	A	8	0	0	0	0
4	B	4	0	0	0	0
5	A	87	0	0	3	0
5	B	76	0	0	5	0
5	C	10	0	0	1	0
5	D	8	0	0	0	0
All	All	15532	0	15244	188	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 188 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:177:LEU:O	1:B:181:PRO:HD2	1.71	0.89
1:A:308:ILE:O	1:A:311:VAL:HG22	1.79	0.83
1:C:105:GLY:HA2	1:C:127:SER:OG	1.87	0.75
1:D:346:GLU:HG2	1:D:365:LEU:HD12	1.70	0.74
1:D:92:ILE:HD12	1:D:414:ILE:HD11	1.70	0.72

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	475/491 (97%)	453 (95%)	22 (5%)	0	100	100
1	B	468/491 (95%)	447 (96%)	16 (3%)	5 (1%)	14	30
1	C	464/491 (94%)	426 (92%)	34 (7%)	4 (1%)	17	35
1	D	463/491 (94%)	426 (92%)	35 (8%)	2 (0%)	34	57
All	All	1870/1964 (95%)	1752 (94%)	107 (6%)	11 (1%)	25	47

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	354	SER
1	B	209	HIS
1	C	180	GLY
1	C	291	GLU
1	D	275	LYS

5.3.2 Protein sidechains ⓘ

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	426/439 (97%)	401 (94%)	25 (6%)	19	39
1	B	422/439 (96%)	388 (92%)	34 (8%)	11	23
1	C	419/439 (95%)	376 (90%)	43 (10%)	7	13
1	D	418/439 (95%)	387 (93%)	31 (7%)	13	28
All	All	1685/1756 (96%)	1552 (92%)	133 (8%)	12	24

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	77	ARG
1	C	247	SER

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Mol	Chain	Res	Type
1	D	365	LEU
1	C	80	SER
1	C	143	LYS

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

Mol	Chain	Res	Type
1	C	209	HIS
1	C	344	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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$
4	NO3	A	604	-	1,3,3	1.28	0	0,3,3	0.00	-
2	HEM	C	600	1	27,50,50	0.98	1 (3%)	17,82,82	1.51	1 (5%)
3	BHF	C	601	-	22,24,24	2.02	5 (22%)	27,34,34	1.97	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	601	1	27,50,50	1.32	3 (11%)	17,82,82	1.50	3 (17%)
2	HEM	D	600	1	27,50,50	1.36	5 (18%)	17,82,82	1.25	2 (11%)
4	NO3	A	603	-	1,3,3	0.12	0	0,3,3	0.00	-
4	NO3	B	603	-	1,3,3	1.02	0	0,3,3	0.00	-
3	BHF	D	601	-	22,24,24	1.95	5 (22%)	27,34,34	2.02	8 (29%)
2	HEM	B	601	1	27,50,50	1.25	4 (14%)	17,82,82	1.43	2 (11%)
3	BHF	B	602	-	22,24,24	1.96	7 (31%)	27,34,34	2.88	14 (51%)
3	BHF	A	602	-	22,24,24	1.85	6 (27%)	27,34,34	2.74	11 (40%)

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	BHF	C	601	-	-	0/4/4/4	0/4/4/4
2	HEM	A	601	1	-	0/6/54/54	-
2	HEM	D	600	1	-	0/6/54/54	-
2	HEM	C	600	1	-	2/6/54/54	-
3	BHF	D	601	-	-	0/4/4/4	0/4/4/4
2	HEM	B	601	1	-	0/6/54/54	-
3	BHF	B	602	-	-	0/4/4/4	0/4/4/4
3	BHF	A	602	-	-	0/4/4/4	0/4/4/4

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	BHF	C10-C19	5.90	1.49	1.41
3	C	601	BHF	C10-C19	5.72	1.49	1.41
3	D	601	BHF	C10-C19	5.10	1.48	1.41
3	A	602	BHF	C10-C19	3.98	1.47	1.41
3	A	602	BHF	C8-C7	3.97	1.45	1.36

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	BHF	C13-C18-C19	-7.61	114.88	119.31
3	A	602	BHF	C17-C18-C19	-6.25	117.72	122.59
3	B	602	BHF	C8-C9-C10	-5.45	117.01	123.05
3	C	601	BHF	C8-C9-C10	-5.26	117.22	123.05
3	B	602	BHF	C18-C19-C10	4.89	122.75	120.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

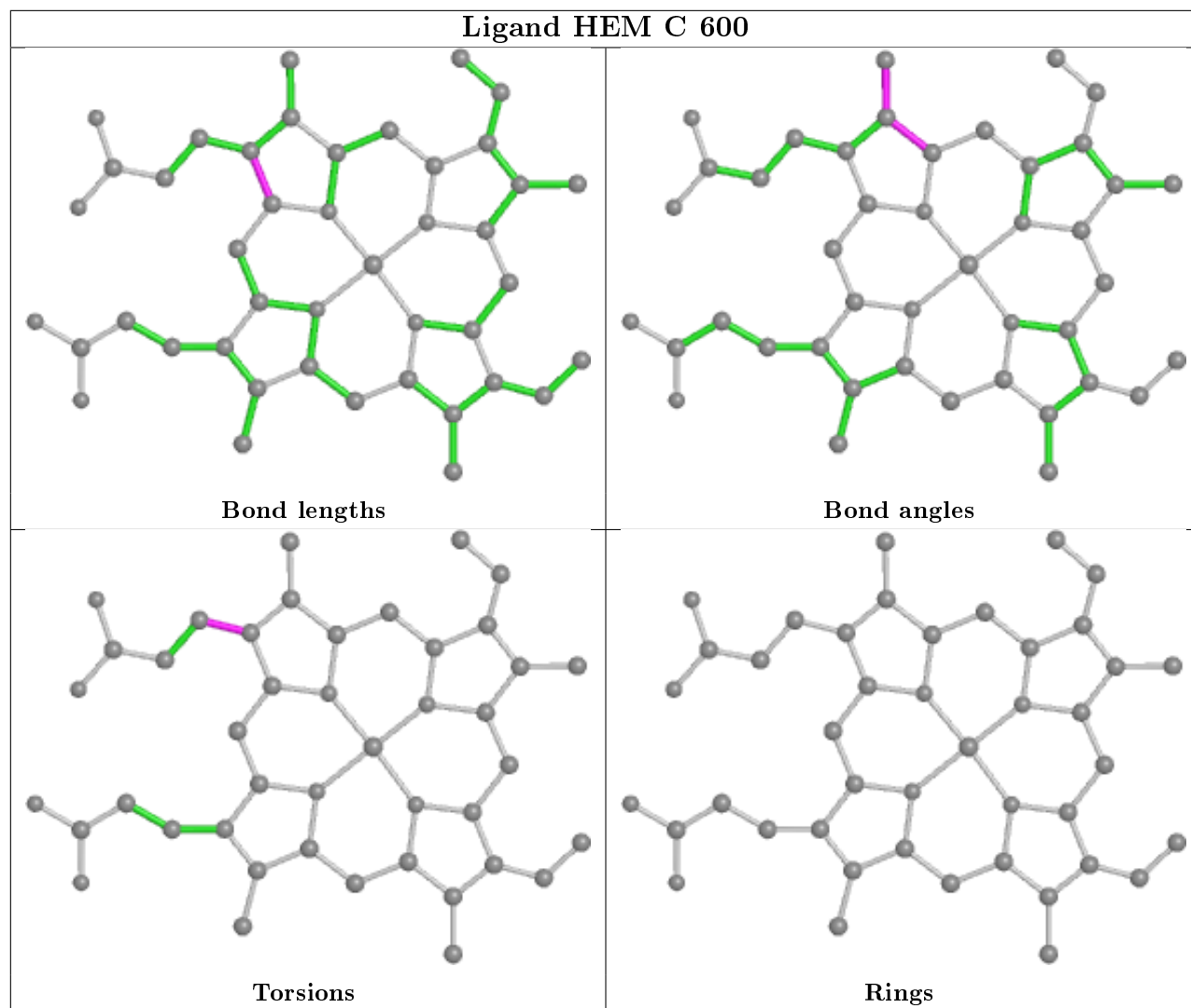
Mol	Chain	Res	Type	Atoms
2	C	600	HEM	C2D-C3D-CAD-CBD
2	C	600	HEM	C4D-C3D-CAD-CBD

