



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:41 am BST

PDB ID : 6OYU
Title : Structure of an ancestral-reconstructed cytochrome P450 1B1 with alpha-naphthoflavone
Authors : Bart, A.G.; Harris, K.L.; Scott, E.E.
Deposited on : 2019-05-15
Resolution : 2.95 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

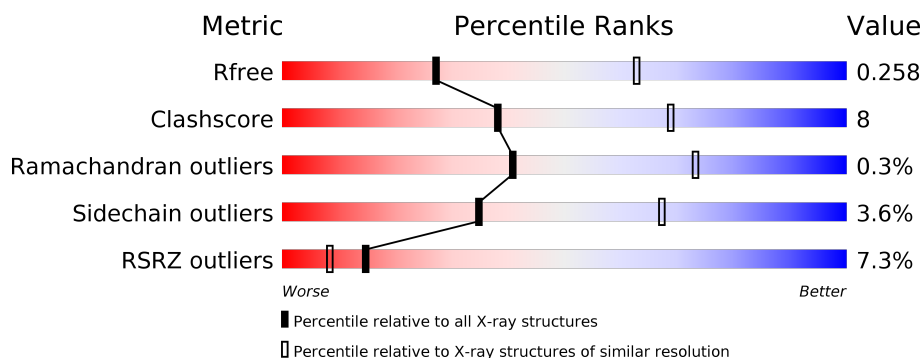
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	493	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>9%</div> </div> </div>
1	B	493	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>7%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BHF	A	603	-	-	X	-

2 Entry composition [i](#)

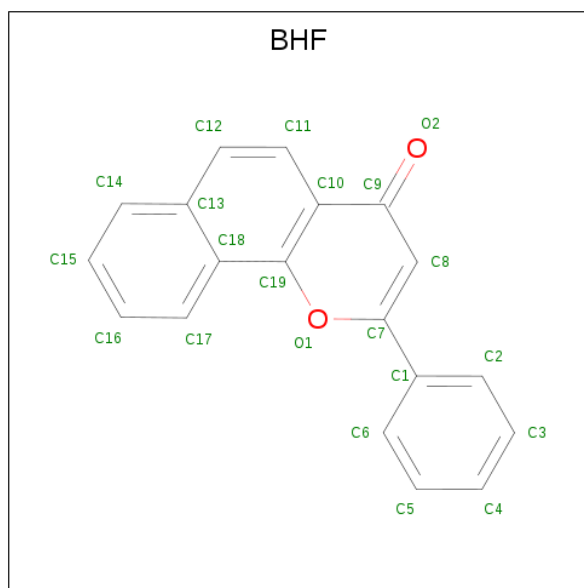
There are 5 unique types of molecules in this entry. The entry contains 14970 atoms, of which 7392 are hydrogens and 0 are deuteriums.

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 1B1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	450	Total	C	H	N	O	S	0	0	0
			7157	2295	3565	652	629	16			
1	B	459	Total	C	H	N	O	S	0	0	0
			7277	2333	3625	663	640	16			

- Molecule 2 is 2-PHENYL-4H-BENZO[H]CHROMEN-4-ONE (three-letter code: BHF) (formula: C₁₉H₁₂O₂) (labeled as "Ligand of Interest" by author).



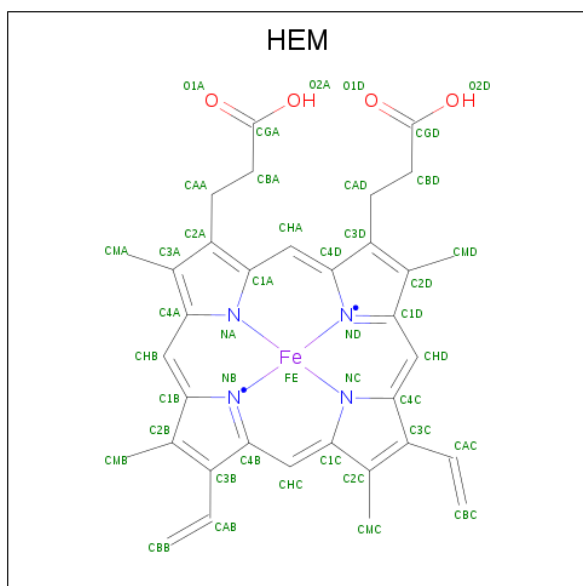
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			33	19	12	2		
2	A	1	Total	C	H	O	0	0
			33	19	12	2		
2	A	1	Total	C	H	O	0	0
			33	19	12	2		
2	A	1	Total	C	H	O	0	0
			33	19	12	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			33	19	12	2		
2	B	1	Total	C	H	O	0	0
			33	19	12	2		
2	B	1	Total	C	H	O	0	0
			33	19	12	2		
2	B	1	Total	C	H	O	0	0
			33	19	12	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	B	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			13	3	7	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			13	3	7	3		

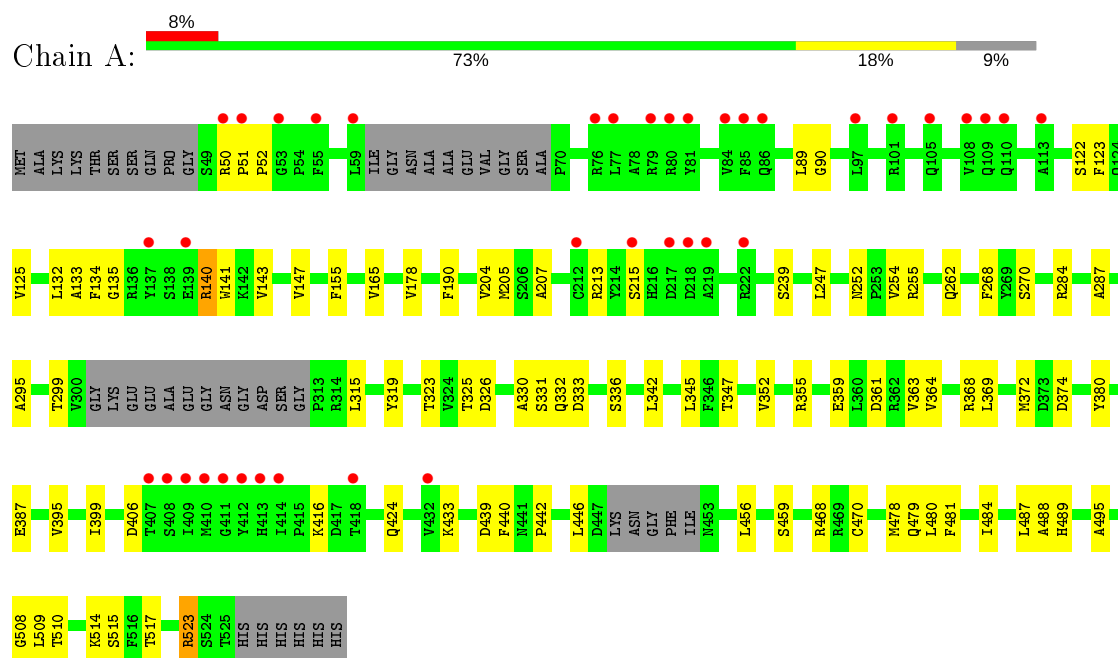
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	24	Total	O	0	0
			24	24		

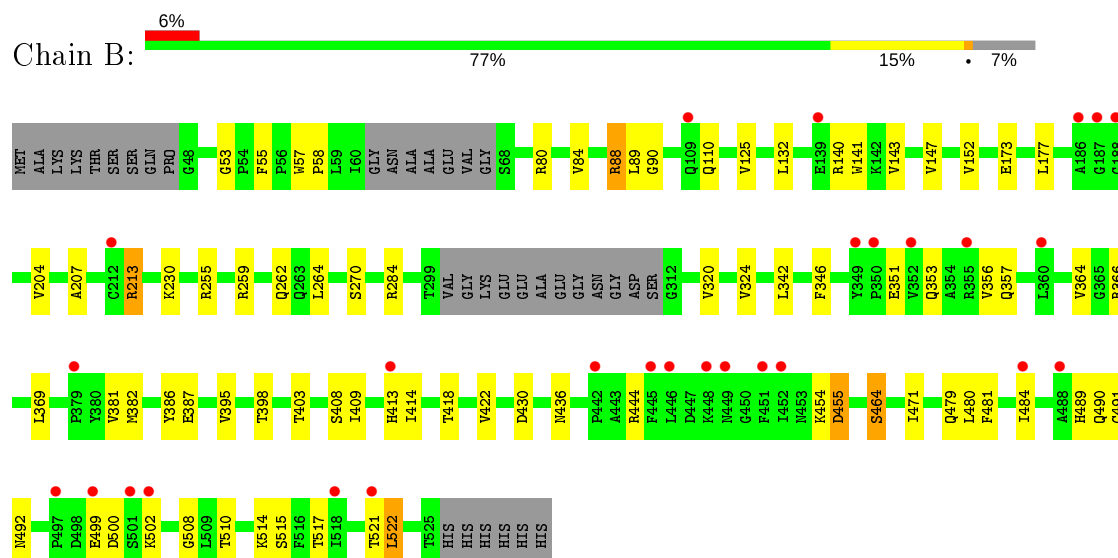
3 Residue-property plots [i](#)

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 1B1



• Molecule 1: Cytochrome P450 1B1



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	164.64 Å 164.64 Å 96.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.15 – 2.95 48.15 – 2.94	Depositor EDS
% Data completeness (in resolution range)	95.5 (48.15-2.95) 89.7 (48.15-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.96 Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472)	Depositor
R, R_{free}	0.199 , 0.258 0.199 , 0.258	Depositor DCC
R_{free} test set	1983 reflections (7.59%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14970	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, HEM, 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	0.26	0/3688	0.43	0/5003
1	B	0.29	0/3750	0.45	0/5088
All	All	0.28	0/7438	0.44	0/10091

