



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2026 – 06:53 am BST

PDB ID : 28PB / pdb_000028pb
Title : Crystal structure of CbcA periplasmic domain from *Geobacter sulfurreducens*
Authors : Antunes, J.M.A.; Correia, M.A.S.; Santos-Silva, T.; Morgado, L.
Deposited on : 2026-02-12
Resolution : 1.91 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

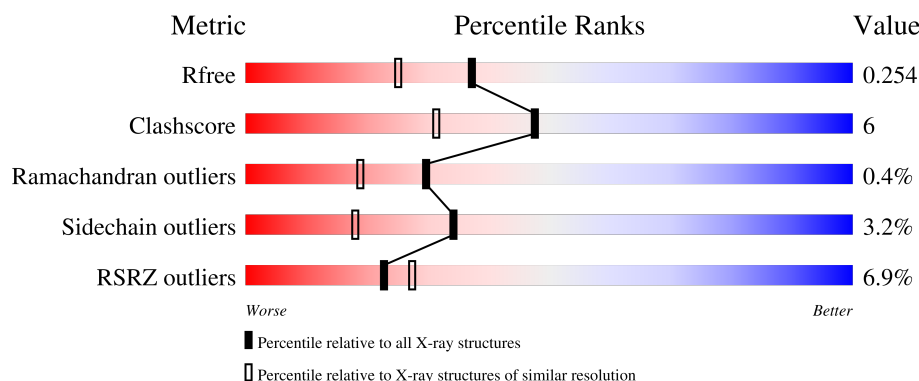
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	278	5% 82% 16%
1	B	278	9% 86% 14%

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	HEC	A	301	X	-	-	-
2	HEC	A	302	X	-	-	-
2	HEC	A	303	X	-	-	-
2	HEC	A	304	X	-	-	-
2	HEC	A	305	X	-	-	-
2	HEC	A	306	X	-	-	-
2	HEC	A	307	X	-	-	-
2	HEC	B	301	X	-	-	-
2	HEC	B	302	X	-	-	-
2	HEC	B	303	X	-	-	-
2	HEC	B	304	X	-	-	-
2	HEC	B	305	X	-	-	-
2	HEC	B	306	X	-	-	-
2	HEC	B	307	X	-	-	-

2 Entry composition [i](#)

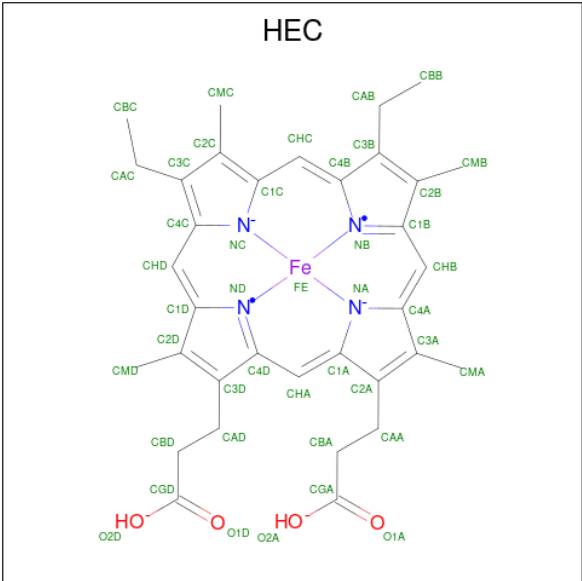
There are 5 unique types of molecules in this entry. The entry contains 5184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	1	0
			2131	1312	385	413	21			
1	B	277	Total	C	N	O	S	0	1	0
			2132	1312	385	414	21			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca		
			1	1	0	0
3	B	1	Total	Ca		
			1	1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg		
			1	1	0	0

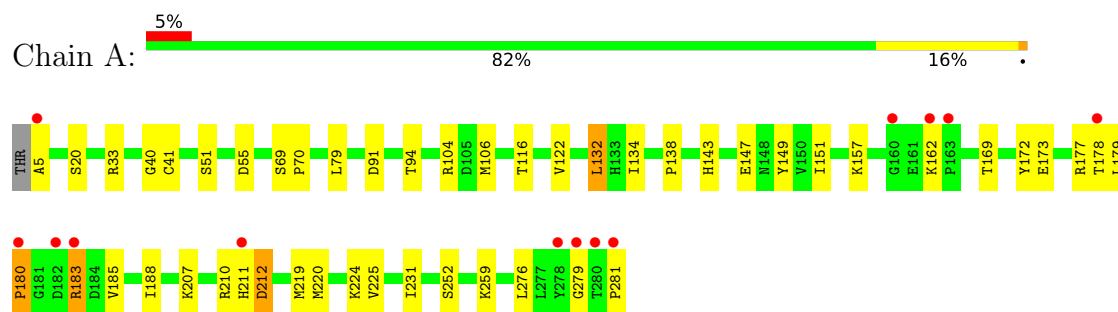
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	199	Total	O		
			199	199	0	0
5	B	117	Total	O		
			117	117	0	0

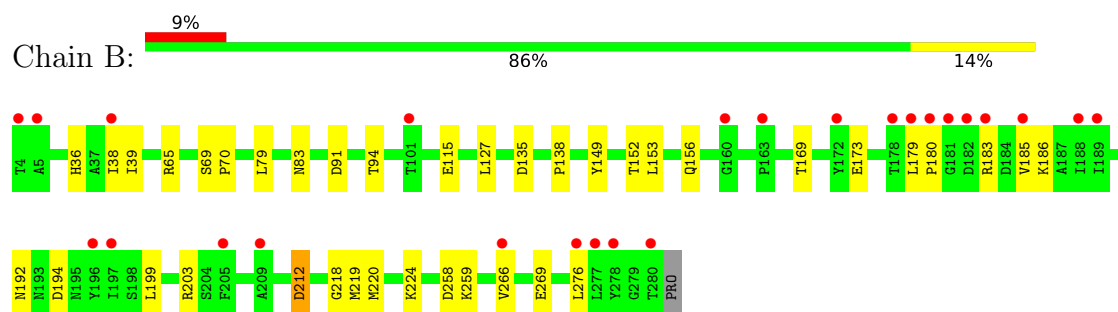
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome c



• Molecule 1: Cytochrome c



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.44Å 94.17Å 114.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.75 – 1.91 72.65 – 1.91	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.75-1.91) 100.0 (72.65-1.91)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, R_{free}	0.199 , 0.253 0.200 , 0.254	Depositor DCC
R_{free} test set	2876 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5184	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: MG, CA, HEC

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	0.57	0/2184	1.14	6/2962 (0.2%)
1	B	0.54	0/2184	1.14	1/2963 (0.0%)
All	All	0.55	0/4368	1.14	7/5925 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	LEU	N-CA-CB	-6.14	101.17	110.07
1	A	147	GLU	CB-CG-CD	5.67	122.23	112.60
1	B	135	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	173	GLU	CB-CG-CD	5.32	121.64	112.60
1	A	169	THR	CA-CB-OG1	-5.26	101.71	109.60
1	A	116	THR	CA-CB-OG1	-5.13	101.90	109.60
1	A	212	ASP	CA-CB-CG	5.03	117.63	112.60

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	2131	0	2037	28	0
1	B	2132	0	2036	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	301	0	210	2	0
2	B	301	0	210	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	1	0	0	0	0
5	A	199	0	0	7	2
5	B	117	0	0	6	2
All	All	5184	0	4493	52	2

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.

All (52) 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:179:LEU:HD13	1:B:183:ARG:O	1.82	0.79
1:A:279:GLY:O	1:A:281:PRO:HD3	1.90	0.72
1:A:5:ALA:HA	1:A:41:CYS:SG	2.34	0.67
1:B:152:THR:HG23	5:B:407:HOH:O	1.95	0.66
1:A:5:ALA:HB2	1:A:40:GLY:HA2	1.78	0.65
1:B:91:ASP:OD2	1:B:94:THR:HG23	1.97	0.64
1:B:199:LEU:HG	1:B:269:GLU:HB3	1.79	0.64
1:B:180:PRO:HG2	1:B:183:ARG:NH1	2.16	0.60
1:A:91:ASP:OD2	1:A:94:THR:HG23	2.06	0.56
1:A:224:LYS:NZ	5:A:405:HOH:O	2.38	0.56
1:A:225:VAL:HG11	2:A:304:HEC:HBA2	1.88	0.54
1:B:173:GLU:H	1:B:173:GLU:CD	2.14	0.54
1:A:276:LEU:C	1:A:276:LEU:HD23	2.33	0.53
1:A:33:ARG:NH2	1:B:115:GLU:OE1	2.38	0.53
1:B:149:TYR:CD1	1:B:220:MET:HE3	2.44	0.53
1:B:192:ASN:HB2	5:B:417:HOH:O	2.08	0.53
1:A:51:SER:HB2	1:A:55:ASP:OD2	2.09	0.53
1:A:224:LYS:HD3	5:A:524:HOH:O	2.10	0.52
1:A:185:VAL:O	1:A:188:ILE:HG13	2.10	0.52
1:A:210:ARG:HG3	1:A:211:HIS:CD2	2.45	0.52
1:A:104:ARG:HG3	5:A:559:HOH:O	2.09	0.51
1:B:127:LEU:HD11	2:B:306:HEC:HBC2	1.92	0.51
1:B:194:ASP:CG	5:B:417:HOH:O	2.54	0.51
1:B:192:ASN:CB	5:B:417:HOH:O	2.59	0.51
1:A:177:ARG:C	1:A:179:LEU:H	2.19	0.51
1:A:5:ALA:HB3	5:A:582:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ALA:HB2	1:A:41:CYS:H	1.77	0.49
1:B:138:PRO:HG3	1:B:219:MET:HE2	1.96	0.47
1:A:69:SER:N	1:A:70:PRO:CD	2.78	0.47
1:B:156:GLN:HG2	1:B:169:THR:HA	1.96	0.47
1:A:104:ARG:CG	5:A:559:HOH:O	2.63	0.46
2:A:304:HEC:HMC3	2:A:304:HEC:HBC3	1.98	0.46
1:B:153:LEU:HD23	1:B:218:GLY:HA3	1.98	0.46
1:B:203:ARG:NH2	1:B:276:LEU:HD21	2.30	0.46
1:B:212:ASP:N	1:B:212:ASP:OD1	2.49	0.46
1:A:94:THR:HG22	5:A:504:HOH:O	2.17	0.45
1:B:69:SER:N	1:B:70:PRO:CD	2.79	0.45
1:B:36:HIS:HB3	1:B:39:ILE:HG12	1.99	0.44
1:A:149:TYR:CD1	1:A:220:MET:HE3	2.52	0.44
1:B:83:ASN:HB3	2:B:304:HEC:C2D	2.47	0.44
1:B:224:LYS:NZ	5:B:410:HOH:O	2.50	0.43
1:B:65:ARG:HG3	5:B:404:HOH:O	2.18	0.43
1:A:138:PRO:HD3	1:A:219:MET:CE	2.49	0.42
1:B:203:ARG:NH2	1:B:276:LEU:CD2	2.83	0.42
1:A:180:PRO:HG2	1:A:183:ARG:HD3	2.02	0.42
1:A:172:TYR:CZ	1:A:259:LYS:HG2	2.55	0.42
1:A:138:PRO:HD3	1:A:219:MET:HE2	2.01	0.41
1:A:79:LEU:O	5:A:401:HOH:O	2.21	0.41
1:A:143:HIS:CE1	1:A:231:ILE:HD11	2.56	0.41
1:B:186:LYS:HG2	1:B:266:VAL:HG21	2.03	0.41
1:A:134:ILE:HD13	1:A:134:ILE:HA	1.99	0.40
1:A:151:ILE:O	1:A:252:SER:HA	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:590:HOH:O	5:B:513:HOH:O[3_645]	2.00	0.20
5:A:594:HOH:O	5:B:511:HOH:O[3_645]	2.02	0.18

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	276/278 (99%)	264 (96%)	10 (4%)	2 (1%)	18	9
1	B	276/278 (99%)	260 (94%)	16 (6%)	0	100	100
All	All	552/556 (99%)	524 (95%)	26 (5%)	2 (0%)	30	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	THR
1	A	180	PRO

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	234/234 (100%)	225 (96%)	9 (4%)	29	14
1	B	234/234 (100%)	228 (97%)	6 (3%)	40	24
All	All	468/468 (100%)	453 (97%)	15 (3%)	34	18

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

Mol	Chain	Res	Type
1	A	20	SER
1	A	106	MET
1	A	122	VAL
1	A	132	LEU
1	A	157	LYS
1	A	162	LYS
1	A	183	ARG
1	A	207	LYS
1	A	212	ASP
1	B	38	ILE

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Mol	Chain	Res	Type
1	B	79	LEU
1	B	185	VAL
1	B	212	ASP
1	B	258	ASP
1	B	259	LYS

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

Mol	Chain	Res	Type
1	A	211	HIS
1	B	129	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 for Mogul analysis.