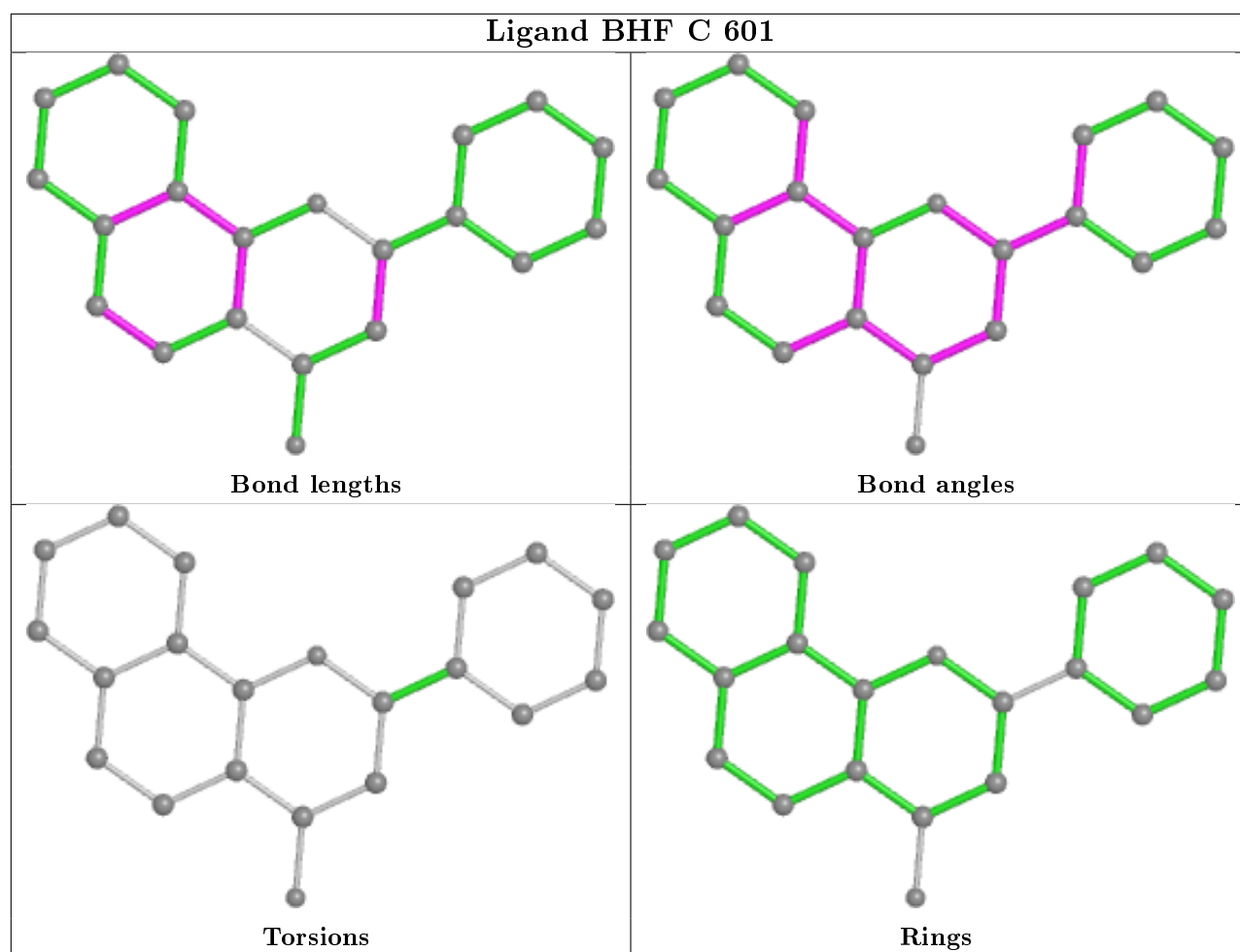
There are no ring outliers.