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

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	3592	3565	3563	65	0
1	B	3652	3625	3622	41	0
2	A	84	48	48	17	0
2	B	84	48	48	0	0
3	A	43	30	30	7	0
3	B	43	30	30	4	0
4	A	12	15	16	1	0
4	B	24	31	32	0	0
5	A	20	0	0	2	0
5	B	24	0	0	0	0
All	All	7578	7392	7389	114	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (114) 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:399:ILE:HG12	2:A:602:BHF:C14	1.97	0.94
1:A:178:VAL:HG12	1:A:487:LEU:HD23	1.68	0.75
1:B:125:VAL:HG21	1:B:262:GLN:HG2	1.70	0.73
1:A:488:ALA:O	1:A:523:ARG:NH1	2.23	0.72
1:B:57:TRP:HE3	1:B:89:LEU:HD13	1.55	0.71
1:B:403:THR:OG1	1:B:418:THR:HG22	1.93	0.69
1:A:508:GLY:HA2	2:A:604:BHF:H16	1.76	0.67
3:B:605:HEM:HBB2	3:B:605:HEM:HMB2	1.78	0.65
1:A:122:SER:CB	2:A:603:BHF:H16	2.26	0.64
4:A:606:GOL:O3	4:A:606:GOL:O1	2.05	0.63
1:B:356:VAL:HG13	1:B:381:VAL:HG22	1.81	0.62
1:A:155:PHE:HE2	1:A:165:VAL:HG21	1.64	0.61
3:A:605:HEM:HBB2	3:A:605:HEM:HMB2	1.81	0.61
1:A:295:ALA:O	1:A:299:THR:HG23	2.02	0.60
1:A:508:GLY:O	1:A:510:THR:N	2.33	0.60
1:A:122:SER:HB3	2:A:603:BHF:C16	2.34	0.57
1:A:122:SER:HB3	2:A:603:BHF:H16	1.85	0.57
1:B:492:ASN:HB2	1:B:521:THR:OG1	2.05	0.57
1:A:125:VAL:HG21	1:A:262:GLN:HG2	1.87	0.56
1:A:399:ILE:CG1	2:A:602:BHF:C14	2.80	0.56
1:A:509:LEU:HA	2:A:603:BHF:C2	2.37	0.55
1:A:406:ASP:OD1	1:A:416:LYS:N	2.40	0.55
1:B:125:VAL:HG21	1:B:262:GLN:CG	2.37	0.54
1:A:89:LEU:HD11	2:A:604:BHF:H3	1.91	0.53
1:A:330:ALA:HB1	5:A:710:HOH:O	2.08	0.52
1:A:347:THR:HB	1:A:495:ALA:HB2	1.90	0.52
3:B:605:HEM:HBB2	3:B:605:HEM:CMB	2.39	0.52
1:A:122:SER:HB3	2:A:603:BHF:C15	2.40	0.52
1:B:414:ILE:CG2	1:B:418:THR:HG21	2.40	0.51
1:A:207:ALA:HB2	1:A:213:ARG:HB2	1.93	0.51
1:A:178:VAL:HG12	1:A:487:LEU:CD2	2.37	0.51
3:A:605:HEM:HBB2	3:A:605:HEM:CMB	2.40	0.51
1:B:395:VAL:HG11	3:B:605:HEM:HMA3	1.92	0.50
1:A:399:ILE:HG12	2:A:602:BHF:H14	1.89	0.50
1:A:204:VAL:HG11	1:A:479:GLN:OE1	2.10	0.50
1:A:247:LEU:O	1:A:252:ASN:ND2	2.45	0.50
1:B:173:GLU:O	1:B:177:LEU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PHE:CE2	1:A:165:VAL:HG21	2.46	0.49
1:A:319:TYR:O	1:A:323:THR:HG23	2.12	0.49
1:B:204:VAL:HG11	1:B:479:GLN:OE1	2.12	0.49
1:B:408:SER:HB3	1:B:413:HIS:HA	1.95	0.49
1:B:464:SER:HB2	3:B:605:HEM:HBA1	1.95	0.49
1:A:252:ASN:OD1	1:A:255:ARG:N	2.35	0.48
1:A:143:VAL:O	1:A:147:VAL:HG12	2.15	0.47
1:B:207:ALA:HB2	1:B:213:ARG:HB2	1.96	0.47
1:B:508:GLY:O	1:B:510:THR:N	2.47	0.47
1:A:123:PHE:HB3	1:A:134:PHE:HB3	1.96	0.47
3:A:605:HEM:HMC2	3:A:605:HEM:HBC2	1.97	0.47
1:B:110:GLN:NE2	1:B:408:SER:O	2.46	0.47
1:B:84:VAL:HG21	1:B:409:ILE:HD12	1.97	0.47
1:A:132:LEU:HD12	1:A:141:TRP:NE1	2.29	0.46
1:A:399:ILE:CG1	2:A:602:BHF:C15	2.93	0.46
1:A:205:MET:HG3	1:A:331:SER:OG	2.16	0.46
1:B:499:GLU:OE1	1:B:517:THR:OG1	2.25	0.46
1:A:395:VAL:HG11	3:A:605:HEM:HMA3	1.98	0.46
3:A:605:HEM:HBC2	3:A:605:HEM:CMC	2.46	0.46
1:A:380:TYR:HD1	1:A:446:LEU:HD11	1.82	0.45
2:A:603:BHF:O2	5:A:701:HOH:O	2.21	0.45
1:B:398:THR:CG2	1:B:422:VAL:HB	2.46	0.45
1:A:50:ARG:HB2	1:A:51:PRO:HD2	1.99	0.45
1:B:132:LEU:HD12	1:B:141:TRP:NE1	2.32	0.45
1:A:514:LYS:HE3	1:A:515:SER:OG	2.17	0.45
1:B:480:LEU:O	1:B:484:ILE:HG12	2.17	0.45
1:A:333:ASP:HB2	2:A:601:BHF:C3	2.46	0.45
1:B:140:ARG:HB2	1:B:140:ARG:NH1	2.33	0.44
1:B:489:HIS:ND1	1:B:490:GLN:OE1	2.47	0.44
1:A:135:GLY:O	1:A:468:ARG:NH2	2.50	0.44
1:A:315:LEU:HB3	1:A:319:TYR:CD2	2.52	0.44
1:A:395:VAL:O	1:A:424:GLN:NE2	2.50	0.44
1:A:122:SER:HB3	2:A:603:BHF:H15	1.98	0.44
1:B:353:GLN:O	1:B:357:GLN:HG3	2.17	0.44
1:B:490:GLN:O	1:B:522:LEU:HD23	2.18	0.44
1:B:88:ARG:NE	1:B:90:GLY:O	2.45	0.44
1:A:361:ASP:OD1	1:A:523:ARG:NH2	2.51	0.44
1:B:255:ARG:O	1:B:259:ARG:HG2	2.18	0.44
1:A:372:MET:HB3	1:A:478:MET:HE2	1.99	0.44
1:B:346:PHE:O	1:B:353:GLN:NE2	2.51	0.43
1:B:414:ILE:HG22	1:B:418:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:TRP:CE3	1:B:89:LEU:HD13	2.44	0.43
1:A:252:ASN:OD1	1:A:254:VAL:N	2.50	0.43
1:A:133:ALA:CB	2:A:601:BHF:H15	2.48	0.43
1:A:399:ILE:HG13	2:A:602:BHF:C15	2.49	0.43
1:A:342:LEU:HD13	1:A:484:ILE:HG21	2.01	0.43
1:A:352:VAL:HG11	1:A:442:PRO:HG2	1.99	0.43
1:A:456:LEU:O	1:A:459:SER:OG	2.36	0.43
1:A:345:LEU:HD13	1:A:440:PHE:CE1	2.54	0.42
1:A:395:VAL:HG21	3:A:605:HEM:HMB1	2.02	0.42
1:A:364:VAL:HG22	1:A:374:ASP:OD2	2.18	0.42
1:A:480:LEU:O	1:A:484:ILE:HG12	2.19	0.42
1:B:342:LEU:HD13	1:B:484:ILE:CG2	2.50	0.42
1:A:433:LYS:NZ	1:A:459:SER:HB2	2.35	0.42
1:B:369:LEU:N	1:B:369:LEU:HD12	2.35	0.42
1:A:140:ARG:HD3	1:A:140:ARG:H	1.85	0.41
1:B:364:VAL:O	1:B:364:VAL:HG12	2.20	0.41
1:A:268:PHE:CE2	1:A:325:THR:HG23	2.55	0.41
1:A:332:GLN:O	1:A:336:SER:OG	2.28	0.41
1:A:489:HIS:O	1:A:523:ARG:NH1	2.53	0.41
1:B:382:MET:O	1:B:386:TYR:N	2.49	0.41
1:A:326:ASP:OD1	2:A:601:BHF:H14	2.21	0.41
1:B:455:ASP:N	1:B:455:ASP:OD1	2.54	0.41
1:A:51:PRO:O	1:A:52:PRO:C	2.59	0.41
1:B:320:VAL:O	1:B:324:VAL:HG23	2.21	0.41
1:A:470:CYS:HB2	3:A:605:HEM:NA	2.34	0.41
1:A:284:ARG:HG3	1:A:287:ALA:HB2	2.03	0.40
1:A:369:LEU:HD12	1:A:369:LEU:N	2.36	0.40
1:B:230:LYS:HB2	1:B:264:LEU:HD11	2.02	0.40
1:B:57:TRP:CG	1:B:58:PRO:HA	2.57	0.40
1:A:359:GLU:O	1:A:363:VAL:HG23	2.21	0.40
1:A:190:PHE:HB3	1:A:517:THR:HB	2.03	0.40
1:B:491:CYS:HA	1:B:521:THR:O	2.22	0.40
1:A:342:LEU:HD13	1:A:484:ILE:CG2	2.52	0.40
1:B:143:VAL:O	1:B:147:VAL:HG23	2.22	0.40
1:B:152:VAL:HG21	1:B:471:ILE:HD12	2.03	0.40
1:B:436:ASN:O	1:B:444:ARG:NH2	2.48	0.40

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	442/493 (90%)	417 (94%)	24 (5%)	1 (0%)	47	79
1	B	453/493 (92%)	428 (94%)	23 (5%)	2 (0%)	34	69
All	All	895/986 (91%)	845 (94%)	47 (5%)	3 (0%)	41	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	464	SER
1	B	53	GLY
1	A	90	GLY

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	389/419 (93%)	379 (97%)	10 (3%)	46	75
1	B	394/419 (94%)	376 (95%)	18 (5%)	27	60
All	All	783/838 (93%)	755 (96%)	28 (4%)	35	67

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ARG
1	A	215	SER
1	A	239	SER

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Mol	Chain	Res	Type
1	A	270	SER
1	A	355	ARG
1	A	368	ARG
1	A	387	GLU
1	A	439	ASP
1	A	481	PHE
1	A	523	ARG
1	B	55	PHE
1	B	80	ARG
1	B	88	ARG
1	B	213	ARG
1	B	270	SER
1	B	284	ARG
1	B	351	GLU
1	B	366	ARG
1	B	387	GLU
1	B	430	ASP
1	B	454	LYS
1	B	455	ASP
1	B	481	PHE
1	B	500	ASP
1	B	502	LYS
1	B	514	LYS
1	B	515	SER
1	B	522	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	110	GLN
1	B	332	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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	GOL	B	606	-	5,5,5	0.78	0	5,5,5	0.92	0
2	BHF	B	602	-	22,24,24	1.19	2 (9%)	27,34,34	2.32	6 (22%)
2	BHF	A	602	-	22,24,24	1.94	3 (13%)	27,34,34	1.78	6 (22%)
4	GOL	B	607	-	5,5,5	0.85	0	5,5,5	1.00	0
2	BHF	B	603	-	22,24,24	1.21	2 (9%)	27,34,34	2.24	6 (22%)
2	BHF	A	601	-	22,24,24	1.94	3 (13%)	27,34,34	1.80	6 (22%)
3	HEM	A	605	1	27,50,50	1.85	4 (14%)	17,82,82	1.36	1 (5%)
2	BHF	A	604	-	22,24,24	1.94	3 (13%)	27,34,34	1.79	6 (22%)
4	GOL	A	606	-	5,5,5	0.74	0	5,5,5	0.90	0
2	BHF	B	604	-	22,24,24	1.18	2 (9%)	27,34,34	2.29	7 (25%)
4	GOL	B	609	-	5,5,5	0.84	0	5,5,5	1.00	0
4	GOL	A	607	-	5,5,5	0.84	0	5,5,5	0.97	0
2	BHF	B	601	-	22,24,24	1.20	2 (9%)	27,34,34	2.27	6 (22%)
2	BHF	A	603	-	22,24,24	1.94	3 (13%)	27,34,34	1.80	6 (22%)
3	HEM	B	605	1	27,50,50	1.84	4 (14%)	17,82,82	1.50	2 (11%)
4	GOL	B	608	-	5,5,5	0.77	0	5,5,5	0.91	0