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	$\# Z > 2$
2	HEC	A	305	1	50,50,50	1.86	14 (28%)	68,82,82	1.25	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	B	306	1	50,50,50	1.89	10 (20%)	68,82,82	2.32	8 (11%)
2	HEC	B	305	1	50,50,50	1.80	11 (22%)	68,82,82	0.93	3 (4%)
2	HEC	A	307	1	50,50,50	1.67	12 (24%)	68,82,82	0.91	2 (2%)
2	HEC	B	301	1	50,50,50	1.86	14 (28%)	68,82,82	1.26	5 (7%)
2	HEC	A	302	1	50,50,50	1.79	14 (28%)	68,82,82	1.06	5 (7%)
2	HEC	A	304	1	50,50,50	1.86	11 (22%)	68,82,82	0.98	2 (2%)
2	HEC	A	306	1	50,50,50	1.72	11 (22%)	68,82,82	1.10	4 (5%)
2	HEC	B	302	1	50,50,50	1.72	11 (22%)	68,82,82	0.90	4 (5%)
2	HEC	B	303	1	50,50,50	1.79	9 (18%)	68,82,82	1.02	4 (5%)
2	HEC	A	301	1	50,50,50	1.72	12 (24%)	68,82,82	1.28	5 (7%)
2	HEC	A	303	1	50,50,50	1.78	11 (22%)	68,82,82	1.33	4 (5%)
2	HEC	B	307	1	50,50,50	1.74	11 (22%)	68,82,82	1.31	5 (7%)
2	HEC	B	304	4,1	50,50,50	1.74	12 (24%)	68,82,82	1.06	6 (8%)

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
2	HEC	A	305	1	1/1/3/7	7/14/54/54	-
2	HEC	B	306	1	1/1/3/7	4/14/54/54	-
2	HEC	B	305	1	1/1/3/7	5/14/54/54	-
2	HEC	A	307	1	1/1/3/7	7/14/54/54	-
2	HEC	B	301	1	1/1/3/7	9/14/54/54	-
2	HEC	A	302	1	1/1/3/7	7/14/54/54	-
2	HEC	A	304	1	1/1/3/7	4/14/54/54	-
2	HEC	A	306	1	1/1/3/7	6/14/54/54	-
2	HEC	B	302	1	1/1/3/7	9/14/54/54	-
2	HEC	B	303	1	1/1/3/7	8/14/54/54	-
2	HEC	A	301	1	1/1/3/7	9/14/54/54	-
2	HEC	A	303	1	1/1/3/7	8/14/54/54	-
2	HEC	B	307	1	1/1/3/7	6/14/54/54	-
2	HEC	B	304	4,1	1/1/3/7	6/14/54/54	-

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	307	HEC	FE-ND	5.74	2.12	1.94
2	B	306	HEC	FE-NB	5.09	2.10	1.94
2	A	304	HEC	FE-NC	4.79	2.11	1.95
2	B	305	HEC	C4A-C3A	-4.76	1.35	1.45
2	B	301	HEC	C4D-C3D	-4.70	1.36	1.45
2	B	301	HEC	FE-NC	4.55	2.10	1.95
2	B	305	HEC	C1A-C2A	-4.53	1.37	1.45
2	B	306	HEC	C1B-C2B	-4.51	1.35	1.44
2	B	303	HEC	FE-ND	4.50	2.08	1.94
2	B	304	HEC	C4D-C3D	-4.49	1.37	1.45
2	A	303	HEC	C4D-C3D	-4.47	1.37	1.45
2	B	305	HEC	C4D-C3D	-4.41	1.37	1.45
2	A	305	HEC	FE-NC	4.35	2.09	1.95
2	A	303	HEC	C4A-C3A	-4.32	1.36	1.45
2	A	306	HEC	C4A-C3A	-4.30	1.36	1.45
2	A	301	HEC	C4A-C3A	-4.27	1.36	1.45
2	B	303	HEC	C1A-C2A	-4.24	1.37	1.45
2	B	306	HEC	C4D-C3D	-4.24	1.37	1.45
2	A	306	HEC	FE-NB	4.23	2.08	1.94
2	B	301	HEC	C1A-C2A	-4.22	1.37	1.45
2	B	306	HEC	C4A-C3A	-4.11	1.37	1.45
2	B	306	HEC	FE-ND	4.10	2.07	1.94
2	B	305	HEC	C1D-C2D	-4.10	1.36	1.44
2	B	302	HEC	C1A-C2A	-4.09	1.37	1.45
2	A	307	HEC	C1A-C2A	-4.08	1.38	1.45
2	A	307	HEC	FE-NA	4.06	2.08	1.95
2	A	304	HEC	C4A-C3A	-4.06	1.37	1.45
2	B	304	HEC	FE-NC	4.00	2.08	1.95
2	A	303	HEC	C1A-C2A	-3.98	1.38	1.45
2	A	305	HEC	FE-NB	3.98	2.07	1.94
2	A	303	HEC	C1D-C2D	-3.95	1.36	1.44
2	A	302	HEC	FE-NC	3.92	2.08	1.95
2	B	302	HEC	C4D-C3D	-3.91	1.38	1.45
2	B	302	HEC	C4A-C3A	-3.91	1.37	1.45
2	A	302	HEC	C1B-C2B	-3.90	1.37	1.44
2	A	305	HEC	C4A-C3A	-3.89	1.37	1.45
2	A	304	HEC	C4D-C3D	-3.89	1.38	1.45
2	A	304	HEC	C1A-C2A	-3.88	1.38	1.45
2	A	301	HEC	C4D-C3D	-3.86	1.38	1.45
2	B	302	HEC	C1D-C2D	-3.86	1.37	1.44
2	B	303	HEC	C4A-C3A	-3.86	1.37	1.45
2	B	303	HEC	C4D-C3D	-3.85	1.38	1.45
2	B	301	HEC	FE-NA	3.84	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	304	HEC	C1D-C2D	-3.83	1.37	1.44
2	B	302	HEC	FE-NC	3.82	2.08	1.95
2	A	301	HEC	C1A-C2A	-3.81	1.38	1.45
2	A	306	HEC	C1A-C2A	-3.79	1.38	1.45
2	A	305	HEC	C4D-C3D	-3.79	1.38	1.45
2	A	304	HEC	C1D-C2D	-3.79	1.37	1.44
2	B	301	HEC	C4A-C3A	-3.78	1.37	1.45
2	A	302	HEC	C1D-C2D	-3.77	1.37	1.44
2	A	305	HEC	C1B-C2B	-3.75	1.37	1.44
2	B	305	HEC	C1B-C2B	-3.74	1.37	1.44
2	A	301	HEC	C1D-C2D	-3.73	1.37	1.44
2	A	302	HEC	C4D-C3D	-3.73	1.38	1.45
2	B	304	HEC	C1A-C2A	-3.72	1.38	1.45
2	B	301	HEC	C1D-C2D	-3.70	1.37	1.44
2	B	307	HEC	C4A-C3A	-3.67	1.38	1.45
2	A	304	HEC	FE-NB	3.67	2.06	1.94
2	A	304	HEC	C1B-C2B	-3.64	1.37	1.44
2	B	304	HEC	FE-NA	3.63	2.07	1.95
2	B	305	HEC	C4B-C3B	-3.63	1.38	1.45
2	A	307	HEC	C4A-C3A	-3.58	1.38	1.45
2	A	307	HEC	C1D-C2D	-3.58	1.37	1.44
2	B	304	HEC	C1B-C2B	-3.57	1.37	1.44
2	A	306	HEC	FE-ND	3.55	2.05	1.94
2	A	301	HEC	FE-NC	3.53	2.07	1.95
2	A	302	HEC	C4A-C3A	-3.50	1.38	1.45
2	B	302	HEC	C1B-C2B	-3.49	1.37	1.44
2	B	306	HEC	C1D-C2D	-3.48	1.37	1.44
2	A	303	HEC	C1B-C2B	-3.48	1.37	1.44
2	B	303	HEC	C1D-ND	-3.48	1.34	1.40
2	A	306	HEC	C4D-C3D	-3.47	1.39	1.45
2	A	302	HEC	C1A-C2A	-3.43	1.39	1.45
2	A	301	HEC	C1B-C2B	-3.41	1.38	1.44
2	B	307	HEC	FE-NB	3.40	2.05	1.94
2	B	303	HEC	C4B-NB	-3.39	1.34	1.40
2	A	305	HEC	C1D-C2D	-3.35	1.38	1.44
2	B	307	HEC	C1A-C2A	-3.34	1.39	1.45
2	A	306	HEC	C1D-C2D	-3.33	1.38	1.44
2	B	306	HEC	C4B-NB	-3.33	1.34	1.40
2	A	306	HEC	C1D-ND	-3.33	1.34	1.40
2	A	307	HEC	FE-NB	3.30	2.05	1.94
2	A	303	HEC	FE-ND	3.27	2.05	1.94
2	B	307	HEC	C4D-C3D	-3.26	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	306	HEC	C1D-ND	-3.25	1.34	1.40
2	B	303	HEC	C1D-C2D	-3.22	1.38	1.44
2	A	303	HEC	C1D-ND	-3.19	1.34	1.40
2	B	306	HEC	C1A-C2A	-3.18	1.39	1.45
2	A	305	HEC	C1A-C2A	-3.17	1.39	1.45
2	A	307	HEC	C4D-C3D	-3.16	1.39	1.45
2	B	303	HEC	C1B-C2B	-3.16	1.38	1.44
2	A	302	HEC	C4C-C3C	-3.14	1.38	1.44
2	A	303	HEC	C4B-NB	-3.13	1.34	1.40
2	B	307	HEC	C1D-ND	-3.13	1.34	1.40
2	A	306	HEC	C1B-C2B	-3.08	1.38	1.44
2	B	301	HEC	C1B-C2B	-3.07	1.38	1.44
2	B	304	HEC	C4A-C3A	-3.02	1.39	1.45
2	A	302	HEC	C4B-C3B	-3.01	1.39	1.45
2	A	302	HEC	FE-NA	2.96	2.05	1.95
2	A	307	HEC	C1B-C2B	-2.84	1.39	1.44
2	B	305	HEC	C4B-NB	-2.83	1.35	1.40
2	A	301	HEC	C4C-C3C	-2.82	1.39	1.44
2	B	307	HEC	C1D-C2D	-2.81	1.39	1.44
2	A	306	HEC	C4B-NB	-2.80	1.35	1.40
2	B	302	HEC	C4B-C3B	-2.74	1.40	1.45
2	A	307	HEC	FE-NC	2.72	2.04	1.95
2	A	304	HEC	C4B-C3B	-2.68	1.40	1.45
2	A	301	HEC	C1C-C2C	-2.68	1.36	1.43
2	A	305	HEC	C1C-C2C	-2.58	1.37	1.43
2	B	304	HEC	C1C-C2C	-2.57	1.37	1.43
2	A	305	HEC	FE-NA	2.56	2.03	1.95
2	B	302	HEC	C4A-NA	-2.56	1.34	1.39
2	B	306	HEC	C1C-C2C	-2.55	1.37	1.43
2	B	307	HEC	C1B-C2B	-2.55	1.39	1.44
2	B	305	HEC	C1C-C2C	-2.54	1.37	1.43
2	B	302	HEC	FE-NA	2.54	2.03	1.95
2	A	301	HEC	C4C-NC	-2.53	1.34	1.39
2	B	301	HEC	C1C-C2C	-2.53	1.37	1.43
2	A	305	HEC	C1D-ND	-2.51	1.36	1.40
2	A	303	HEC	C1C-C2C	-2.48	1.37	1.43
2	A	301	HEC	C4A-NA	-2.48	1.34	1.39
2	A	305	HEC	C4B-C3B	-2.48	1.40	1.45
2	A	302	HEC	C1C-NC	-2.47	1.35	1.39
2	A	304	HEC	C1C-NC	-2.46	1.35	1.39
2	B	301	HEC	C1A-NA	-2.46	1.35	1.39
2	B	304	HEC	C4B-C3B	-2.46	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	HEC	C4C-NC	-2.46	1.35	1.39
2	A	305	HEC	C4B-NB	-2.45	1.36	1.40
2	A	302	HEC	FE-NB	2.42	2.02	1.94
2	A	304	HEC	FE-ND	2.41	2.02	1.94
2	A	302	HEC	C1C-C2C	-2.39	1.37	1.43
2	B	305	HEC	C4C-NC	-2.35	1.35	1.39
2	A	301	HEC	C1C-NC	-2.34	1.35	1.39
2	A	307	HEC	C4B-C3B	-2.32	1.41	1.45
2	A	305	HEC	C4C-C3C	-2.32	1.40	1.44
2	A	303	HEC	C4B-C3B	-2.29	1.41	1.45
2	A	307	HEC	C4C-NC	-2.28	1.35	1.39
2	B	301	HEC	C4B-C3B	-2.26	1.41	1.45
2	B	303	HEC	C1C-C2C	-2.24	1.38	1.43
2	B	301	HEC	C4A-NA	-2.23	1.35	1.39
2	B	302	HEC	C1C-C2C	-2.22	1.38	1.43
2	B	301	HEC	C1C-NC	-2.22	1.35	1.39
2	A	305	HEC	FE-ND	2.22	2.01	1.94
2	B	307	HEC	C1C-C2C	-2.21	1.38	1.43
2	A	304	HEC	C1C-C2C	-2.21	1.38	1.43
2	A	301	HEC	FE-NB	2.20	2.01	1.94
2	A	302	HEC	C1A-NA	-2.19	1.35	1.39
2	A	306	HEC	C3B-C2B	2.19	1.41	1.36
2	A	306	HEC	C1C-C2C	-2.15	1.38	1.43
2	A	302	HEC	C4B-NB	-2.14	1.36	1.40
2	B	302	HEC	C4C-C3C	-2.12	1.40	1.44
2	A	303	HEC	FE-NB	2.12	2.01	1.94
2	B	304	HEC	C4A-NA	-2.11	1.35	1.39
2	B	307	HEC	C4C-C3C	-2.11	1.40	1.44
2	B	307	HEC	C4D-ND	-2.10	1.34	1.38
2	B	305	HEC	FE-NA	2.09	2.02	1.95
2	A	307	HEC	C4A-NA	-2.08	1.35	1.39
2	B	304	HEC	C4B-NB	-2.07	1.36	1.40
2	B	305	HEC	FE-ND	2.07	2.01	1.94
2	B	301	HEC	C4C-C3C	-2.06	1.40	1.44
2	B	304	HEC	C1C-NC	-2.05	1.35	1.39
2	A	307	HEC	C1C-C2C	-2.04	1.38	1.43