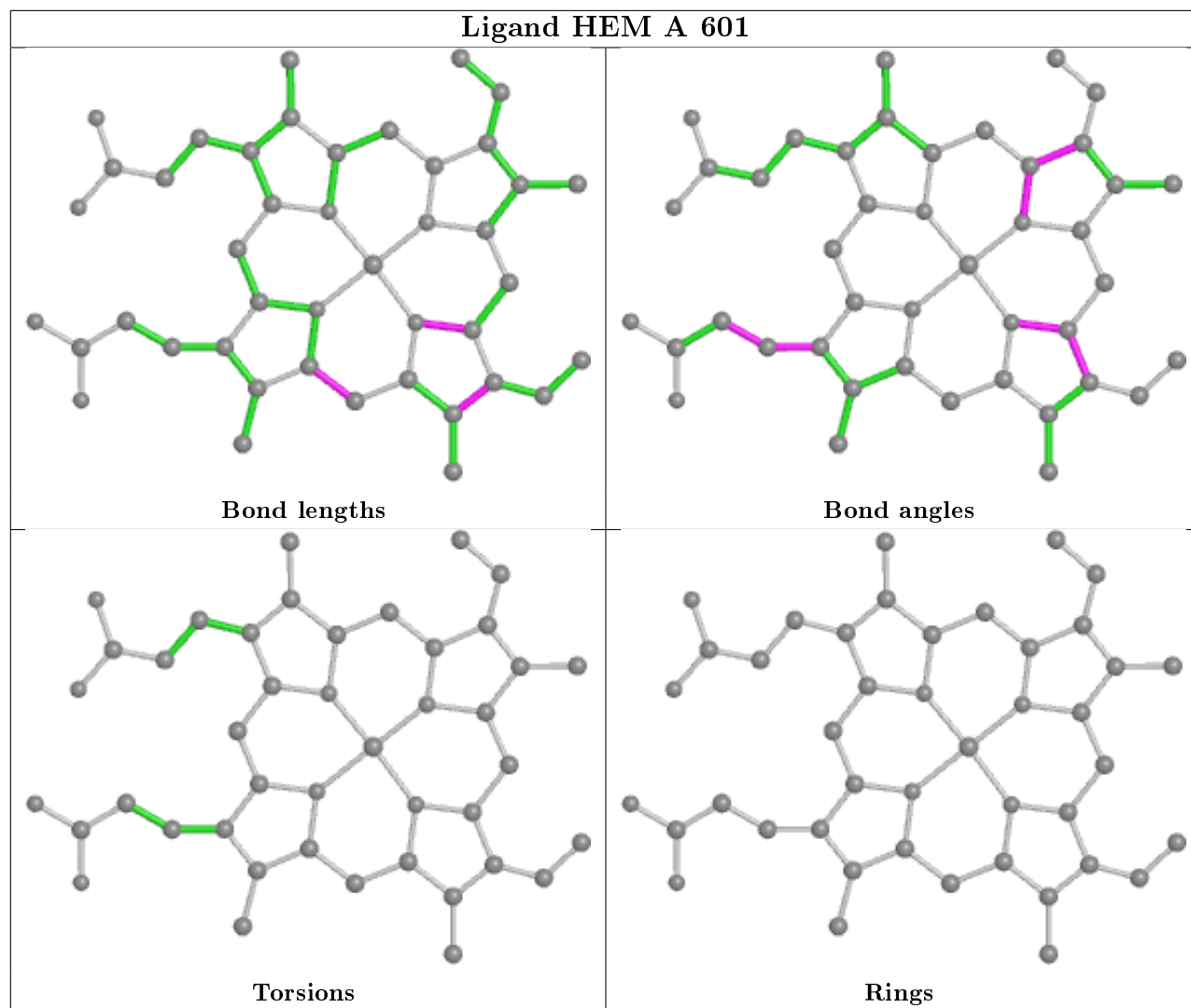
5 monomers are involved in 19 short contacts:

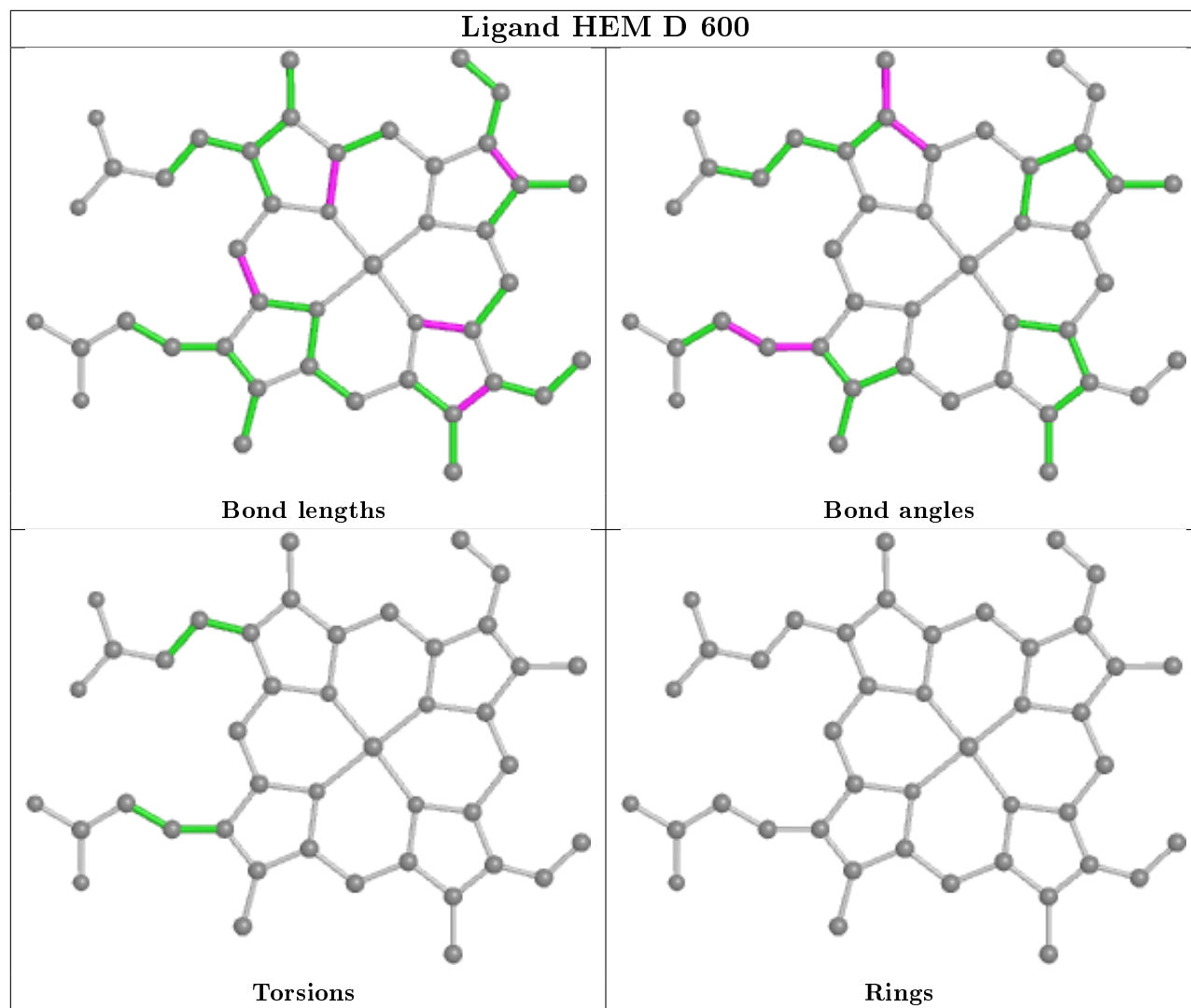
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	600	HEM	3	0
2	A	601	HEM	6	0
2	D	600	HEM	5	0
3	D	601	BHF	1	0
2	B	601	HEM	4	0