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
4	GOL	B	606	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BHF	B	602	-	-	0/4/4/4	0/4/4/4
2	BHF	A	602	-	-	0/4/4/4	0/4/4/4
4	GOL	B	607	-	-	2/4/4/4	-
2	BHF	B	603	-	-	0/4/4/4	0/4/4/4
2	BHF	A	601	-	-	0/4/4/4	0/4/4/4
3	HEM	A	605	1	-	0/6/54/54	-
2	BHF	A	604	-	-	4/4/4/4	0/4/4/4
4	GOL	A	606	-	-	2/4/4/4	-
2	BHF	B	604	-	-	0/4/4/4	0/4/4/4
4	GOL	B	609	-	-	0/4/4/4	-
4	GOL	A	607	-	-	0/4/4/4	-
2	BHF	B	601	-	-	2/4/4/4	0/4/4/4
2	BHF	A	603	-	-	0/4/4/4	0/4/4/4
3	HEM	B	605	1	-	0/6/54/54	-
4	GOL	B	608	-	-	2/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	BHF	C18-C19	5.25	1.48	1.41
2	A	603	BHF	C18-C19	5.23	1.48	1.41
2	A	601	BHF	C18-C19	5.19	1.48	1.41
2	A	604	BHF	C18-C19	5.18	1.48	1.41
2	A	604	BHF	C10-C19	5.08	1.48	1.41
2	A	601	BHF	C10-C19	5.03	1.48	1.41
2	A	603	BHF	C10-C19	5.03	1.48	1.41
2	A	602	BHF	C10-C19	4.99	1.48	1.41
2	B	601	BHF	C8-C9	4.47	1.46	1.37
2	B	603	BHF	C8-C9	4.45	1.46	1.37
2	B	604	BHF	C8-C9	4.35	1.46	1.37
2	B	602	BHF	C8-C9	4.31	1.46	1.37
3	A	605	HEM	C3C-C2C	-4.21	1.34	1.40
3	B	605	HEM	C3C-C2C	-4.17	1.34	1.40
3	A	605	HEM	C3B-C2B	-4.05	1.34	1.40
3	B	605	HEM	C3B-C2B	-3.97	1.34	1.40
3	B	605	HEM	C3B-CAB	3.66	1.55	1.47
3	B	605	HEM	C3C-CAC	3.58	1.55	1.47
3	A	605	HEM	C3C-CAC	3.56	1.55	1.47
3	A	605	HEM	C3B-CAB	3.54	1.55	1.47
2	A	602	BHF	C18-C13	3.35	1.48	1.42
2	A	603	BHF	C18-C13	3.34	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	BHF	C18-C13	3.34	1.48	1.42
2	A	604	BHF	C18-C13	3.31	1.48	1.42
2	B	604	BHF	C10-C19	-2.33	1.38	1.41
2	B	603	BHF	C10-C19	-2.31	1.38	1.41
2	B	601	BHF	C10-C19	-2.27	1.38	1.41
2	B	602	BHF	C10-C19	-2.26	1.38	1.41

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	BHF	C8-C9-C10	-8.75	113.36	123.05
2	B	601	BHF	C8-C9-C10	-8.73	113.39	123.05
2	B	604	BHF	C8-C9-C10	-8.68	113.44	123.05
2	B	603	BHF	C8-C9-C10	-8.67	113.45	123.05
2	A	603	BHF	C18-C19-C10	-4.97	117.61	120.20
2	A	601	BHF	C18-C19-C10	-4.96	117.62	120.20
2	A	602	BHF	C18-C19-C10	-4.89	117.66	120.20
2	A	604	BHF	C18-C19-C10	-4.89	117.66	120.20
2	B	602	BHF	O1-C7-C8	4.15	124.32	119.15
2	A	604	BHF	C8-C9-C10	-4.14	118.47	123.05
2	A	601	BHF	C8-C9-C10	-4.13	118.48	123.05
2	B	603	BHF	O1-C7-C8	4.12	124.29	119.15
2	A	603	BHF	C8-C9-C10	-4.12	118.48	123.05
2	A	602	BHF	C8-C9-C10	-4.11	118.49	123.05
2	B	604	BHF	O1-C7-C8	4.02	124.16	119.15
2	B	601	BHF	O1-C7-C8	3.98	124.11	119.15
2	A	603	BHF	C11-C10-C19	3.66	120.74	116.50
2	A	601	BHF	C11-C10-C19	3.66	120.73	116.50
2	A	604	BHF	C11-C10-C19	3.62	120.69	116.50
2	A	602	BHF	C11-C10-C19	3.60	120.67	116.50
2	A	601	BHF	C8-C7-C1	-2.96	118.88	126.73
2	A	603	BHF	C8-C7-C1	-2.93	118.94	126.73
2	B	604	BHF	C11-C10-C19	2.92	119.88	116.50
2	A	604	BHF	C8-C7-C1	-2.92	118.98	126.73
2	A	602	BHF	C8-C7-C1	-2.91	119.00	126.73
2	B	601	BHF	C13-C18-C19	-2.91	117.62	119.31
2	B	602	BHF	C13-C18-C19	-2.90	117.62	119.31
2	B	602	BHF	C11-C10-C19	2.88	119.83	116.50
2	B	603	BHF	C11-C10-C19	2.83	119.78	116.50
2	B	604	BHF	C13-C18-C19	-2.82	117.67	119.31
2	B	601	BHF	C11-C10-C19	2.82	119.76	116.50
3	B	605	HEM	CBA-CAA-C2A	-2.80	107.32	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	BHF	C18-C19-C10	2.71	121.61	120.20
2	B	603	BHF	C13-C18-C19	-2.60	117.80	119.31
2	A	603	BHF	C13-C18-C19	-2.46	117.87	119.31
2	A	602	BHF	C13-C18-C19	-2.45	117.88	119.31
2	A	604	BHF	C13-C18-C19	-2.45	117.88	119.31
2	A	601	BHF	O1-C7-C8	2.41	122.15	119.15
2	A	601	BHF	C13-C18-C19	-2.40	117.91	119.31
2	A	602	BHF	O1-C7-C8	2.40	122.14	119.15
2	B	601	BHF	C18-C19-C10	2.38	121.44	120.20
2	A	603	BHF	O1-C7-C8	2.38	122.12	119.15
3	A	605	HEM	CBD-CAD-C3D	-2.37	108.11	112.48
2	A	604	BHF	O1-C7-C8	2.36	122.09	119.15
3	B	605	HEM	CMD-C2D-C1D	-2.34	124.86	128.46
2	B	604	BHF	O1-C19-C10	2.31	123.44	121.20
2	B	602	BHF	O1-C19-C10	2.30	123.43	121.20
2	B	601	BHF	C6-C1-C7	-2.24	117.59	120.42
2	B	604	BHF	C6-C1-C7	-2.20	117.63	120.42
2	B	603	BHF	C18-C19-C10	2.12	121.30	120.20
2	B	603	BHF	O1-C19-C10	2.09	123.22	121.20
2	B	604	BHF	C18-C19-C10	2.06	121.27	120.20

There are no chirality outliers.

All (14) torsion outliers are listed below:

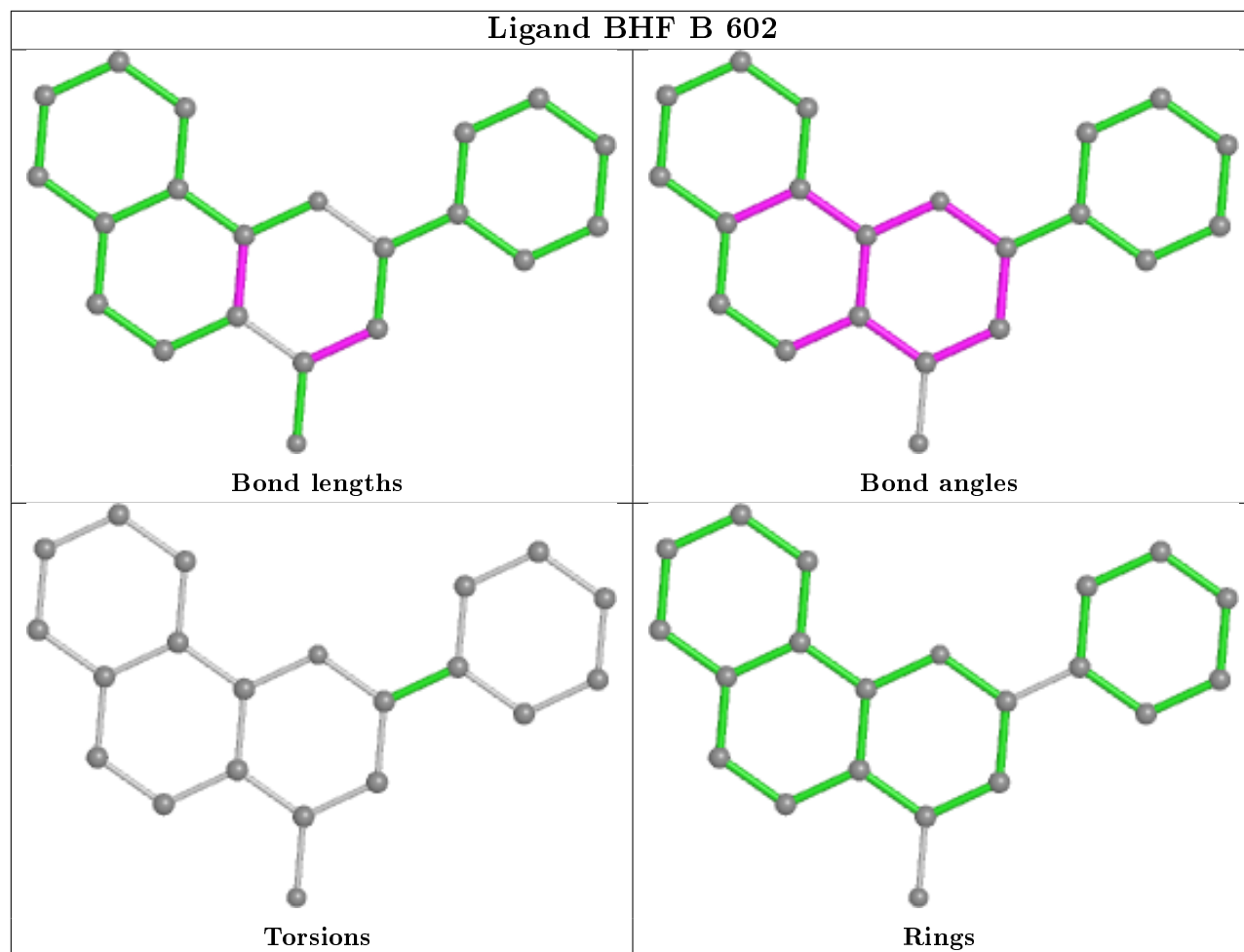
Mol	Chain	Res	Type	Atoms
4	B	607	GOL	C1-C2-C3-O3
4	B	608	GOL	C1-C2-C3-O3
4	B	608	GOL	O2-C2-C3-O3
4	B	606	GOL	C1-C2-C3-O3
4	A	606	GOL	C1-C2-C3-O3
4	B	607	GOL	O2-C2-C3-O3
2	A	604	BHF	C2-C1-C7-C8
2	A	604	BHF	C6-C1-C7-C8
2	A	604	BHF	C2-C1-C7-O1
4	B	606	GOL	O2-C2-C3-O3
2	A	604	BHF	C6-C1-C7-O1
4	A	606	GOL	O2-C2-C3-O3
2	B	601	BHF	C6-C1-C7-C8
2	B	601	BHF	C2-C1-C7-C8