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	306	HEC	CAB-C3B-C4B	13.45	142.26	124.81
2	B	306	HEC	CAB-C3B-C2B	-9.32	111.58	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	303	HEC	CAA-CBA-CGA	6.80	128.24	113.60
2	B	307	HEC	CBA-CAA-C2A	5.54	128.03	112.63
2	A	301	HEC	CAC-C3C-C2C	4.69	134.37	126.86
2	B	301	HEC	CAC-C3C-C2C	4.52	134.10	126.86
2	A	301	HEC	CAC-C3C-C4C	-4.41	118.80	124.92
2	B	307	HEC	CAA-CBA-CGA	-4.32	104.31	113.60
2	B	306	HEC	CHC-C4B-NB	-4.01	119.44	124.37
2	B	301	HEC	CAC-C3C-C4C	-3.92	119.47	124.92
2	A	303	HEC	CAB-C3B-C4B	-3.73	119.97	124.81
2	A	305	HEC	CAA-CBA-CGA	3.69	121.54	113.60
2	B	306	HEC	CHC-C4B-C3B	3.66	132.20	125.33
2	B	303	HEC	CAA-CBA-CGA	3.43	120.98	113.60
2	A	302	HEC	CBA-CAA-C2A	3.35	121.93	112.63
2	A	302	HEC	CAC-C3C-C2C	3.25	132.06	126.86
2	A	305	HEC	CAC-C3C-C2C	3.13	131.88	126.86
2	A	303	HEC	CAB-C3B-C2B	3.08	132.81	127.53
2	B	303	HEC	CBA-CAA-C2A	-3.05	104.16	112.63
2	B	304	HEC	CHB-C4A-NA	-3.00	121.20	124.44
2	A	307	HEC	CAC-C3C-C2C	2.92	131.54	126.86
2	A	304	HEC	CAA-CBA-CGA	2.91	119.86	113.60
2	A	306	HEC	CHB-C4A-NA	2.90	127.57	124.44
2	B	307	HEC	C1D-ND-C4D	2.86	108.03	105.07
2	A	301	HEC	O1A-CGA-CBA	-2.82	114.04	123.08
2	A	306	HEC	C1D-ND-C4D	2.75	107.91	105.07
2	B	306	HEC	CHB-C1B-NB	2.60	127.25	124.42
2	B	307	HEC	C4B-NB-C1B	2.58	107.73	105.07
2	A	305	HEC	C4B-NB-C1B	2.56	107.72	105.07
2	A	305	HEC	CHB-C4A-NA	-2.50	121.74	124.44
2	B	302	HEC	O1A-CGA-CBA	-2.49	115.10	123.08
2	A	305	HEC	C1A-CHA-C4D	2.43	131.29	126.06
2	B	304	HEC	O1D-CGD-CBD	-2.42	115.29	123.08
2	B	303	HEC	O1D-CGD-CBD	-2.39	115.40	123.08
2	A	304	HEC	CBA-CAA-C2A	-2.39	105.98	112.63
2	B	304	HEC	CHA-C4D-ND	2.39	127.01	124.42
2	A	305	HEC	O2A-CGA-CBA	2.38	121.69	114.03
2	A	306	HEC	C4B-NB-C1B	2.33	107.48	105.07
2	B	301	HEC	C4A-NA-C1A	2.32	107.62	105.35
2	B	306	HEC	C4B-NB-C1B	2.29	107.44	105.07
2	A	301	HEC	O2A-CGA-CBA	2.28	121.37	114.03
2	A	307	HEC	O1D-CGD-CBD	-2.26	115.82	123.08
2	B	301	HEC	CBA-CAA-C2A	2.25	118.87	112.63
2	A	303	HEC	CBA-CAA-C2A	-2.24	106.39	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	305	HEC	O1A-CGA-CBA	-2.23	115.92	123.08
2	B	307	HEC	CHA-C4D-C3D	2.20	128.07	124.84
2	B	301	HEC	C4C-NC-C1C	2.19	107.49	105.35
2	A	305	HEC	CHA-C1A-NA	-2.18	122.08	124.44
2	A	305	HEC	C1D-ND-C4D	2.17	107.32	105.07
2	B	304	HEC	CAC-C3C-C2C	2.17	130.34	126.86
2	A	305	HEC	CHA-C1A-C2A	2.17	128.45	124.94
2	B	306	HEC	C1D-ND-C4D	2.15	107.30	105.07
2	A	302	HEC	CHB-C4A-NA	-2.15	122.11	124.44
2	B	302	HEC	CHB-C4A-NA	-2.15	122.12	124.44
2	B	305	HEC	CHB-C4A-NA	2.14	126.76	124.44
2	B	305	HEC	CBA-CAA-C2A	-2.13	106.70	112.63
2	A	305	HEC	C3D-C4D-ND	-2.13	108.29	110.36
2	B	302	HEC	CAC-C3C-C2C	2.13	130.28	126.86
2	A	306	HEC	O1D-CGD-CBD	-2.12	116.28	123.08
2	A	301	HEC	CMC-C2C-C3C	2.11	130.16	125.61
2	B	303	HEC	CHD-C1D-ND	-2.10	121.78	124.37
2	B	304	HEC	O1A-CGA-CBA	-2.09	116.37	123.08
2	A	302	HEC	CHA-C1A-NA	-2.08	122.19	124.44
2	B	306	HEC	CBA-CAA-C2A	-2.05	106.94	112.63
2	A	302	HEC	CHA-C1A-C2A	2.03	128.22	124.94
2	B	302	HEC	O2A-CGA-CBA	2.03	120.54	114.03
2	A	305	HEC	CHB-C1B-NB	2.02	126.61	124.42
2	B	304	HEC	O2A-CGA-CBA	2.01	120.47	114.03

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	HEC	NA
2	A	302	HEC	NA
2	A	303	HEC	NA
2	A	304	HEC	NA
2	A	305	HEC	NA
2	A	306	HEC	NA
2	A	307	HEC	NA
2	B	301	HEC	NA
2	B	302	HEC	NA
2	B	303	HEC	NA
2	B	304	HEC	NA
2	B	305	HEC	NA
2	B	306	HEC	NA
2	B	307	HEC	NA