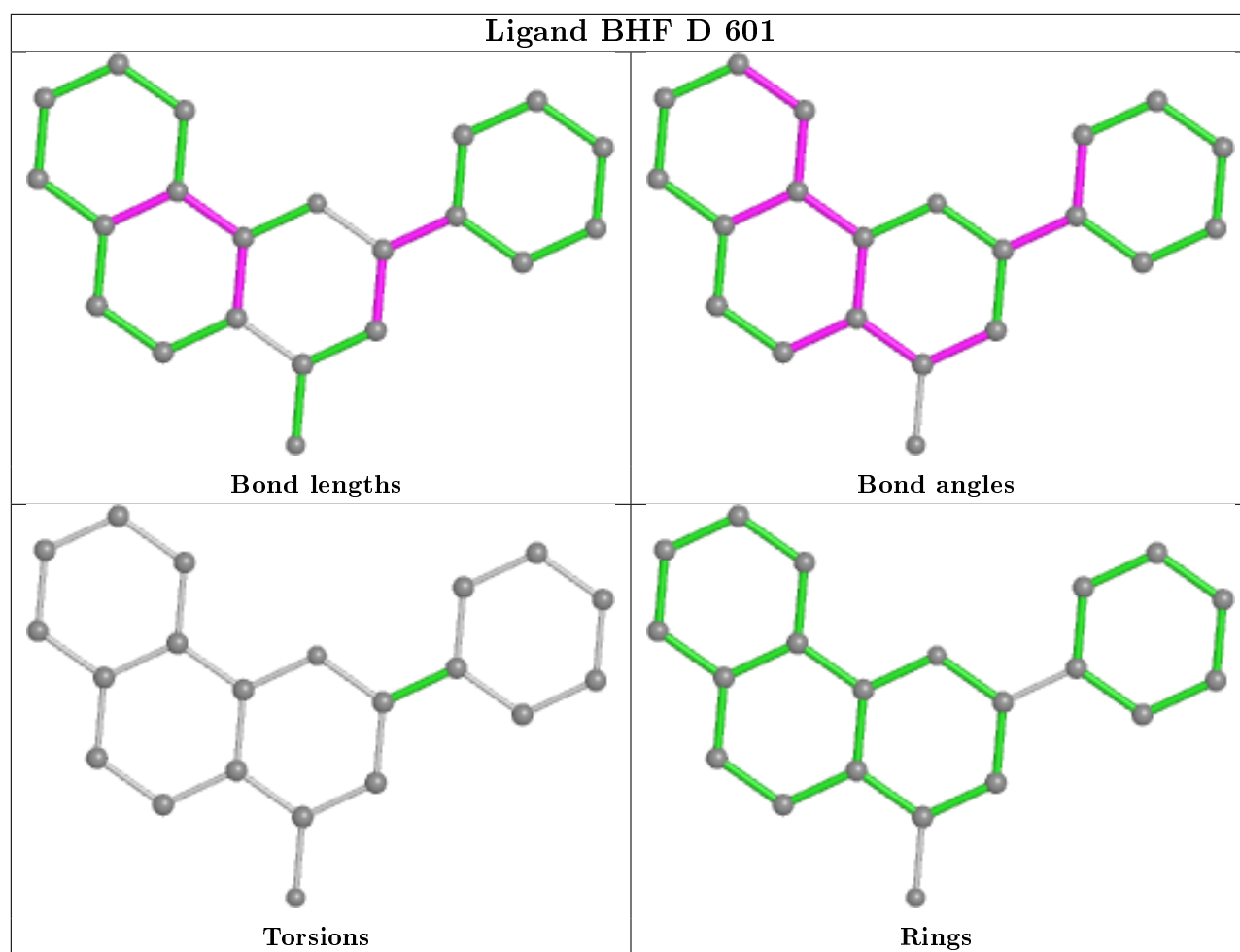
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