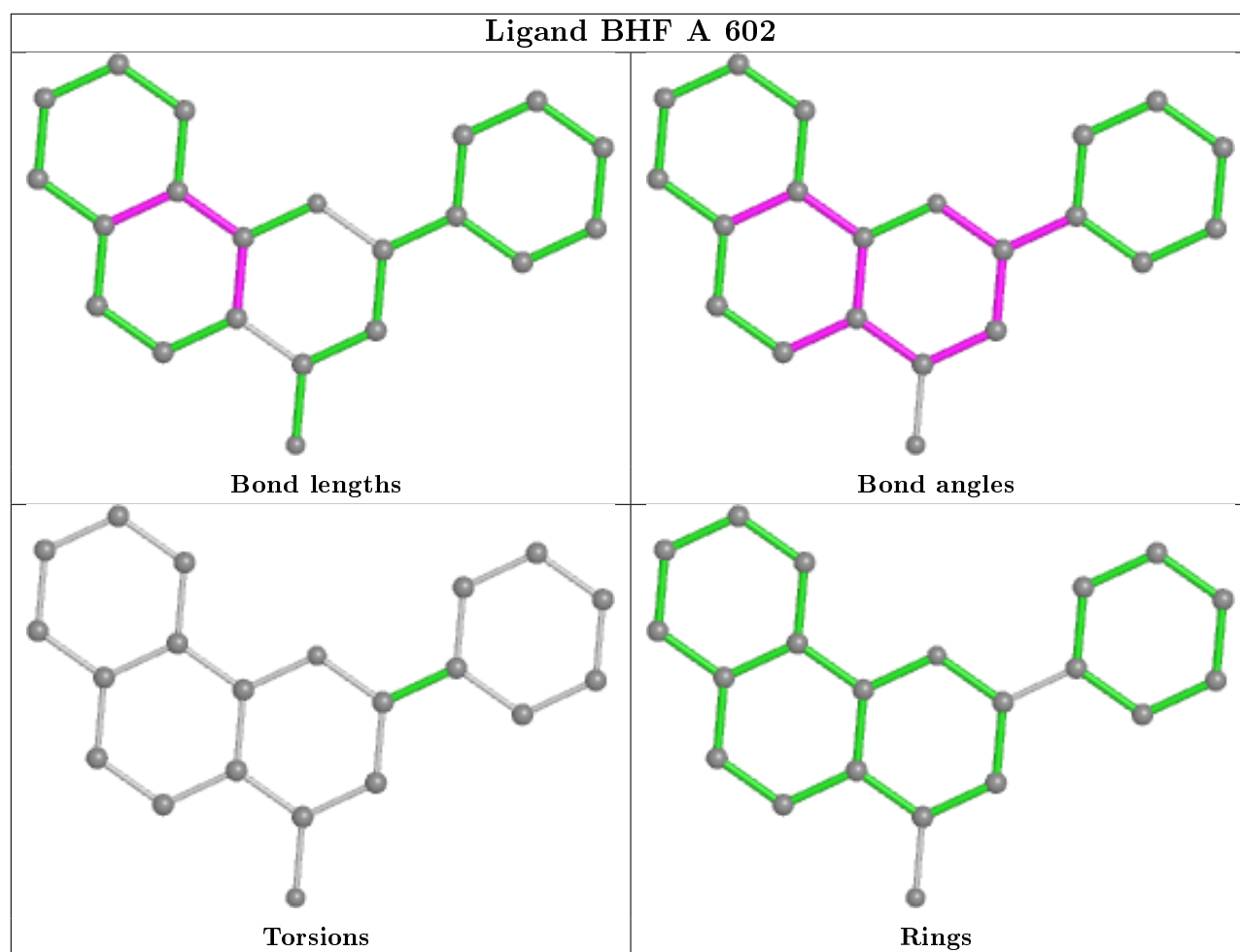
There are no ring outliers.

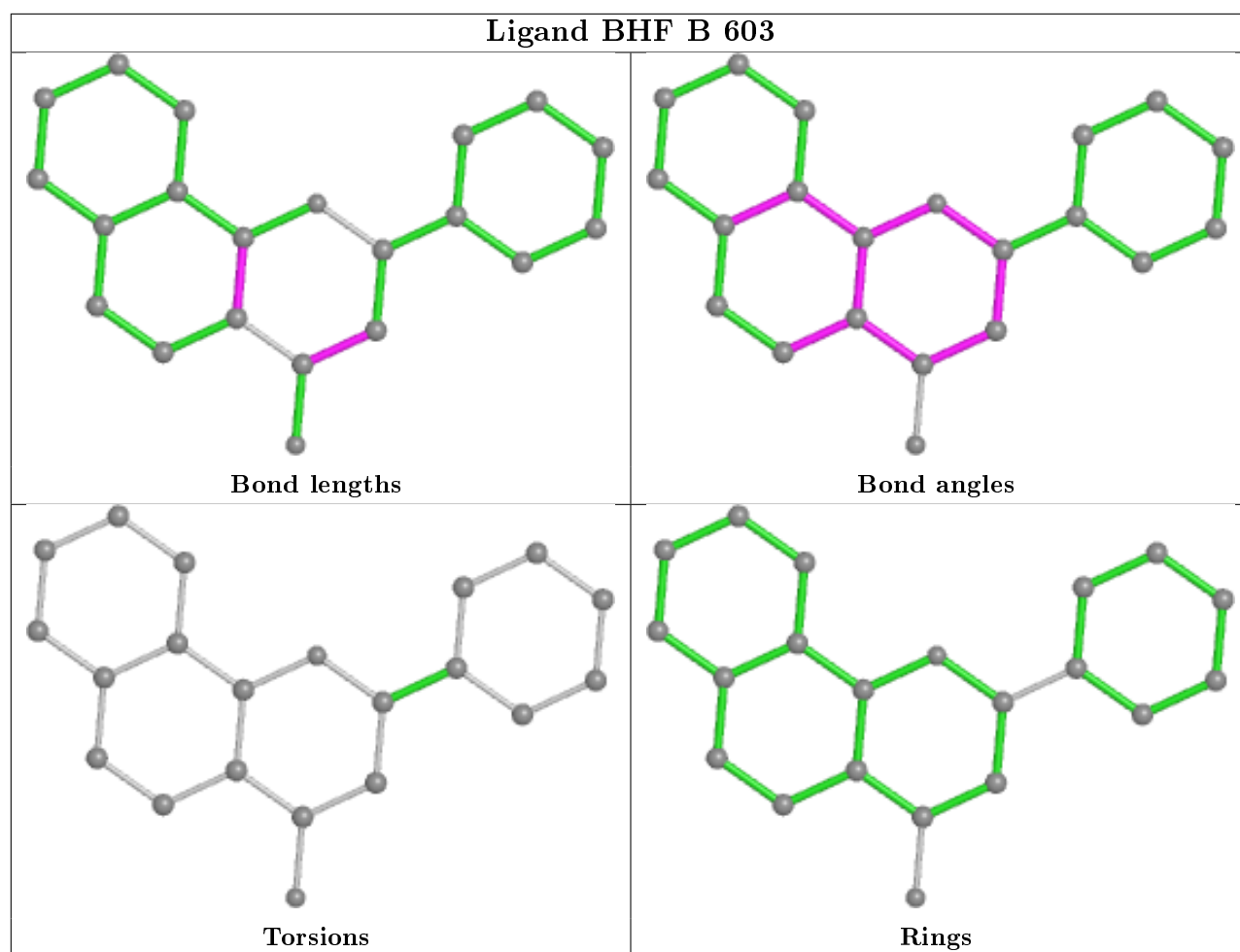
7 monomers are involved in 29 short contacts:

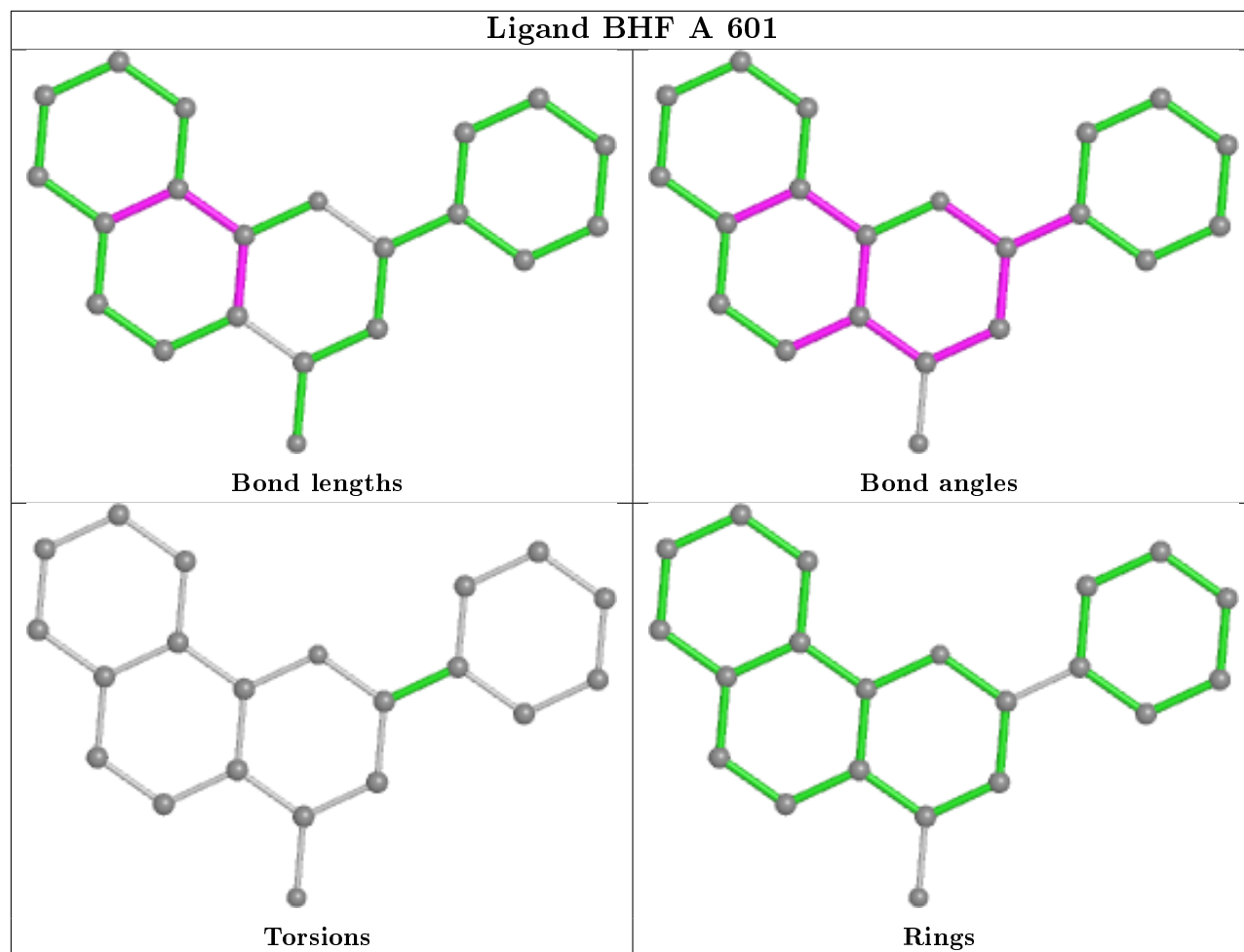
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	BHF	5	0
2	A	601	BHF	3	0
3	A	605	HEM	7	0
2	A	604	BHF	2	0
4	A	606	GOL	1	0
2	A	603	BHF	7	0
3	B	605	HEM	4	0