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	HEC	C2C-C3C-CAC-CBC
2	B	301	HEC	C2C-C3C-CAC-CBC
2	B	301	HEC	C4C-C3C-CAC-CBC
2	A	301	HEC	C4C-C3C-CAC-CBC
2	A	301	HEC	C2D-C3D-CAD-CBD
2	B	302	HEC	C2B-C3B-CAB-CBB
2	A	302	HEC	C2B-C3B-CAB-CBB
2	A	301	HEC	C3D-CAD-CBD-CGD
2	A	301	HEC	C4D-C3D-CAD-CBD
2	B	304	HEC	C2B-C3B-CAB-CBB
2	B	304	HEC	C4C-C3C-CAC-CBC
2	B	306	HEC	C4C-C3C-CAC-CBC
2	B	303	HEC	C2B-C3B-CAB-CBB
2	B	304	HEC	C2C-C3C-CAC-CBC
2	A	307	HEC	C2B-C3B-CAB-CBB
2	B	301	HEC	C3D-CAD-CBD-CGD
2	A	303	HEC	C4C-C3C-CAC-CBC
2	A	303	HEC	C2C-C3C-CAC-CBC
2	A	302	HEC	C4B-C3B-CAB-CBB
2	B	306	HEC	C2C-C3C-CAC-CBC
2	A	306	HEC	C4C-C3C-CAC-CBC
2	B	302	HEC	C3D-CAD-CBD-CGD
2	A	307	HEC	C2C-C3C-CAC-CBC
2	B	302	HEC	C4B-C3B-CAB-CBB
2	A	303	HEC	C2B-C3B-CAB-CBB
2	A	304	HEC	C2B-C3B-CAB-CBB
2	A	307	HEC	C4C-C3C-CAC-CBC
2	B	307	HEC	C4C-C3C-CAC-CBC
2	A	304	HEC	C4C-C3C-CAC-CBC
2	A	306	HEC	C2C-C3C-CAC-CBC
2	A	304	HEC	C2C-C3C-CAC-CBC
2	B	301	HEC	C4D-C3D-CAD-CBD
2	B	306	HEC	C2B-C3B-CAB-CBB
2	A	307	HEC	C4B-C3B-CAB-CBB
2	B	304	HEC	C4B-C3B-CAB-CBB
2	B	301	HEC	C2D-C3D-CAD-CBD
2	A	305	HEC	C4C-C3C-CAC-CBC
2	B	307	HEC	C2C-C3C-CAC-CBC
2	A	305	HEC	C2B-C3B-CAB-CBB
2	B	302	HEC	C4C-C3C-CAC-CBC
2	A	302	HEC	C4C-C3C-CAC-CBC
2	B	303	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	B	305	HEC	C2B-C3B-CAB-CBB
2	A	304	HEC	C4B-C3B-CAB-CBB
2	B	302	HEC	C4D-C3D-CAD-CBD
2	B	302	HEC	C2D-C3D-CAD-CBD
2	B	305	HEC	C4C-C3C-CAC-CBC
2	A	306	HEC	CAA-CBA-CGA-O2A
2	B	303	HEC	C4C-C3C-CAC-CBC
2	B	304	HEC	CAA-CBA-CGA-O1A
2	B	306	HEC	C4B-C3B-CAB-CBB
2	A	303	HEC	CAD-CBD-CGD-O1D
2	A	306	HEC	CAD-CBD-CGD-O2D
2	A	307	HEC	CAA-CBA-CGA-O1A
2	A	301	HEC	CAD-CBD-CGD-O2D
2	B	301	HEC	CAA-CBA-CGA-O1A
2	B	301	HEC	CAA-CBA-CGA-O2A
2	B	307	HEC	CAD-CBD-CGD-O1D
2	A	301	HEC	CAD-CBD-CGD-O1D
2	A	307	HEC	CAA-CBA-CGA-O2A
2	B	304	HEC	CAA-CBA-CGA-O2A
2	A	306	HEC	CAD-CBD-CGD-O1D
2	A	306	HEC	CAA-CBA-CGA-O1A
2	A	301	HEC	CAA-CBA-CGA-O1A
2	A	301	HEC	CAA-CBA-CGA-O2A
2	A	305	HEC	CAA-CBA-CGA-O1A
2	A	305	HEC	CAA-CBA-CGA-O2A
2	B	307	HEC	CAA-CBA-CGA-O2A
2	B	307	HEC	CAD-CBD-CGD-O2D
2	A	302	HEC	CAA-CBA-CGA-O2A
2	A	303	HEC	CAD-CBD-CGD-O2D
2	A	305	HEC	C2C-C3C-CAC-CBC
2	B	301	HEC	CAD-CBD-CGD-O2D
2	A	303	HEC	C2A-CAA-CBA-CGA
2	A	302	HEC	CAA-CBA-CGA-O1A
2	B	303	HEC	CAD-CBD-CGD-O2D
2	B	303	HEC	CAA-CBA-CGA-O1A
2	B	302	HEC	C2C-C3C-CAC-CBC
2	A	305	HEC	CAD-CBD-CGD-O2D
2	B	302	HEC	CAA-CBA-CGA-O2A
2	A	302	HEC	CAD-CBD-CGD-O1D
2	B	301	HEC	CAD-CBD-CGD-O1D
2	B	303	HEC	CAD-CBD-CGD-O1D
2	B	307	HEC	CAA-CBA-CGA-O1A

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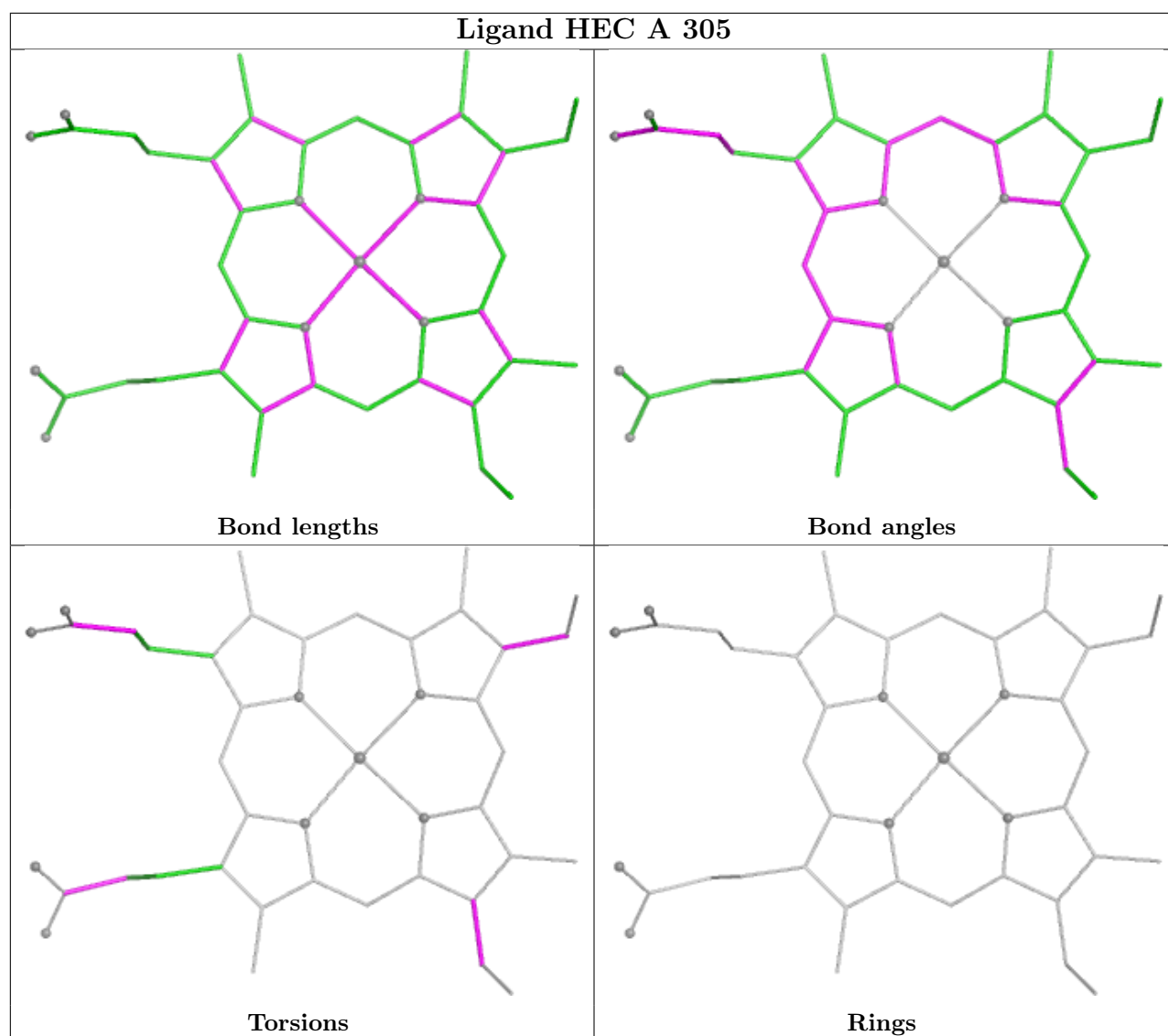
Mol	Chain	Res	Type	Atoms
2	A	303	HEC	C4B-C3B-CAB-CBB
2	A	305	HEC	CAD-CBD-CGD-O1D
2	B	302	HEC	CAA-CBA-CGA-O1A
2	B	305	HEC	C4B-C3B-CAB-CBB
2	A	302	HEC	CAD-CBD-CGD-O2D
2	B	303	HEC	CAA-CBA-CGA-O2A
2	B	305	HEC	CAA-CBA-CGA-O2A
2	B	303	HEC	C2C-C3C-CAC-CBC
2	A	307	HEC	CAD-CBD-CGD-O2D
2	A	303	HEC	CAA-CBA-CGA-O2A
2	B	305	HEC	CAA-CBA-CGA-O1A

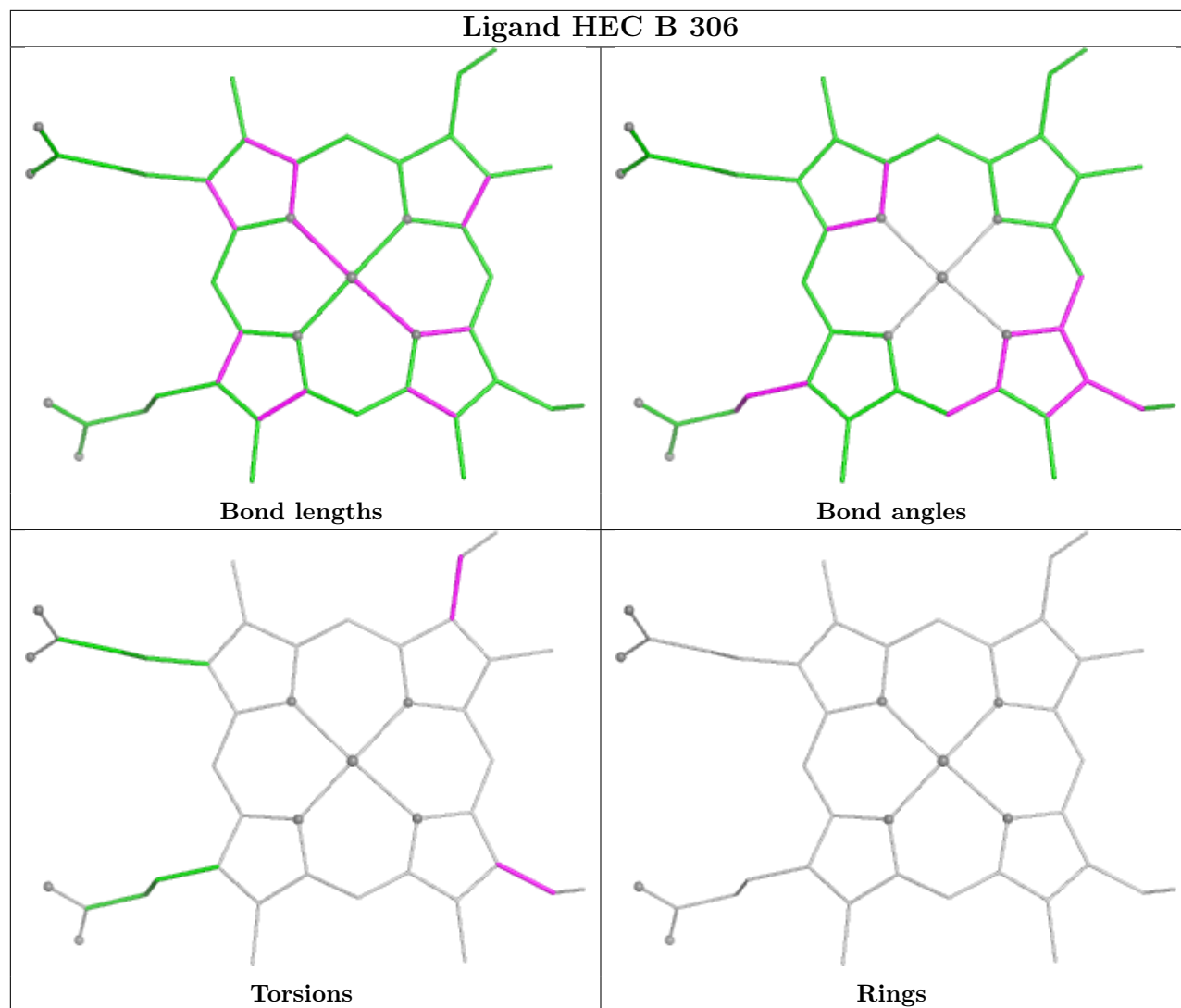
There are no ring outliers.