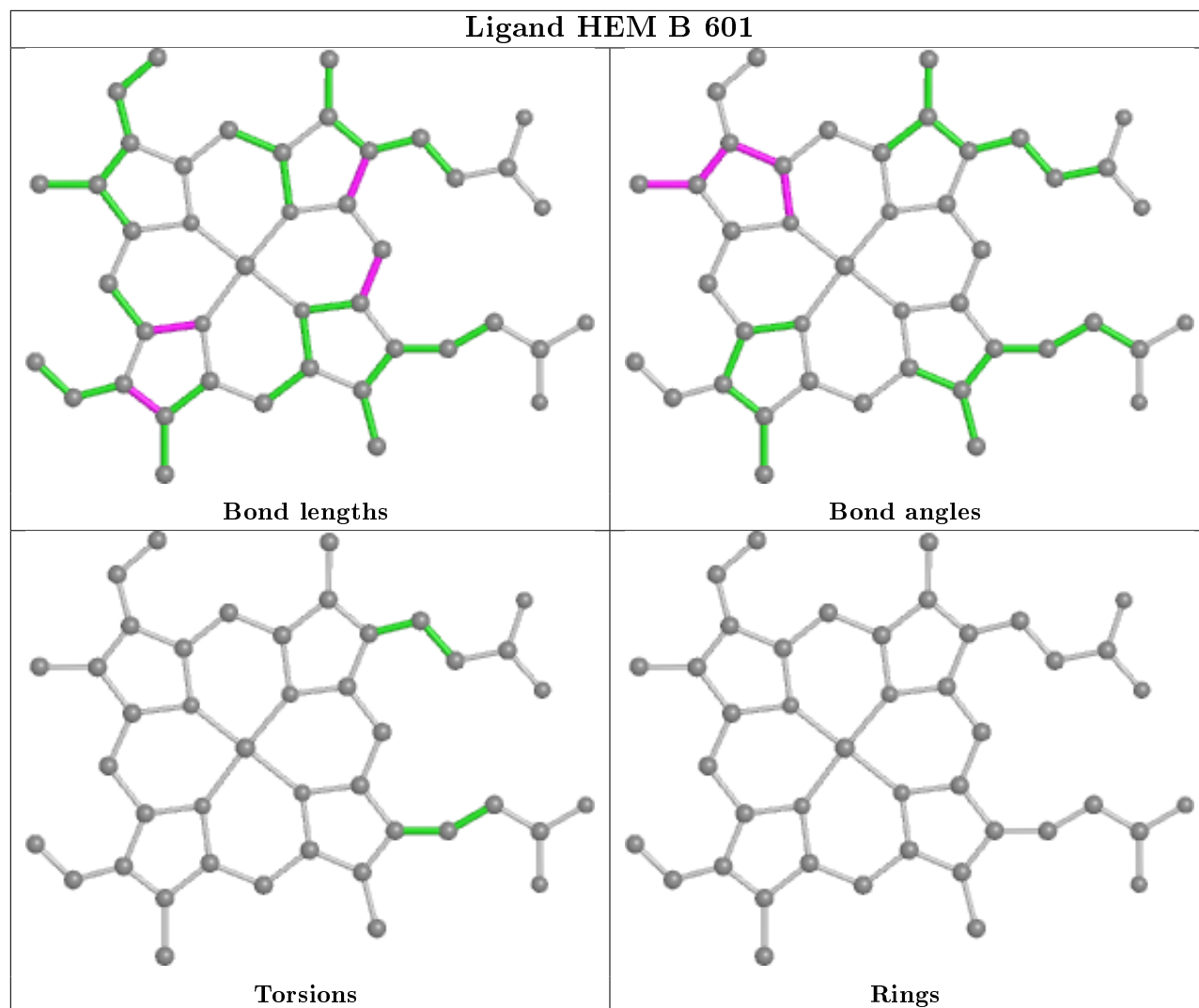


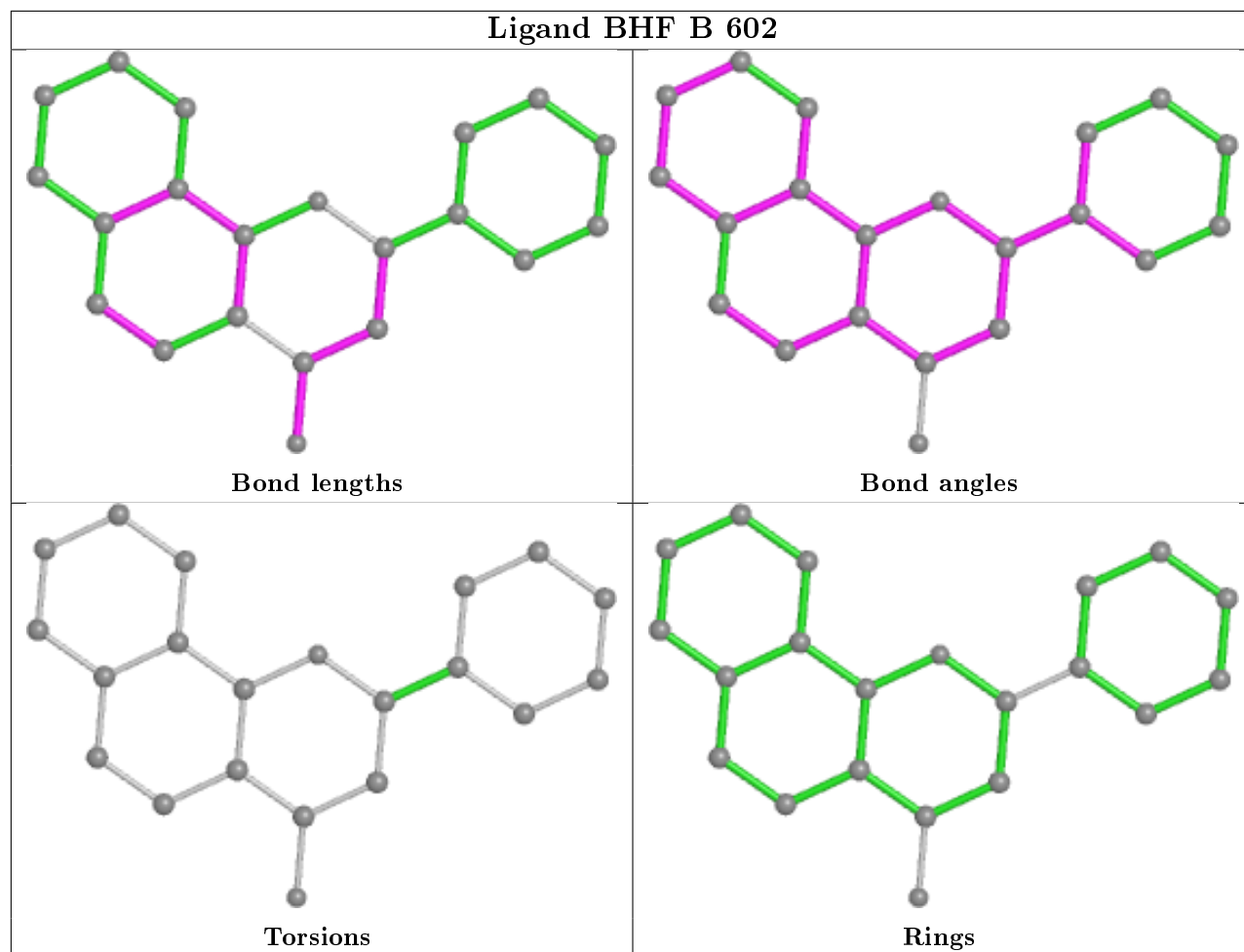


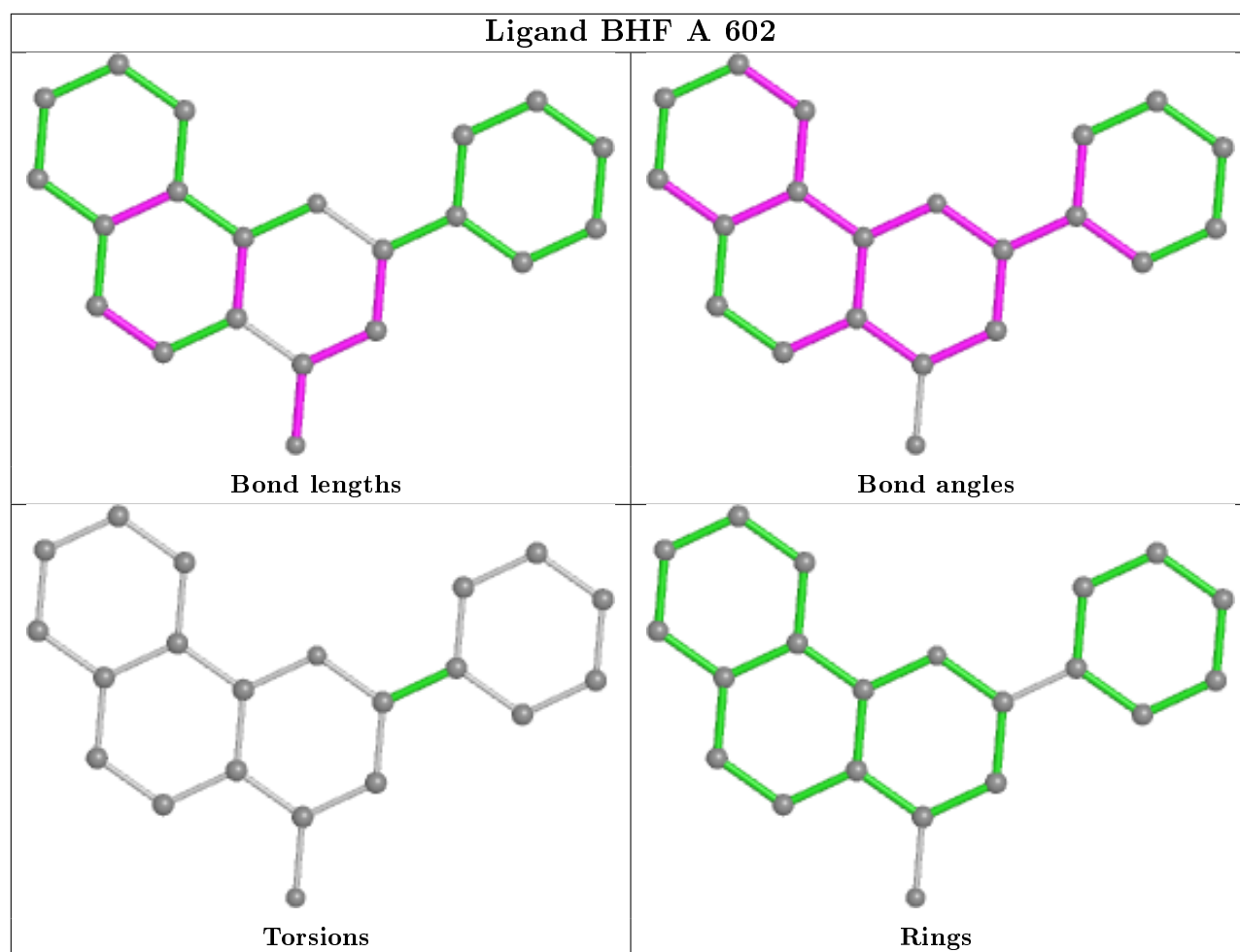












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	477/491 (97%)	-0.23	3 (0%) 89 88	31, 52, 91, 131	0
1	B	472/491 (96%)	-0.11	12 (2%) 57 51	35, 60, 100, 148	0
1	C	468/491 (95%)	0.32	41 (8%) 10 7	59, 90, 118, 146	0