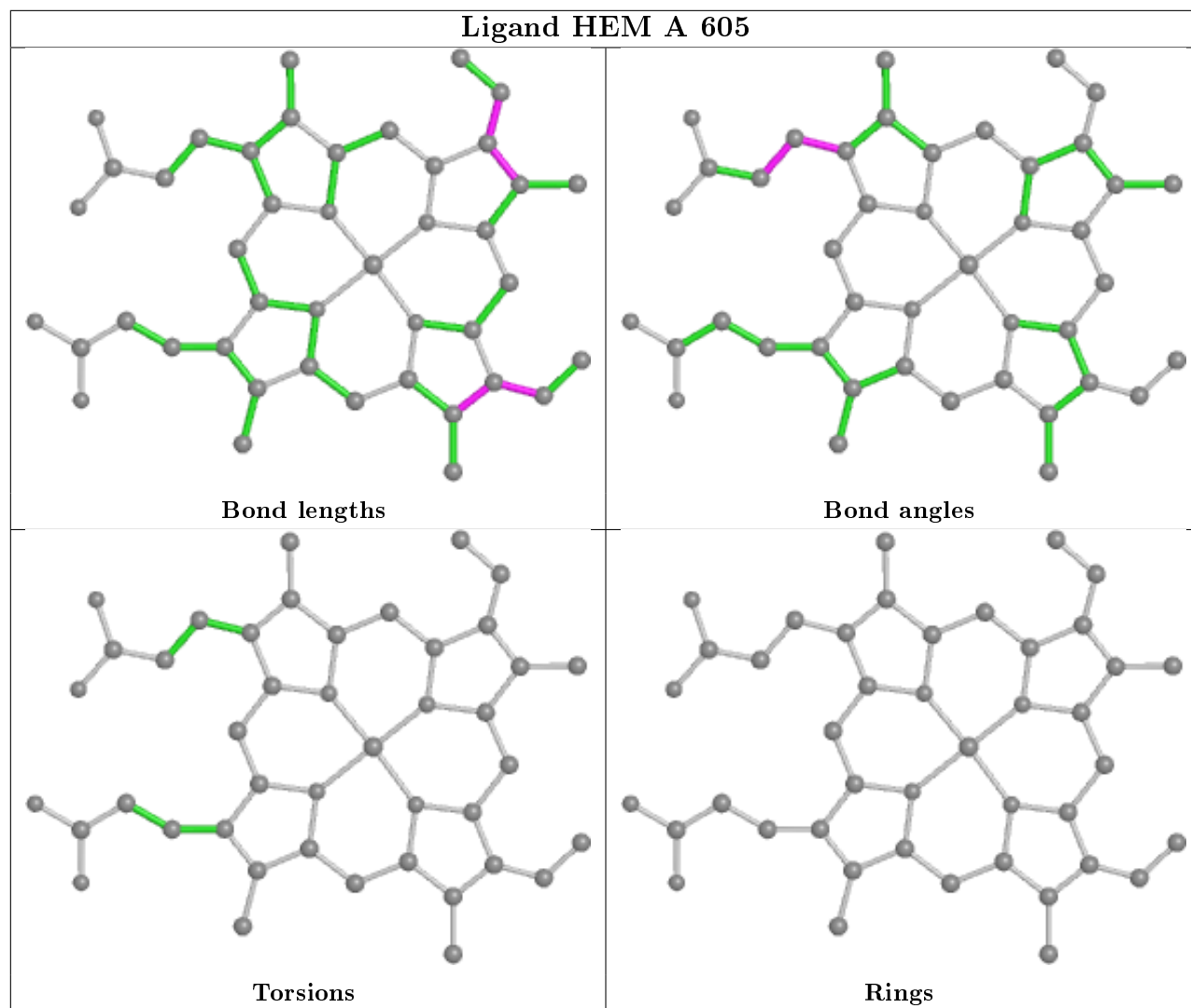
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