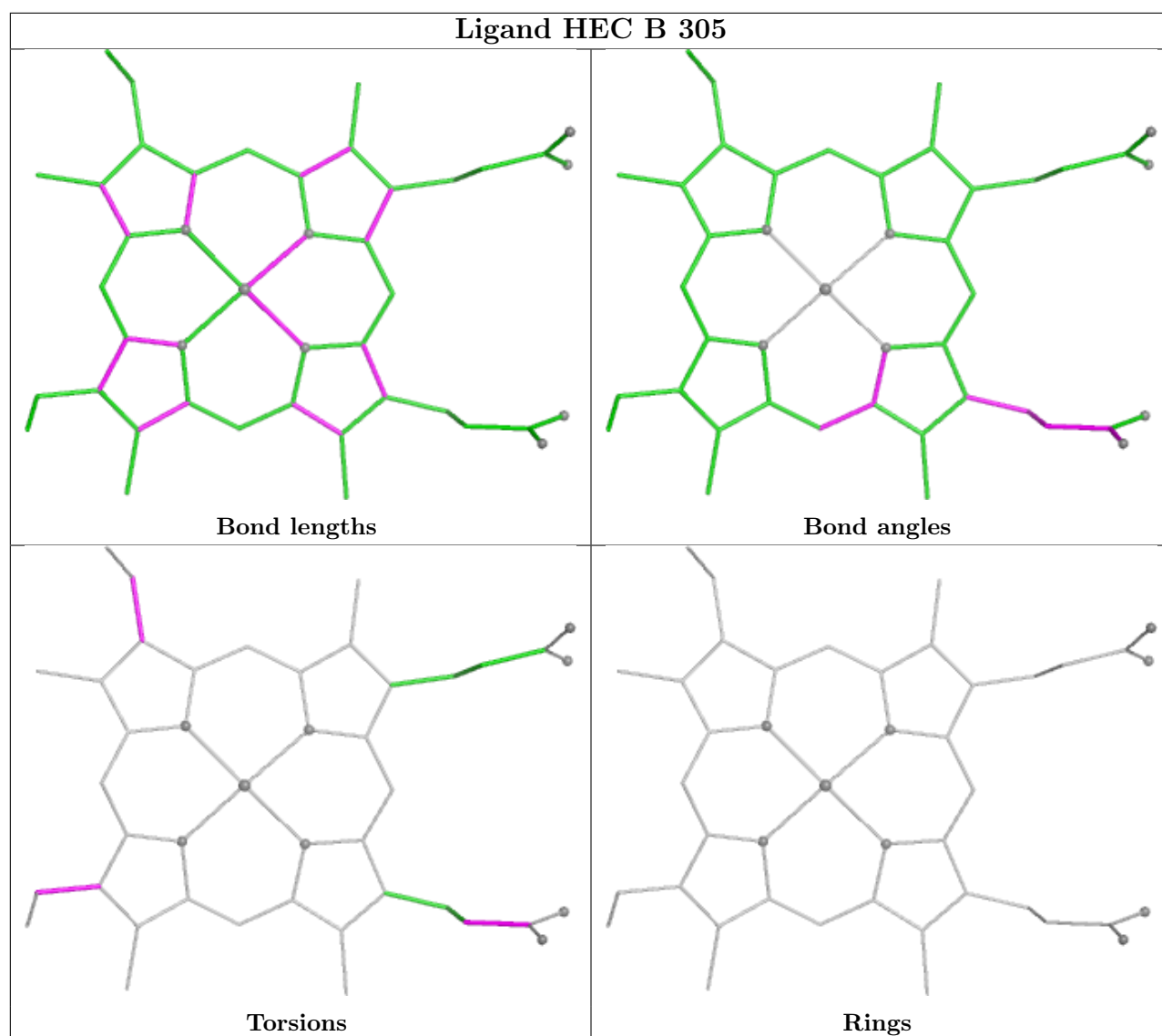
3 monomers are involved in 4 short contacts:

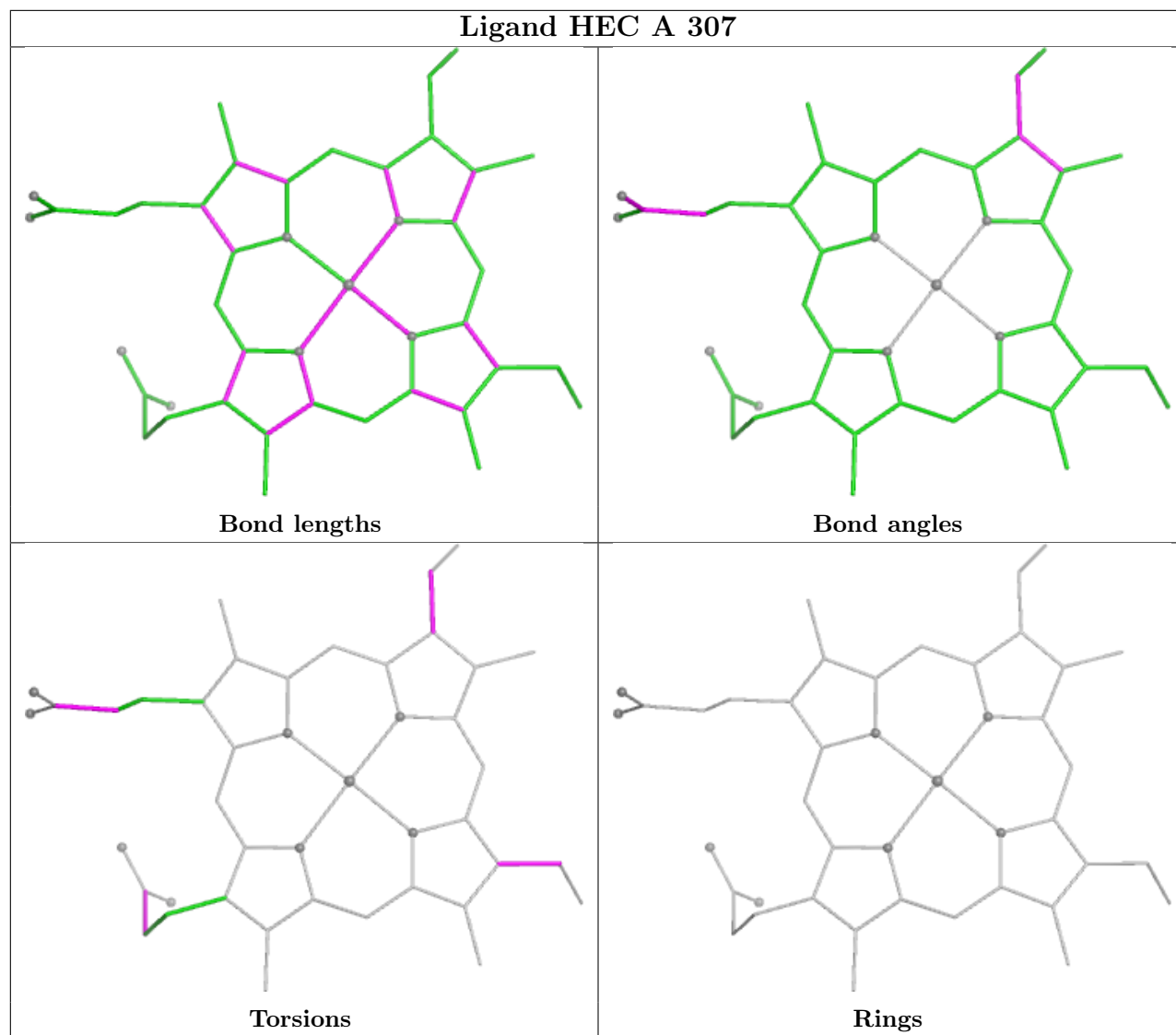
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	306	HEC	1	0
2	A	304	HEC	2	0
2	B	304	HEC	1	0

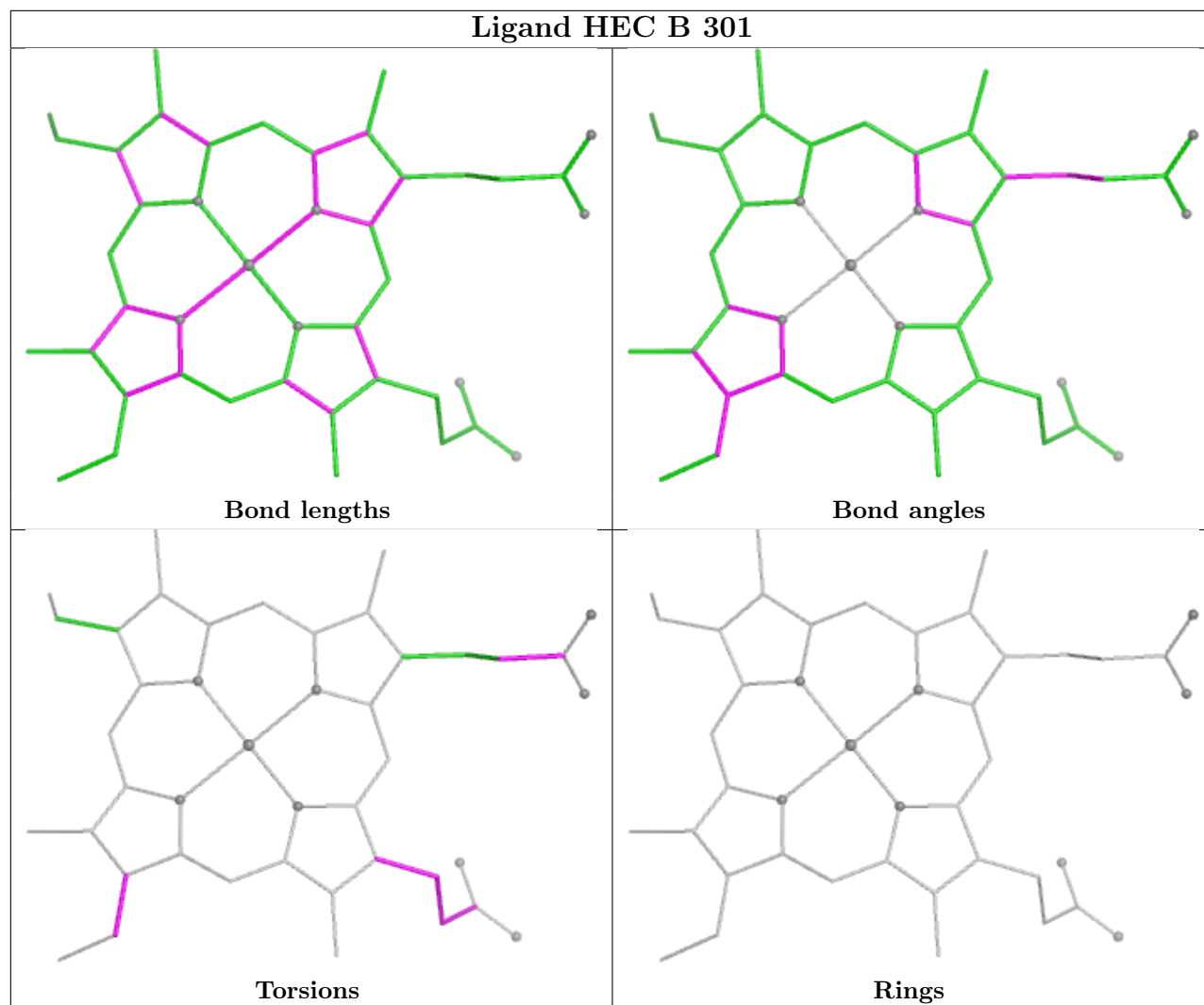
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