1	D	467/491 (95%)	0.28	37 (7%) 12 9	51, 84, 117, 148	0
All	All	1884/1964 (95%)	0.06	93 (4%) 29 23	31, 73, 113, 148	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	GLY	6.4
1	B	301	GLN	6.1
1	C	273	PHE	5.2
1	C	302	LEU	4.7
1	D	317	ALA	4.4

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](#)

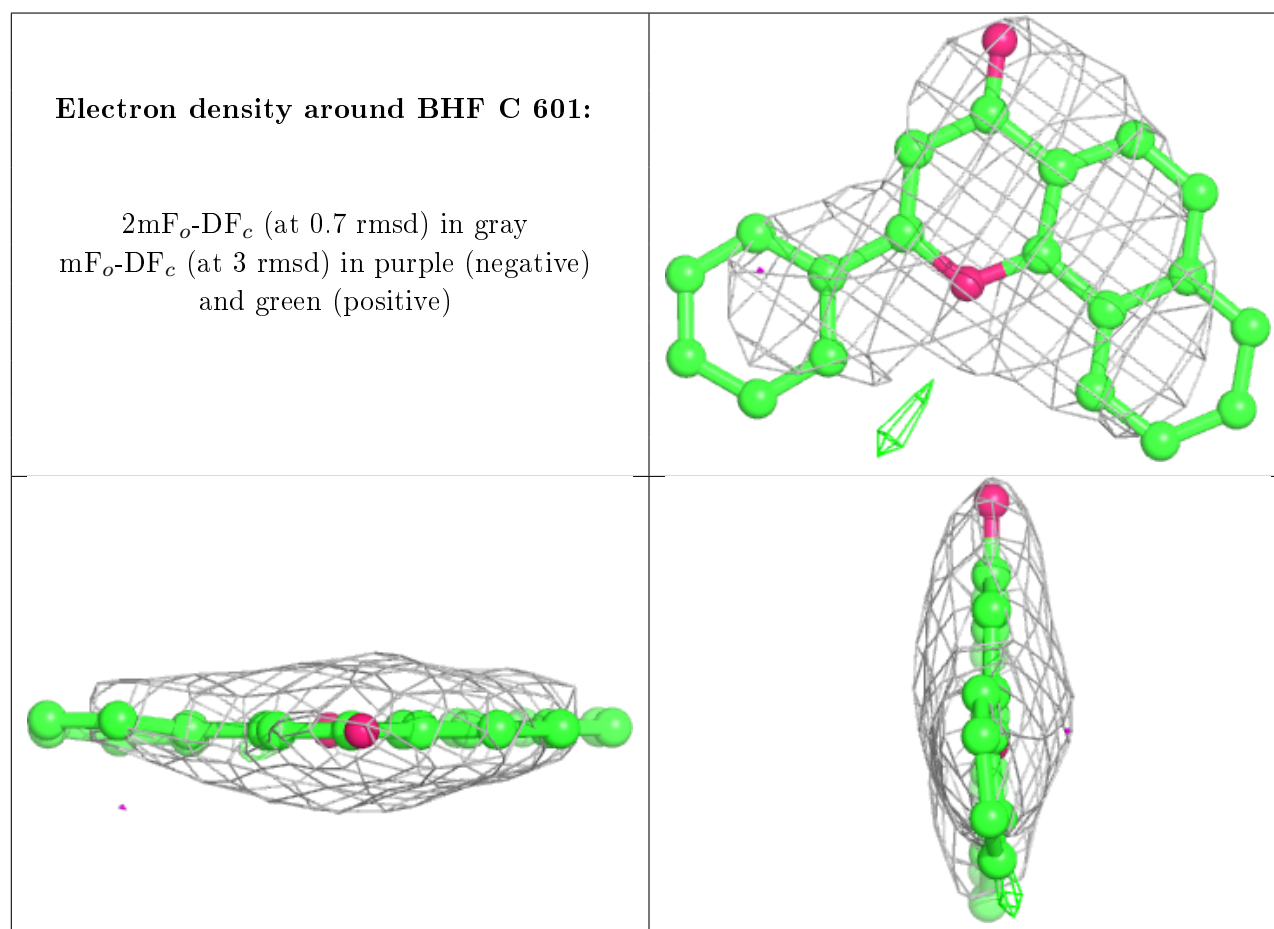
There are no monosaccharides in this entry.