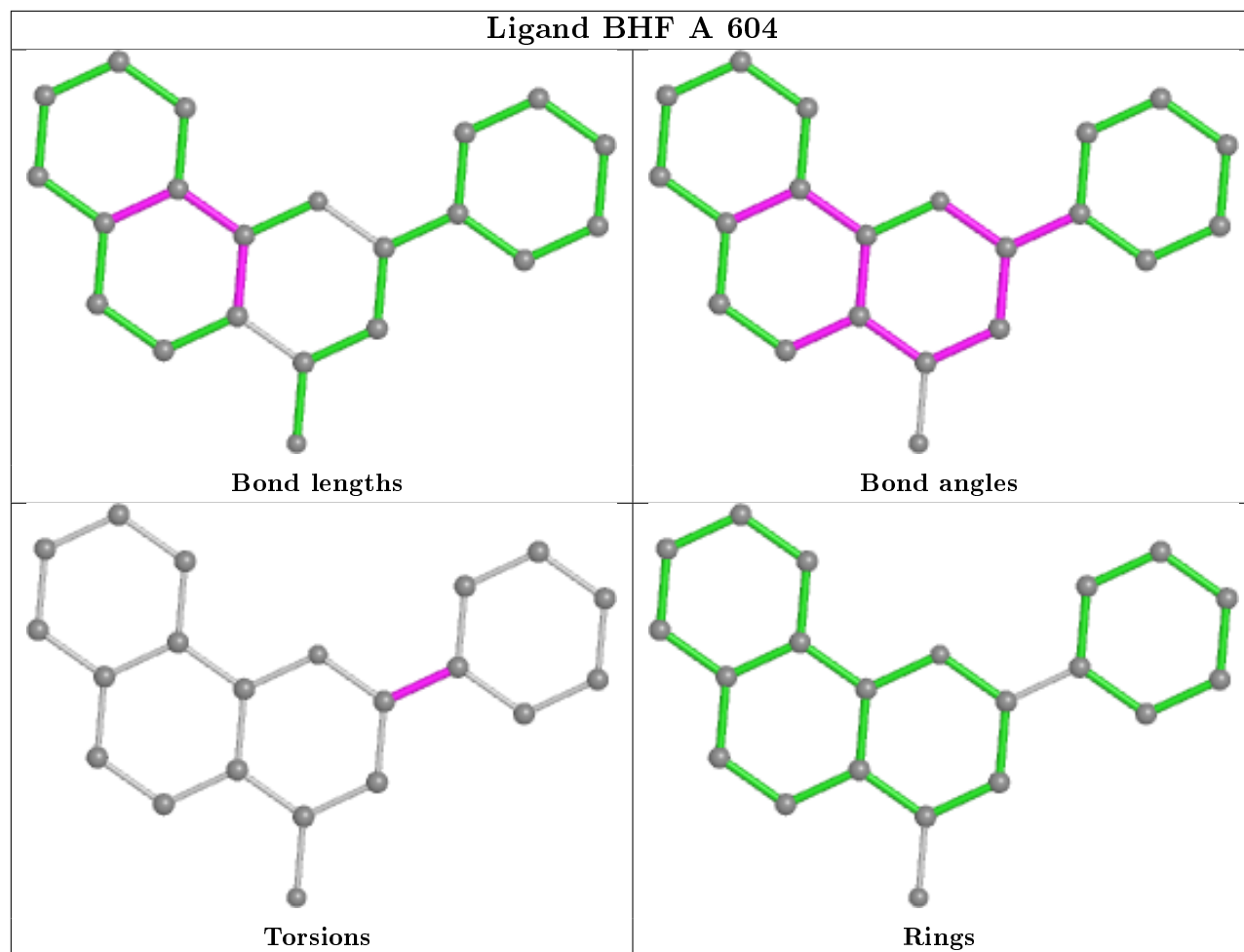


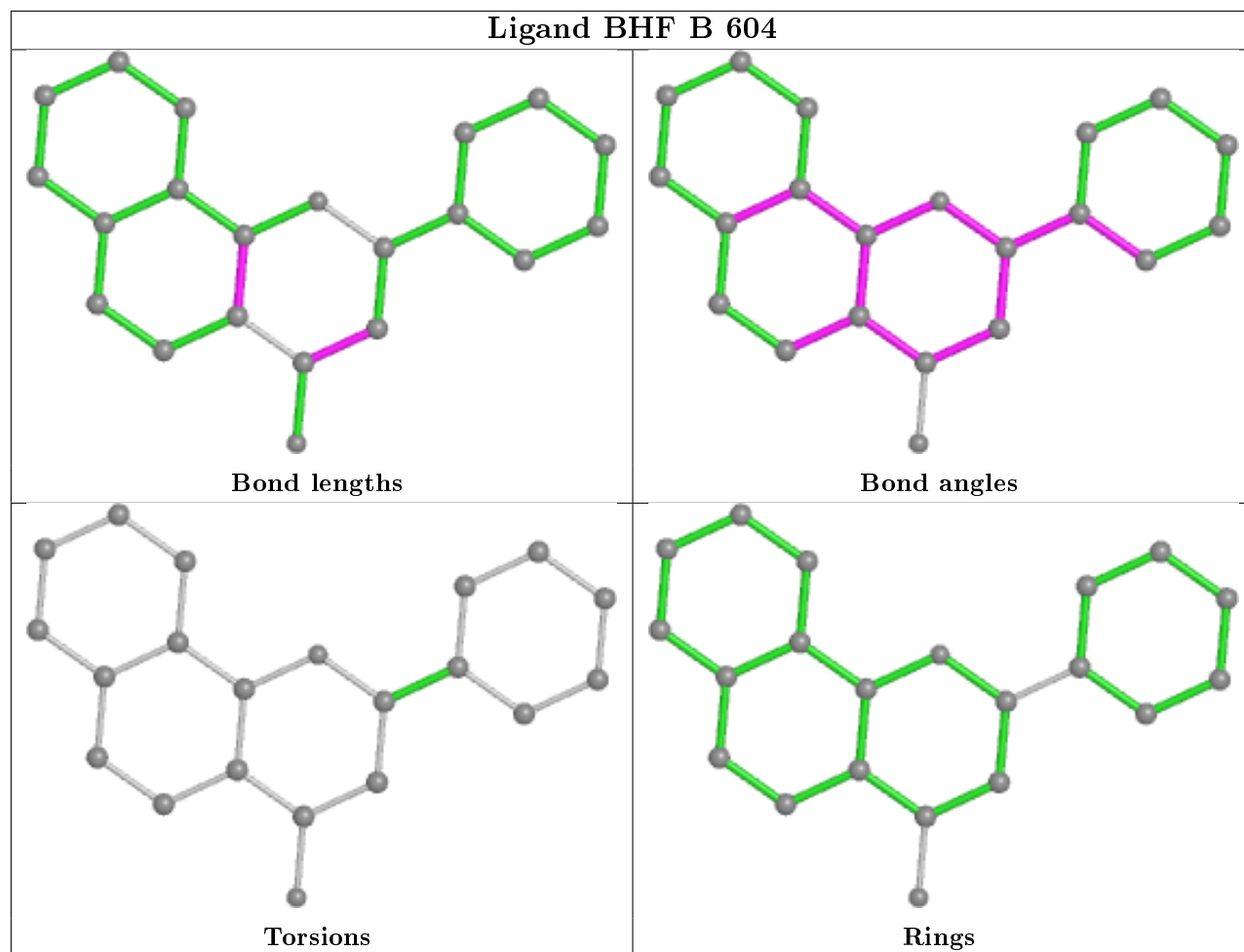


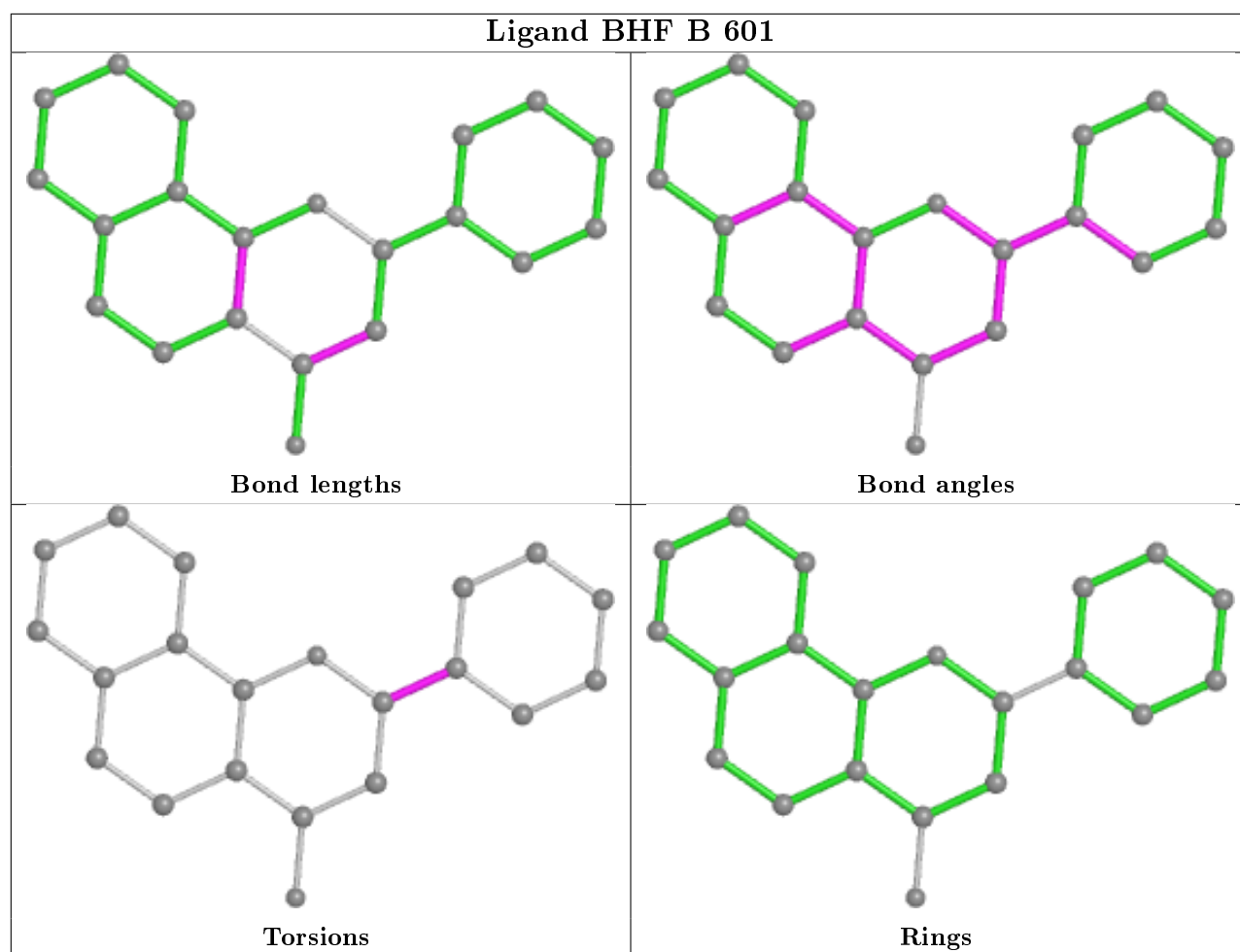


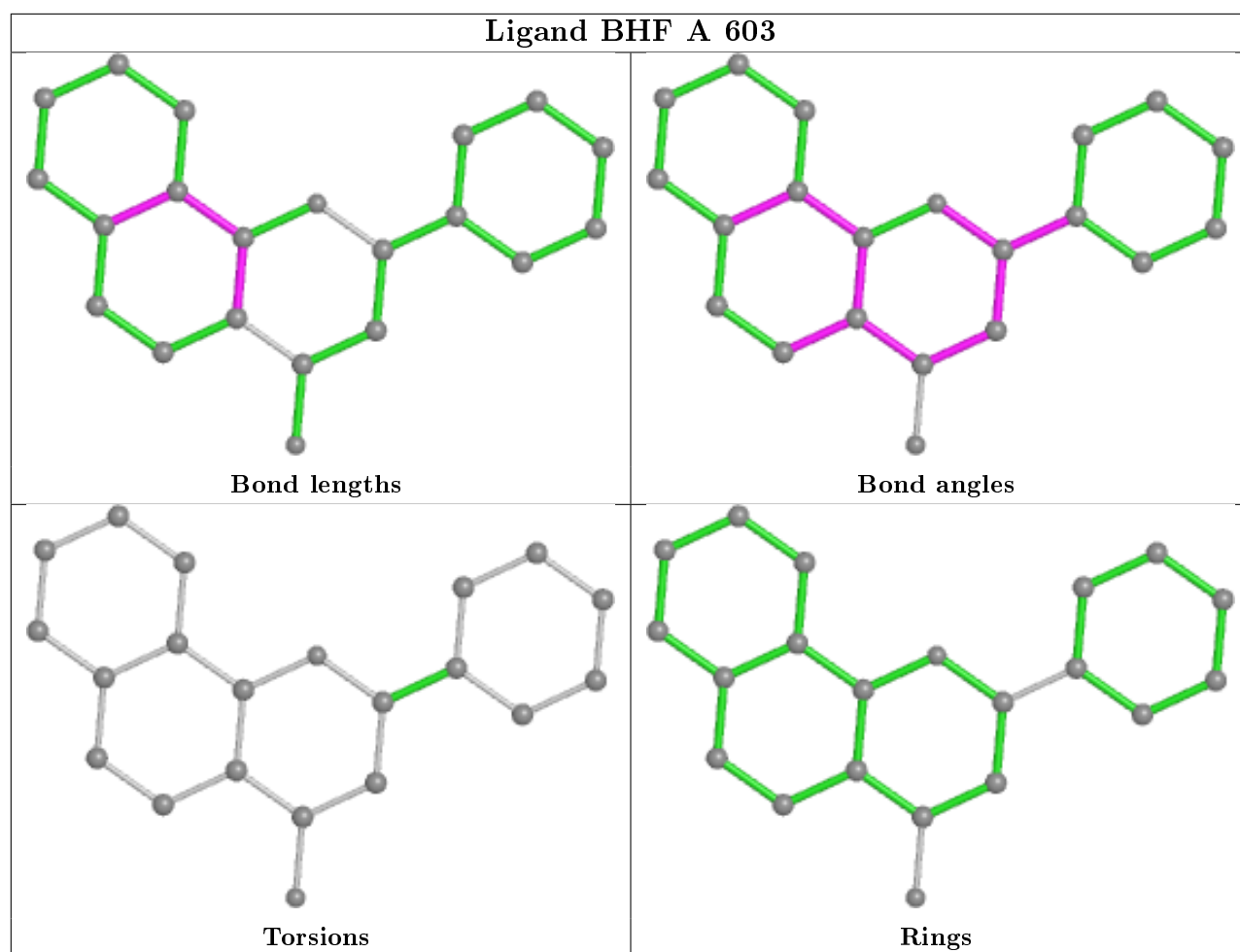


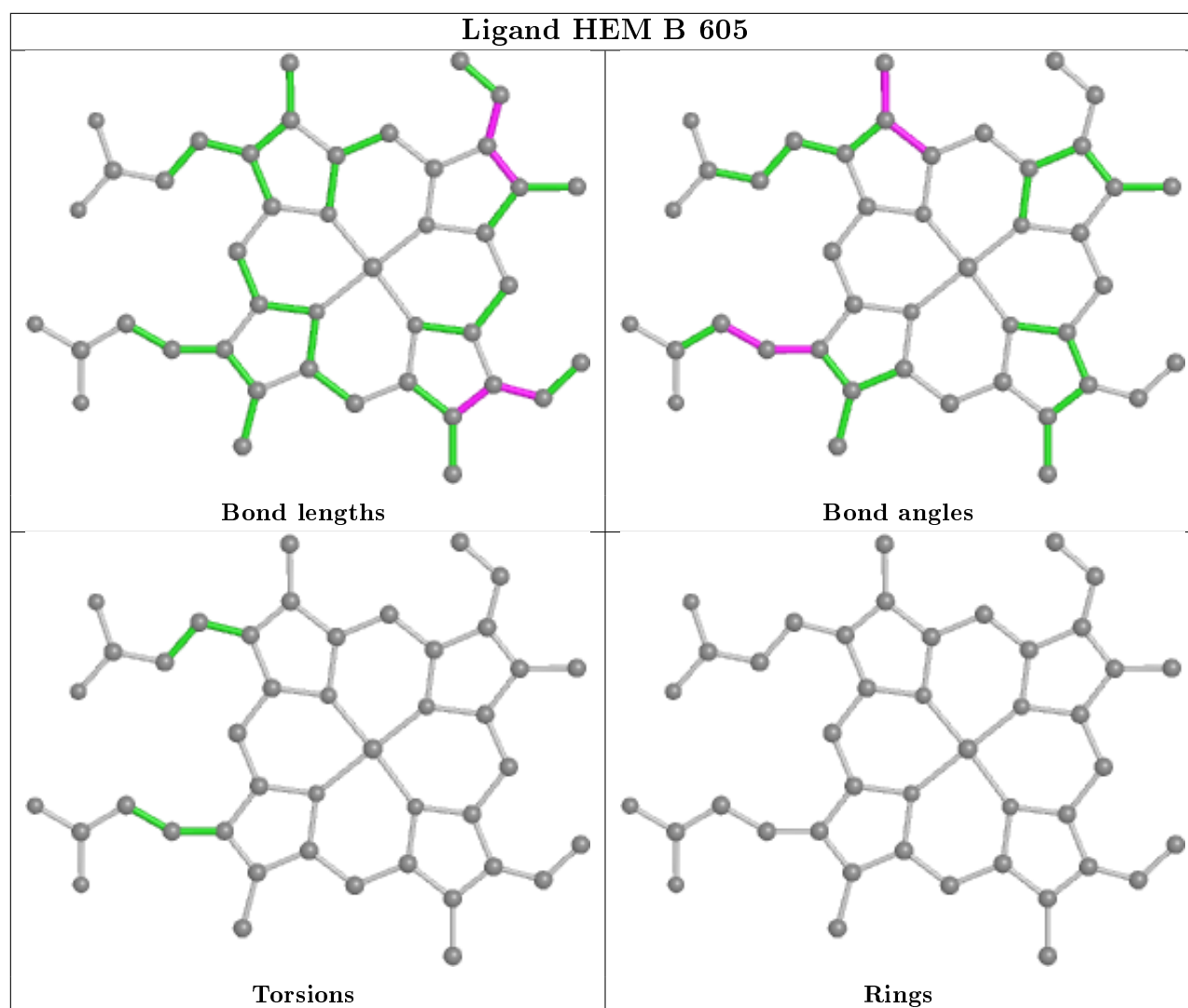












5.7 Other polymers [i](#)

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

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	450/493 (91%)	0.60	38 (8%) 11 6	29, 52, 77, 90	0
1	B	459/493 (93%)	0.61	28 (6%) 21 12	28, 53, 78, 117	0
All	All	909/986 (92%)	0.61	66 (7%) 15 8	28, 52, 77, 117	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	410	MET	4.7
1	B	360	LEU	4.5
1	A	413	HIS	4.3
1	A	217	ASP	4.0
1	B	186	ALA	3.9
1	A	411	GLY	3.8
1	B	449	ASN	3.8
1	A	80	ARG	3.7
1	A	212	CYS	3.5
1	B	452	ILE	3.5
1	A	432	VAL	3.3
1	A	414	ILE	3.3
1	A	408	SER	3.3
1	A	86	GLN	3.2
1	B	349	TYR	3.1
1	A	105	GLN	3.1
1	B	350	PRO	3.1
1	A	101	ARG	3.0
1	A	84	VAL	2.9
1	B	501	SER	2.9
1	A	76	ARG	2.9
1	B	379	PRO	2.8
1	A	218	ASP	2.8
1	A	81	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	187	GLY	2.8
1	B	521	THR	2.8
1	A	110	GLN	2.8
1	A	139	GLU	2.8
1	B	355	ARG	2.7
1	B	352	VAL	2.7
1	A	53	GLY	2.6
1	B	518	ILE	2.6
1	A	109	GLN	2.6
1	B	451	PHE	2.5
1	A	113	ALA	2.5
1	B	109	GLN	2.5
1	A	219	ALA	2.5
1	A	77	LEU	2.5
1	B	188	GLY	2.5
1	A	215	SER	2.4
1	A	108	VAL	2.4
1	B	497	PRO	2.4
1	B	445	PHE	2.4
1	A	412	TYR	2.3
1	A	409	ILE	2.3
1	B	484	ILE	2.3
1	B	413	HIS	2.3
1	B	139	GLU	2.3
1	A	418	THR	2.3
1	A	222	ARG	2.2
1	A	407	THR	2.2
1	B	499	GLU	2.2
1	A	97	LEU	2.2
1	B	448	LYS	2.2
1	B	502	LYS	2.2
1	A	79	ARG	2.1
1	A	50	ARG	2.1
1	A	59	LEU	2.1
1	A	85	PHE	2.1
1	A	137	TYR	2.1
1	A	51	PRO	2.1
1	B	446	LEU	2.1
1	B	442	PRO	2.1
1	A	55	PHE	2.1
1	B	488	ALA	2.0
1	B	212	CYS	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](#)