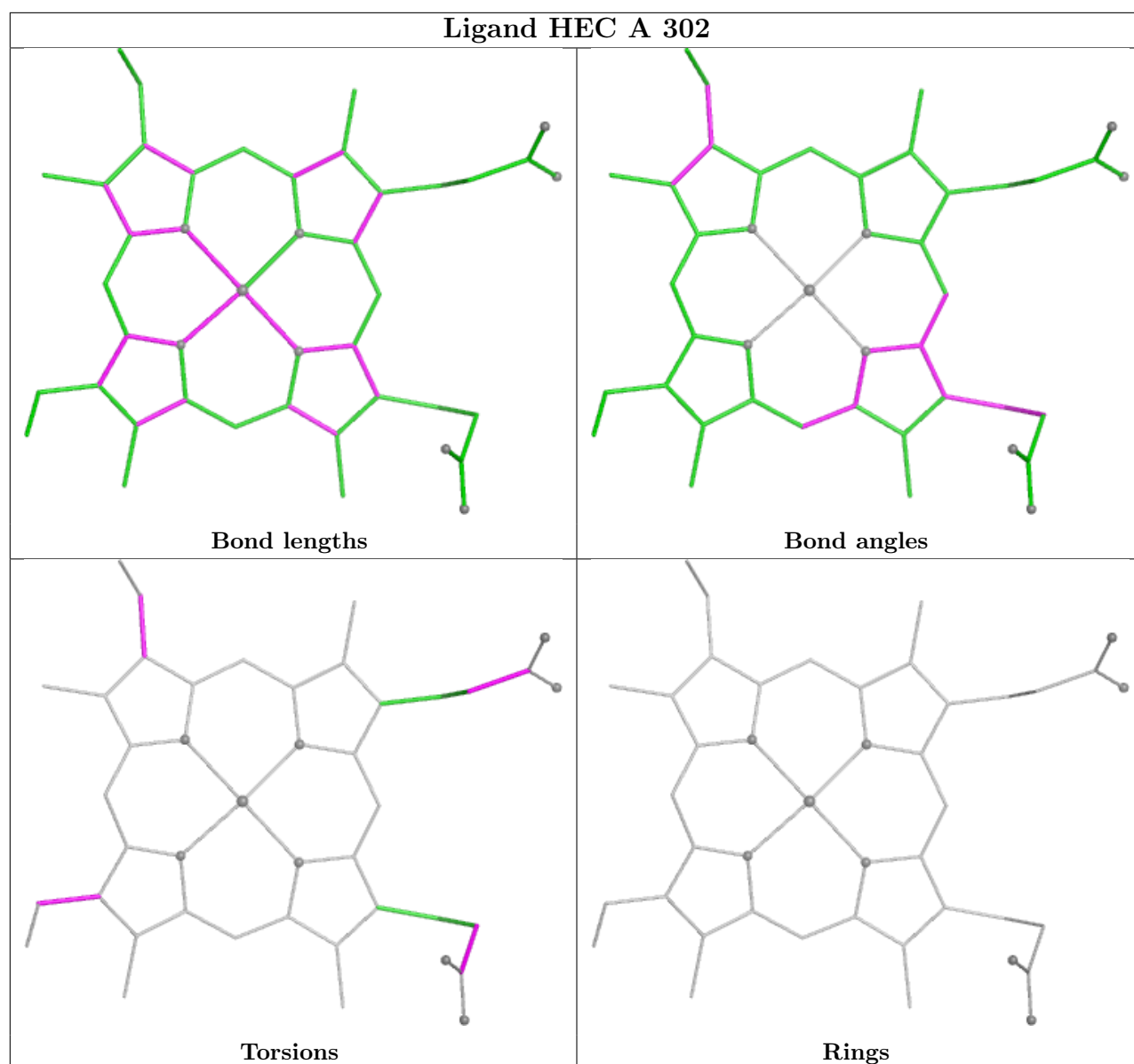


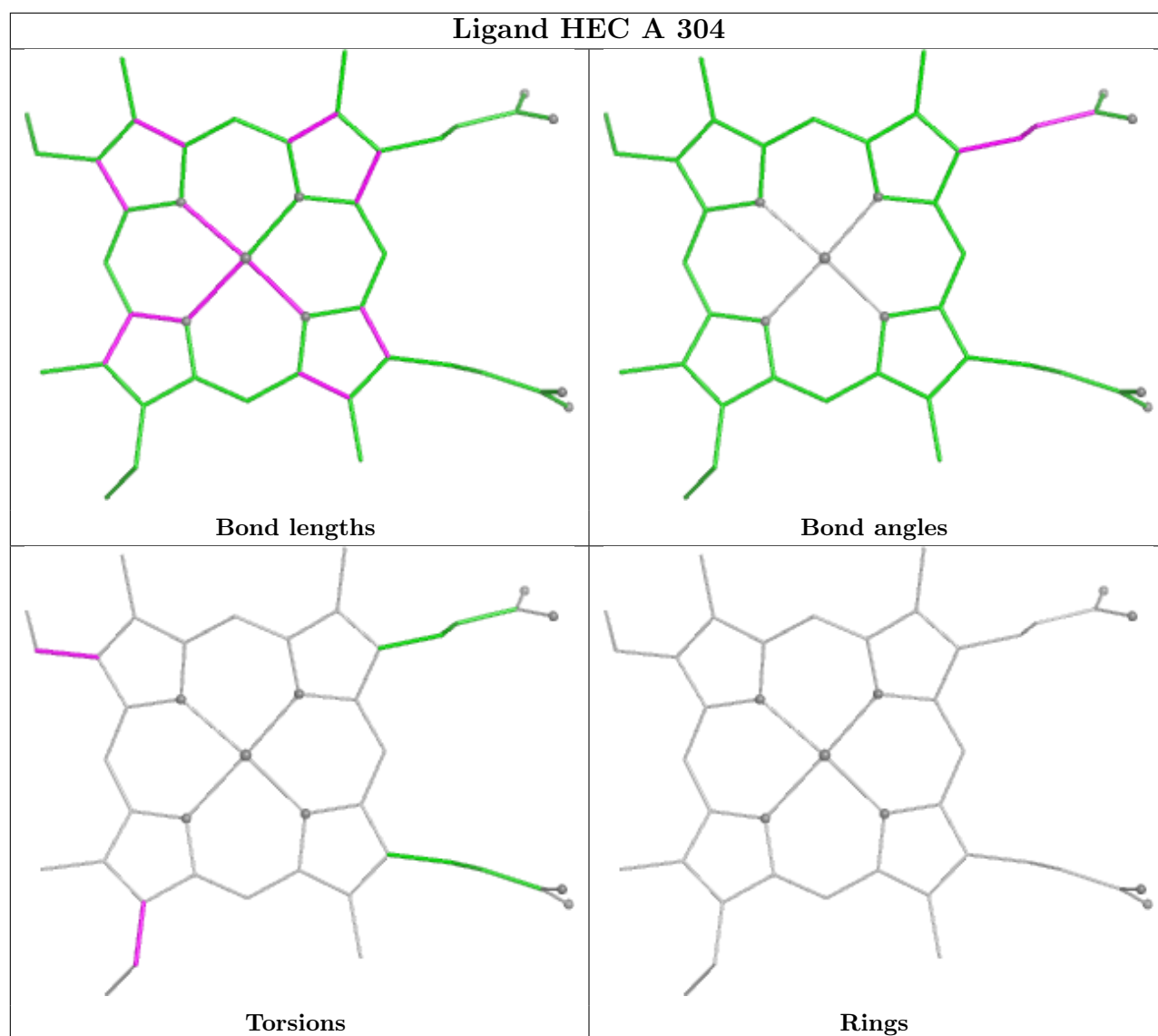


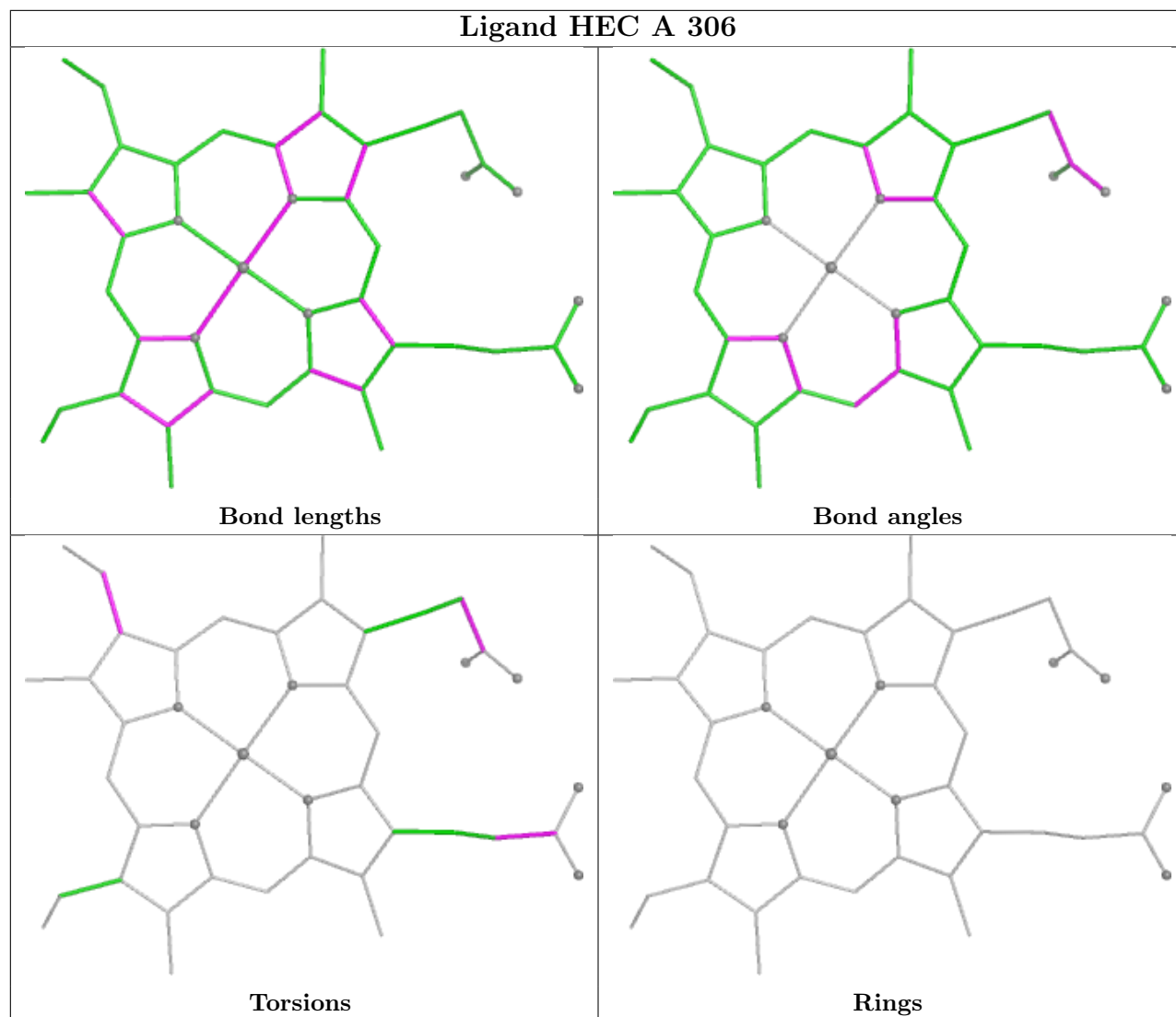


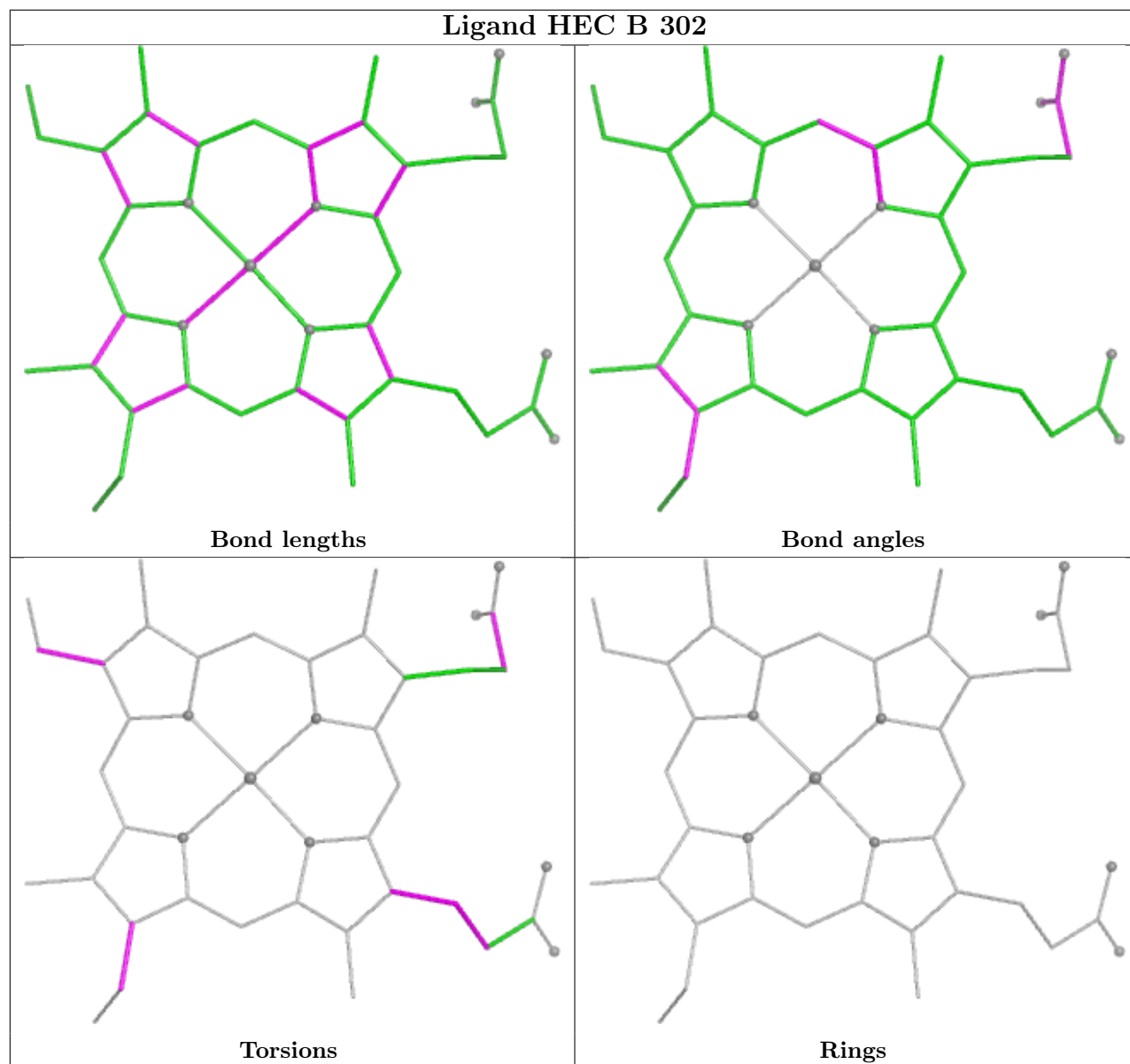


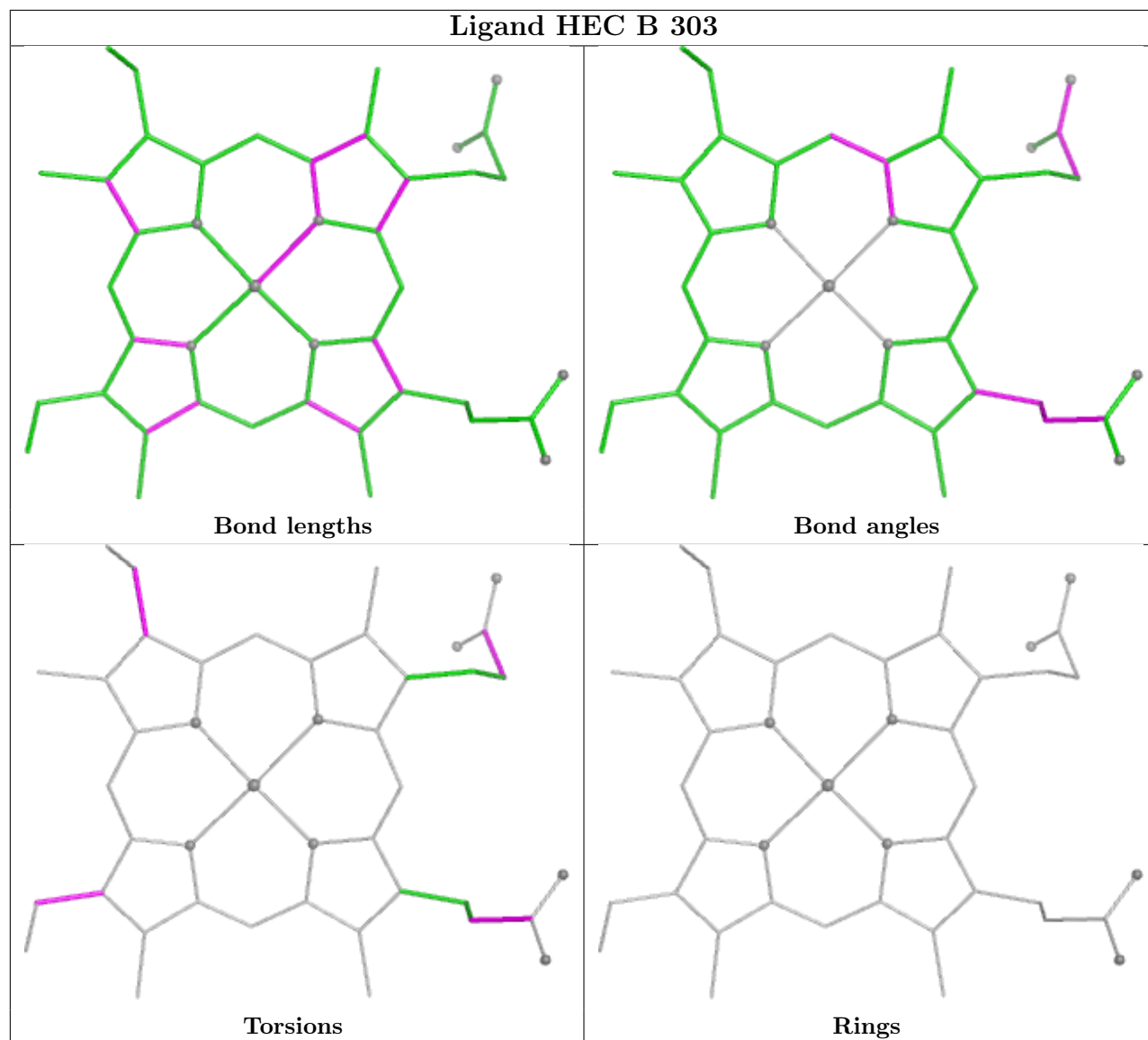


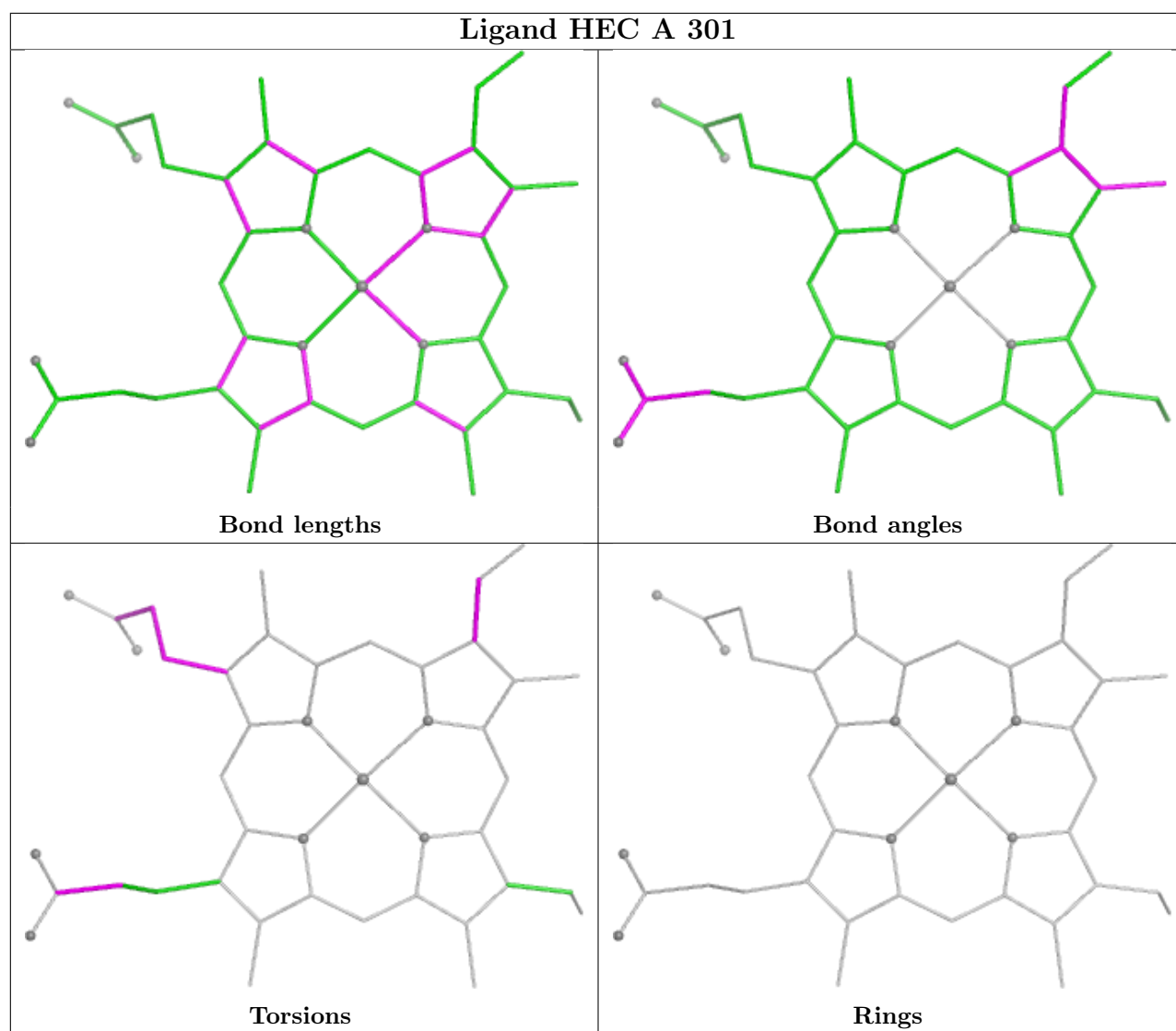


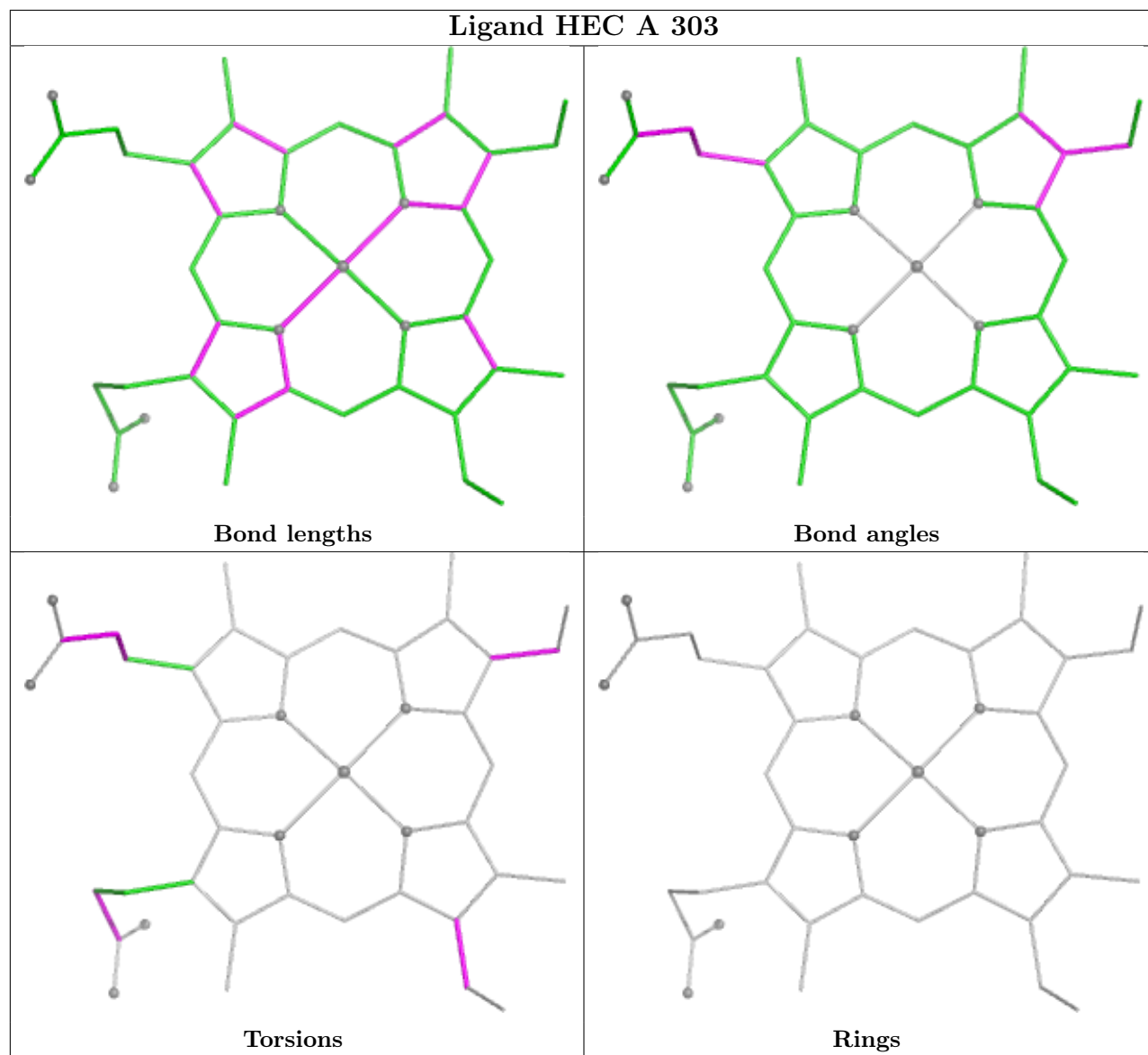


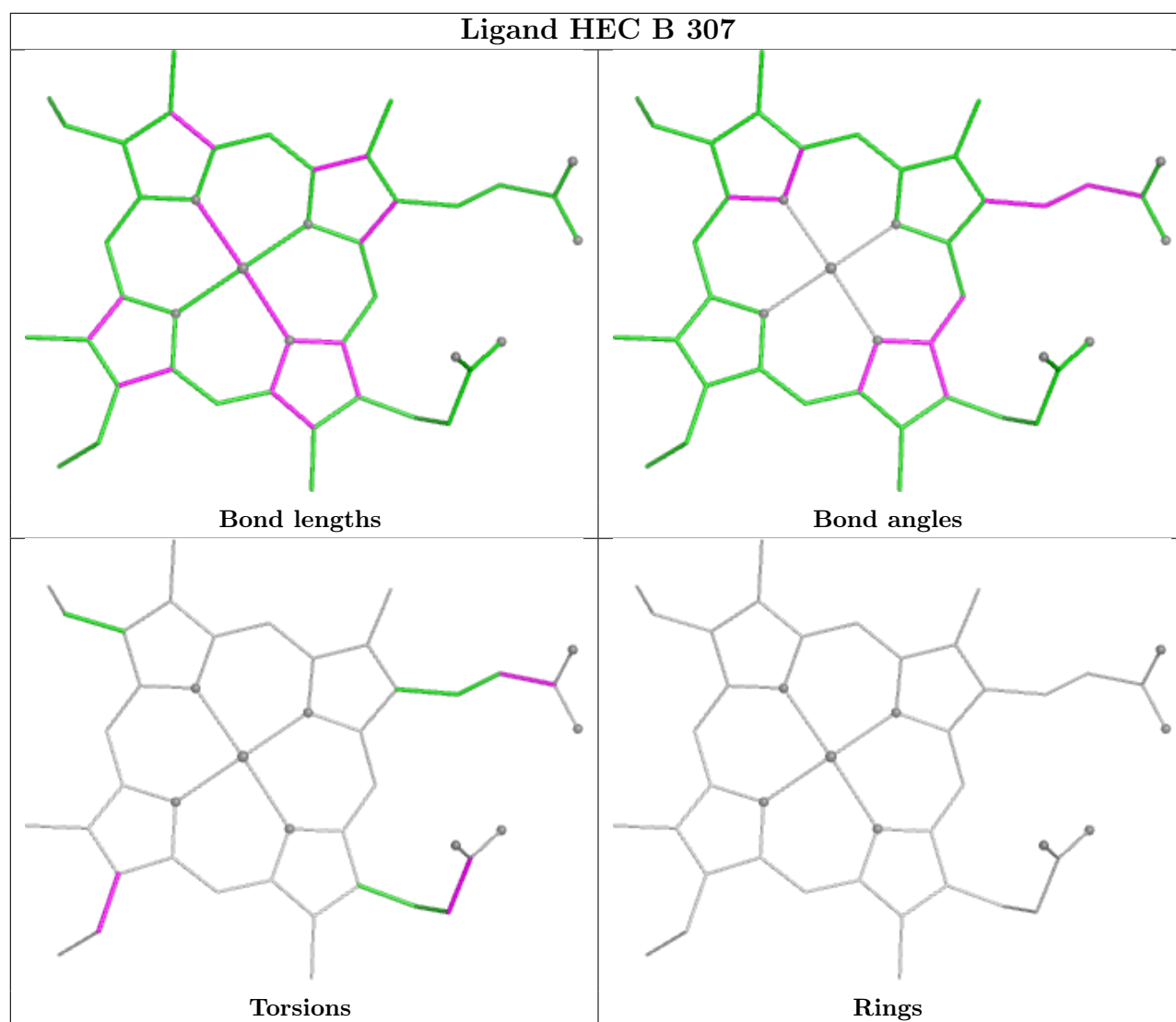


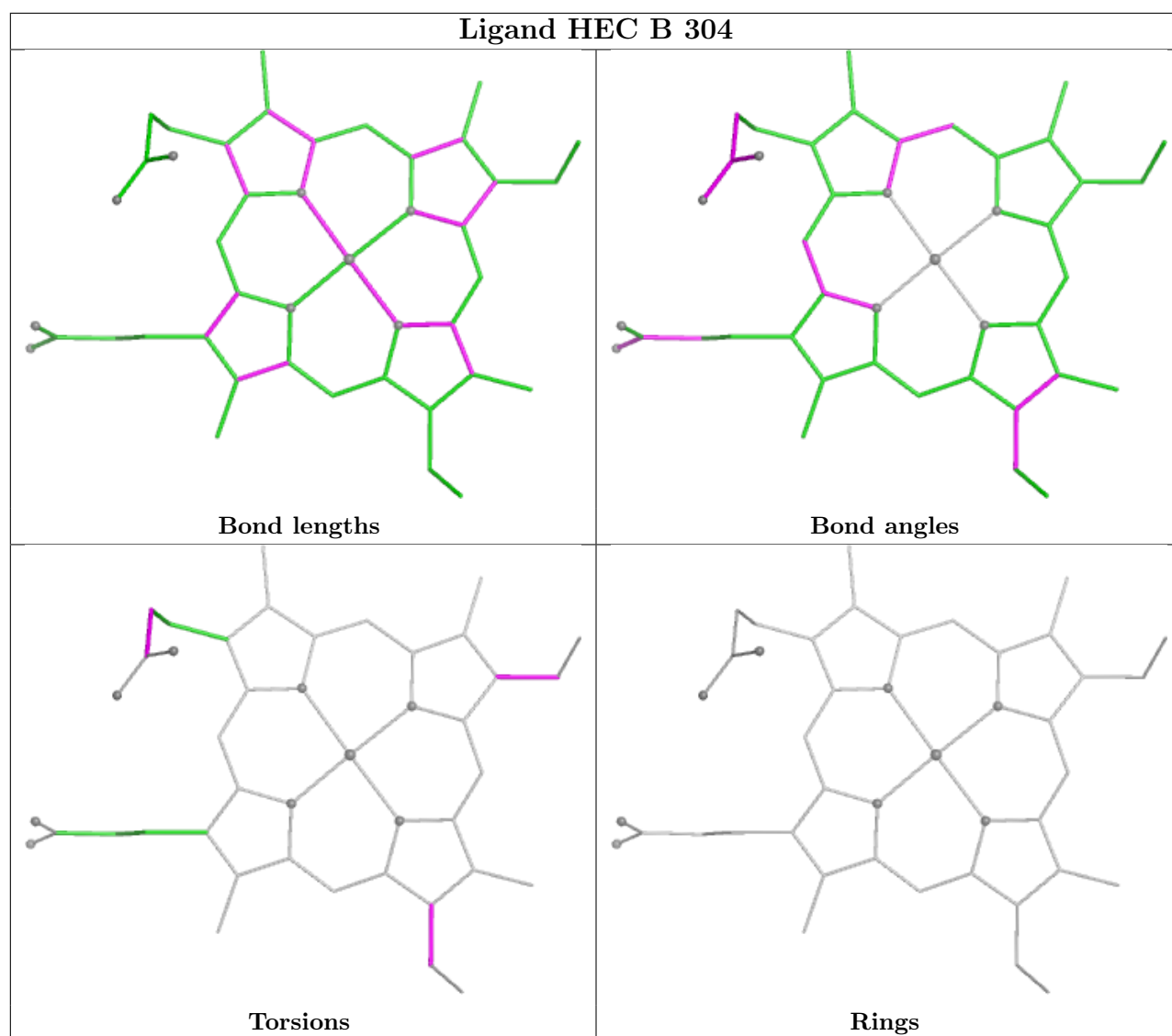












5.7 Other polymers [i](#)