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.

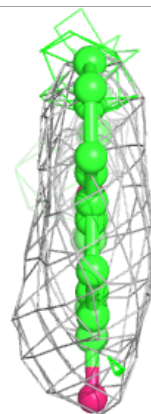
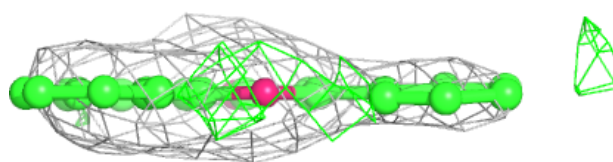
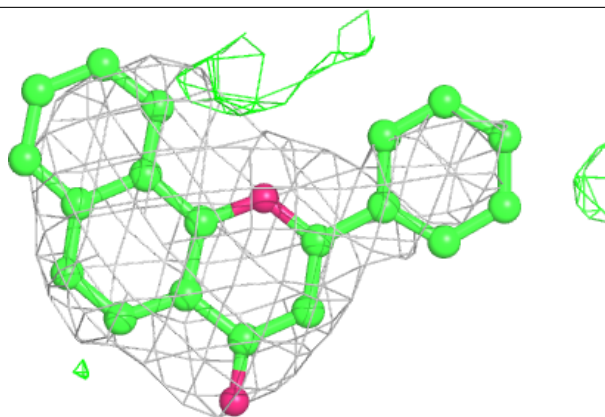
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NO3	A	603	4/4	0.61	0.38	103,103,111,118	0
4	NO3	A	604	4/4	0.63	0.22	64,66,70,101	0
4	NO3	B	603	4/4	0.72	0.28	51,68,73,86	0
3	BHF	C	601	21/21	0.88	0.30	88,104,120,122	0
3	BHF	D	601	21/21	0.89	0.47	94,106,115,121	0
3	BHF	A	602	21/21	0.91	0.29	43,55,72,81	0
3	BHF	B	602	21/21	0.92	0.22	58,62,67,79	0
2	HEM	D	600	43/43	0.97	0.28	40,53,73,80	0
2	HEM	C	600	43/43	0.98	0.21	43,56,80,103	0
2	HEM	B	601	43/43	0.98	0.23	36,46,54,60	0
2	HEM	A	601	43/43	0.99	0.23	32,38,44,52	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.



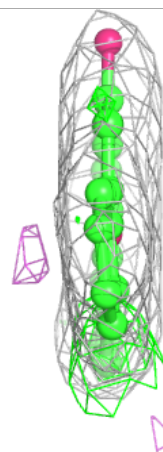
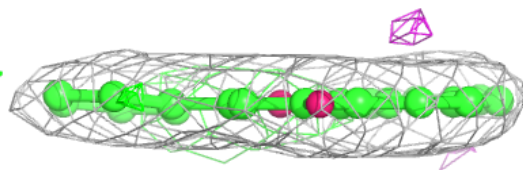
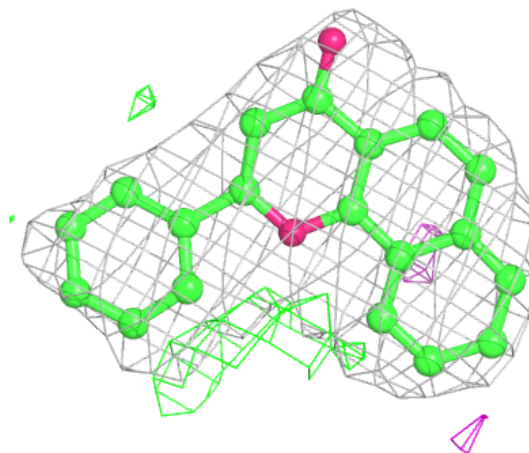
Electron density around BHF D 601:

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



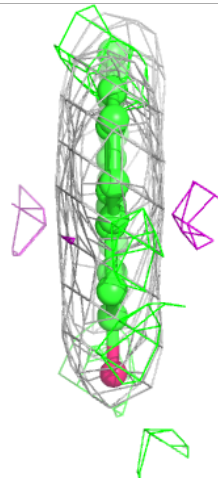
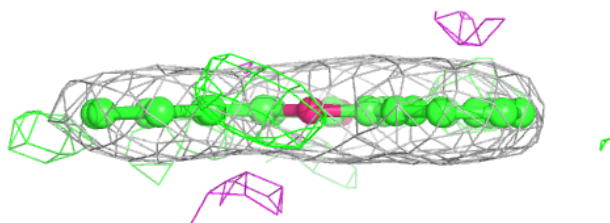
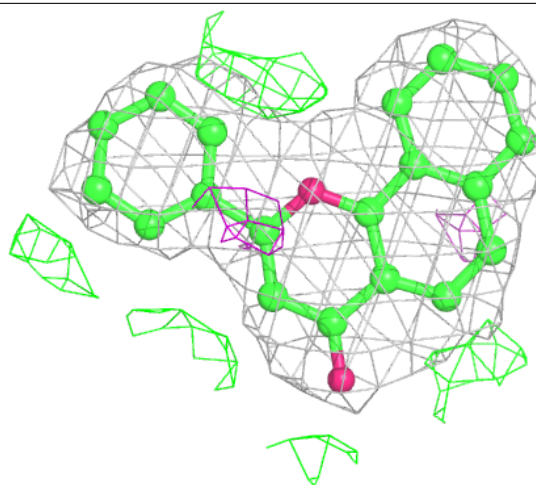
Electron density around BHF A 602:

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



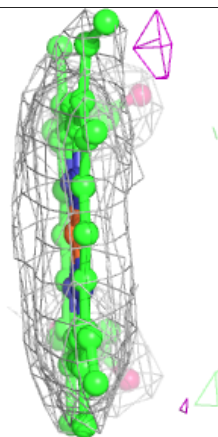
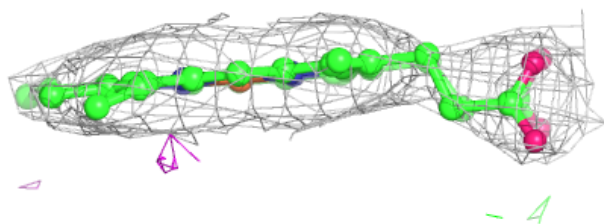
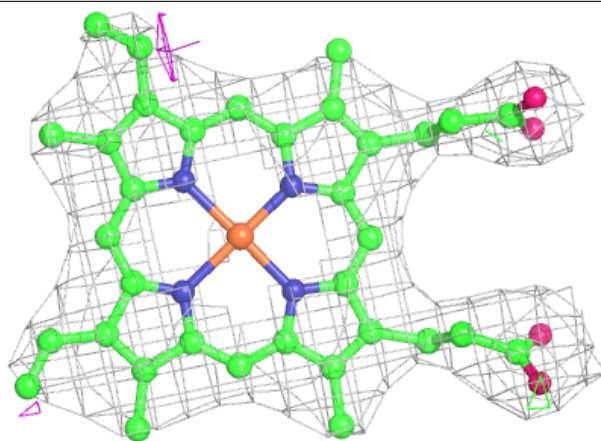
Electron density around BHF B 602:

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



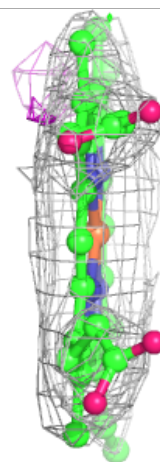
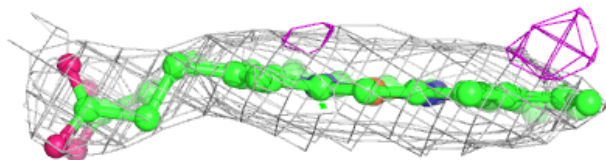
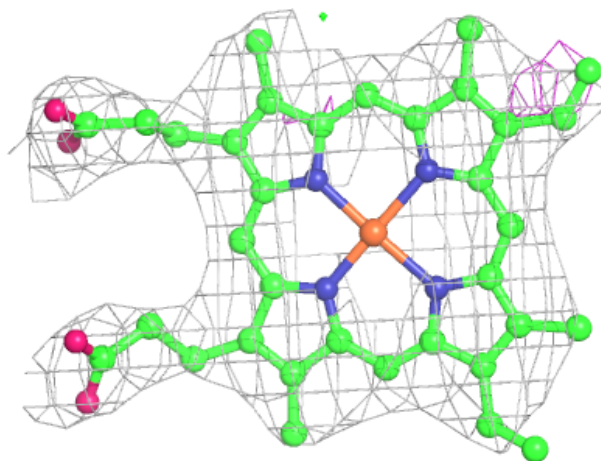
Electron density around HEM D 600:

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



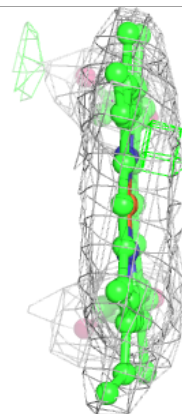
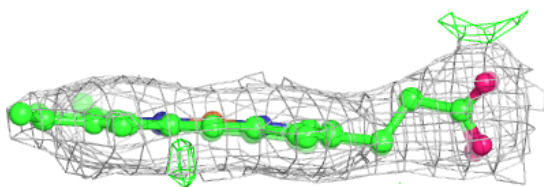
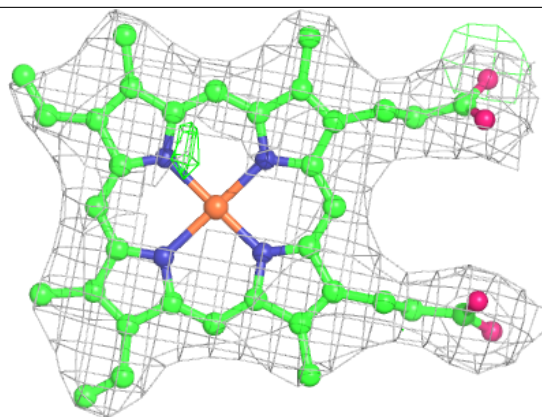
Electron density around HEM C 600:

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

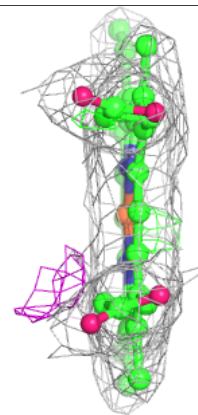
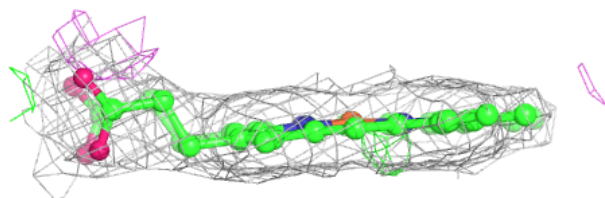
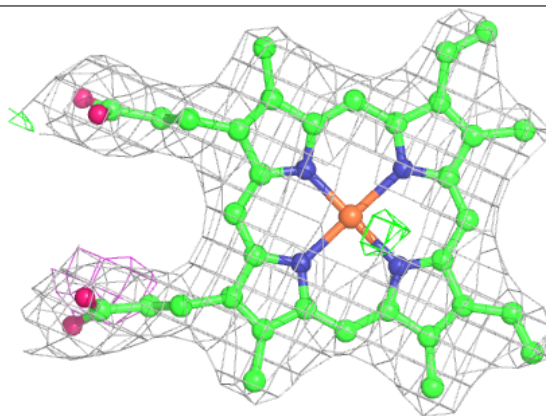


Electron density around HEM B 601:

$2mF_o-DF_c$ (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.