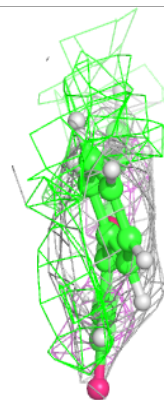
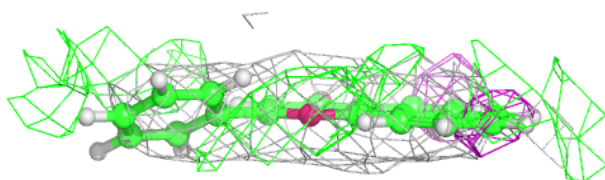
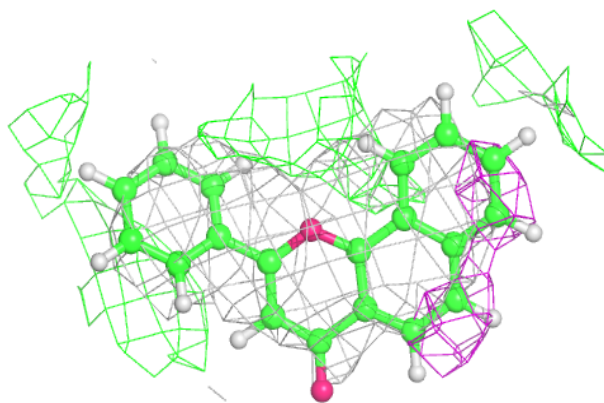
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BHF	A	602	21/21	0.83	0.36	48,63,79,89	0
2	BHF	A	604	21/21	0.85	0.42	52,64,79,82	0
2	BHF	B	602	21/21	0.86	0.27	45,59,74,79	0
4	GOL	A	607	6/6	0.88	0.25	46,60,80,80	0
2	BHF	A	603	21/21	0.89	0.30	32,49,63,67	0
4	GOL	B	608	6/6	0.90	0.22	51,61,71,81	0
4	GOL	B	607	6/6	0.91	0.20	46,70,83,85	0
4	GOL	B	609	6/6	0.92	0.32	43,52,56,63	0
2	BHF	B	604	21/21	0.93	0.26	45,55,68,75	0
4	GOL	B	606	6/6	0.95	0.22	45,58,70,70	0
2	BHF	B	603	21/21	0.95	0.22	34,45,62,70	0
2	BHF	A	601	21/21	0.96	0.25	21,32,43,51	0
2	BHF	B	601	21/21	0.96	0.20	28,39,53,57	0
3	HEM	A	605	43/43	0.97	0.25	24,34,47,51	0
3	HEM	B	605	43/43	0.97	0.23	20,34,45,56	0
4	GOL	A	606	6/6	0.97	0.21	44,53,59,67	0

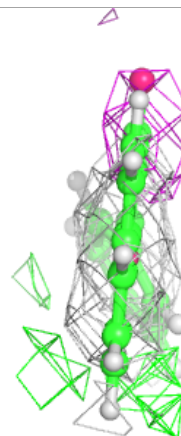
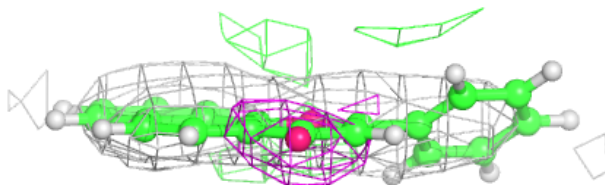
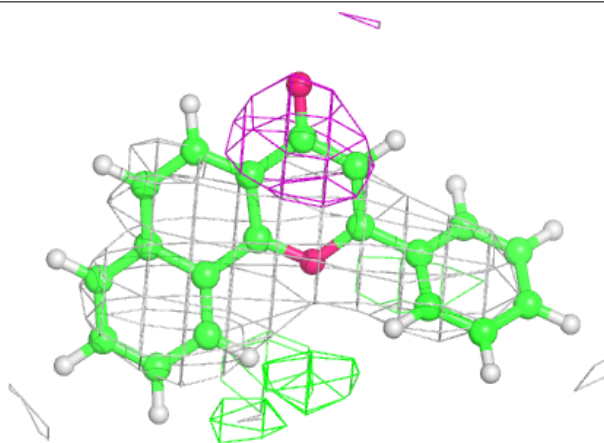
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BHF 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)

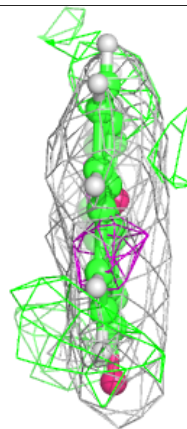
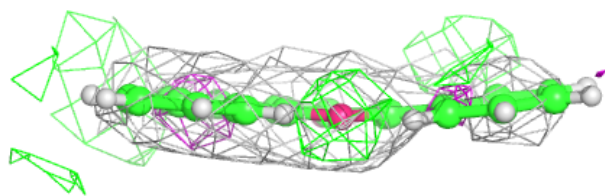
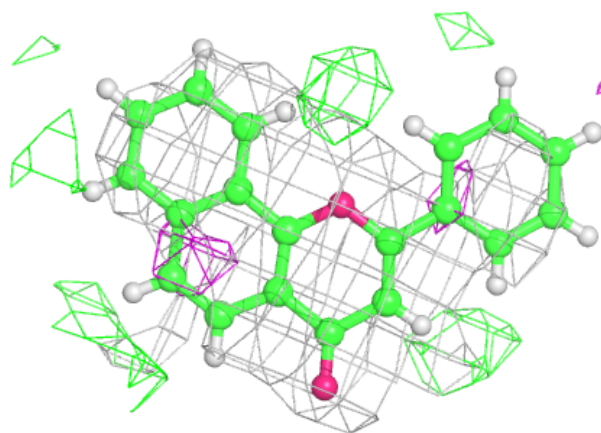
**Electron density around BHF A 604:**

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



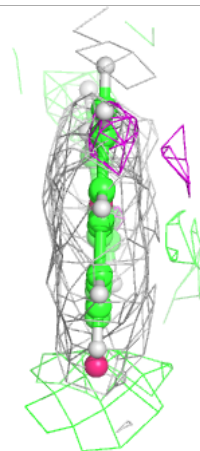
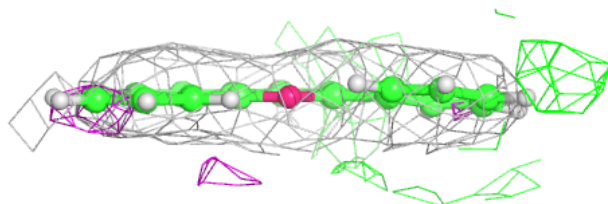
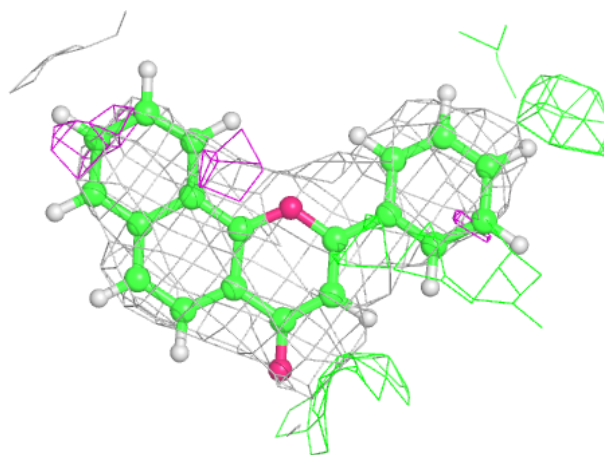
Electron density around BHF B 602:

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



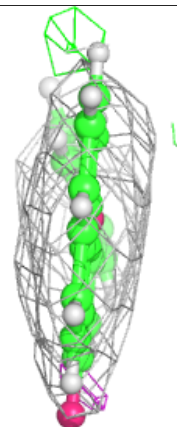
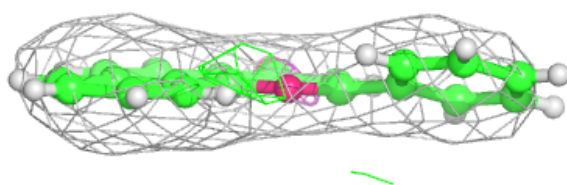
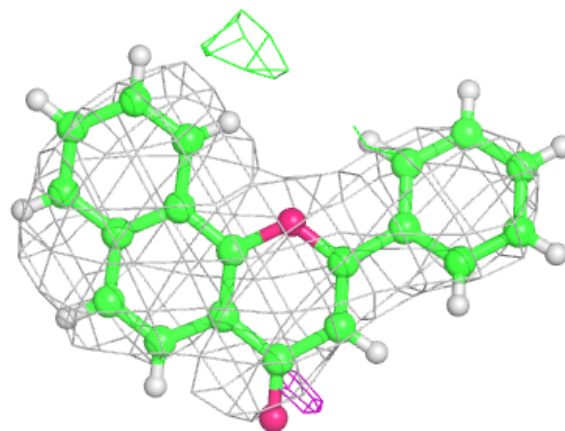
Electron density around BHF A 603:

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



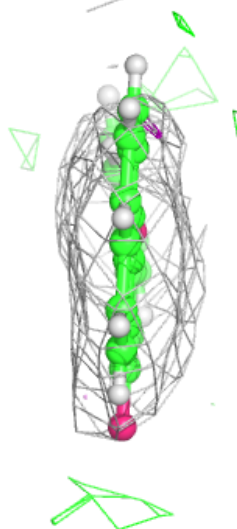
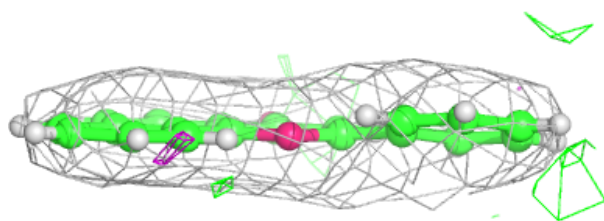
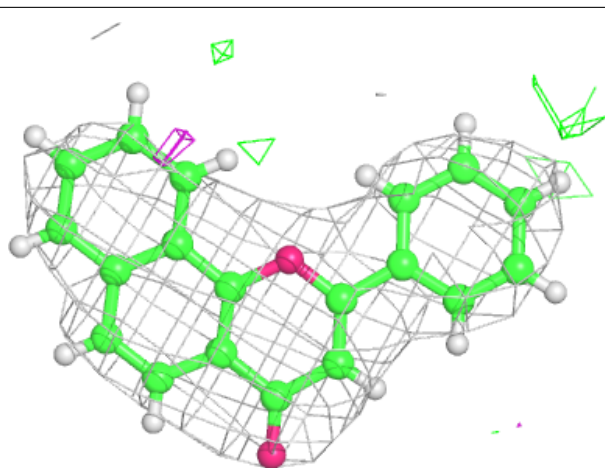
Electron density around BHF B 604:

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



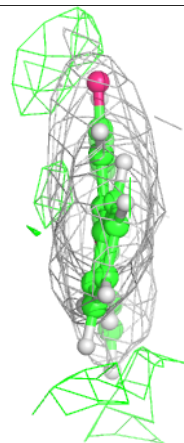
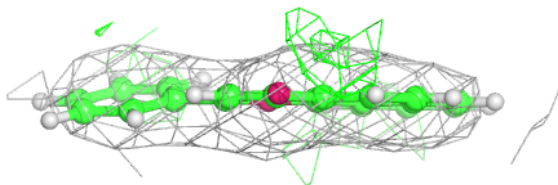
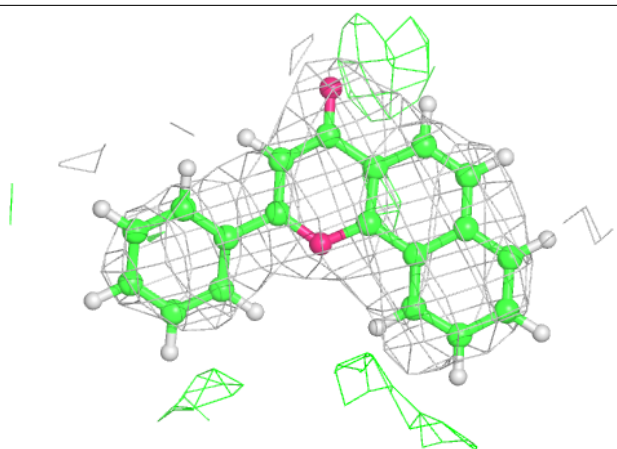
Electron density around BHF B 603:

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



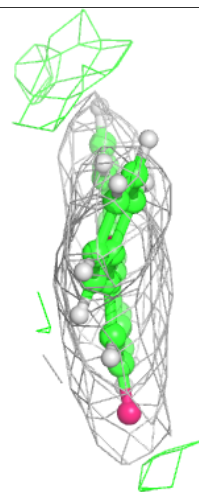
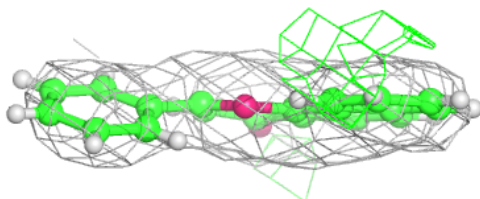
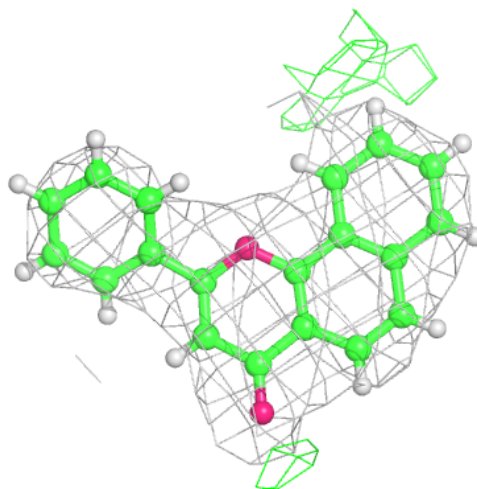
Electron density around BHF A 601:

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



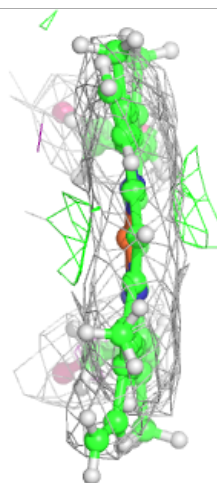
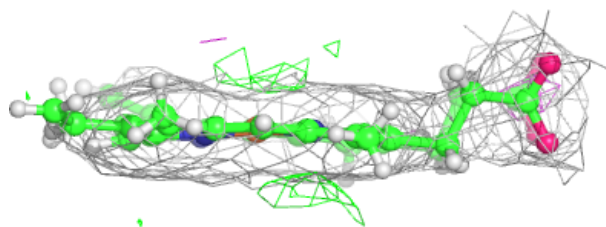
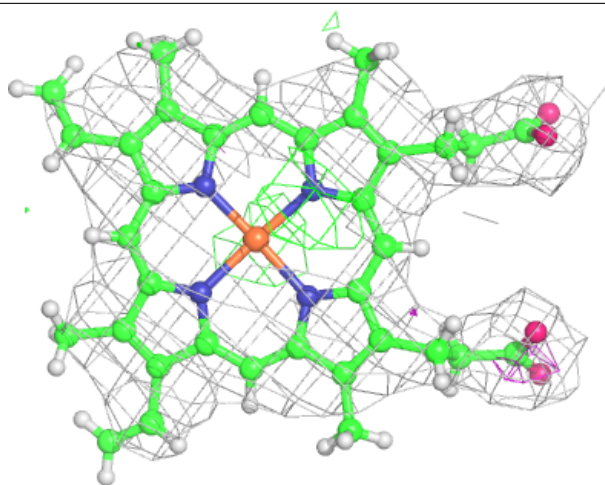
Electron density around BHF B 601:

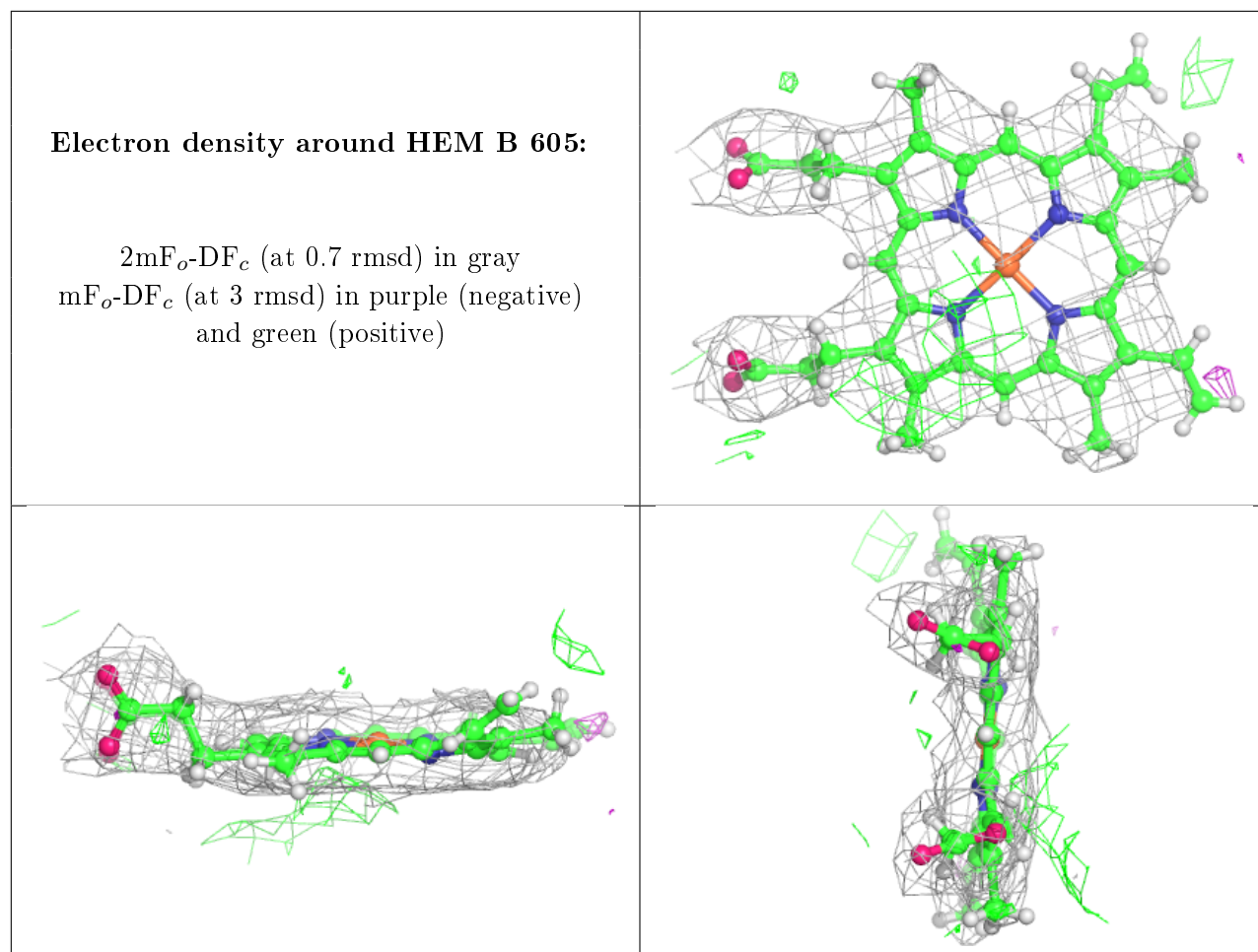
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 605:

$2mF_o-DF_c$ (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.