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	277/278 (99%)	0.13	13 (4%) 36 41	26, 41, 88, 147	1 (0%)
1	B	277/278 (99%)	0.58	25 (9%) 15 18	26, 51, 103, 144	1 (0%)
All	All	554/556 (99%)	0.36	38 (6%) 23 27	26, 46, 96, 147	2 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	THR	5.5
1	A	280	THR	5.0
1	A	182	ASP	4.2
1	B	276	LEU	4.2
1	A	5	ALA	4.1
1	A	160	GLY	4.0
1	A	163	PRO	3.7
1	B	185	VAL	3.6
1	B	280	THR	3.3
1	A	279	GLY	3.2
1	B	188	ILE	3.2
1	A	180	PRO	3.1
1	B	189	ILE	3.1
1	B	179	LEU	3.0
1	B	163	PRO	2.9
1	A	183	ARG	2.9
1	B	277	LEU	2.8
1	B	183	ARG	2.7
1	B	181	GLY	2.6
1	B	205	PHE	2.6
1	A	281	PRO	2.6
1	B	101	THR	2.6
1	B	38	ILE	2.6
1	B	178	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	278	TYR	2.5
1	B	266	VAL	2.5
1	A	278	TYR	2.4
1	B	196	TYR	2.4
1	B	5	ALA	2.4
1	B	209	ALA	2.3
1	A	211	HIS	2.3
1	A	178	THR	2.3
1	B	172	TYR	2.1
1	B	180	PRO	2.1
1	A	162	LYS	2.1
1	B	182	ASP	2.1
1	B	160	GLY	2.0
1	B	197	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

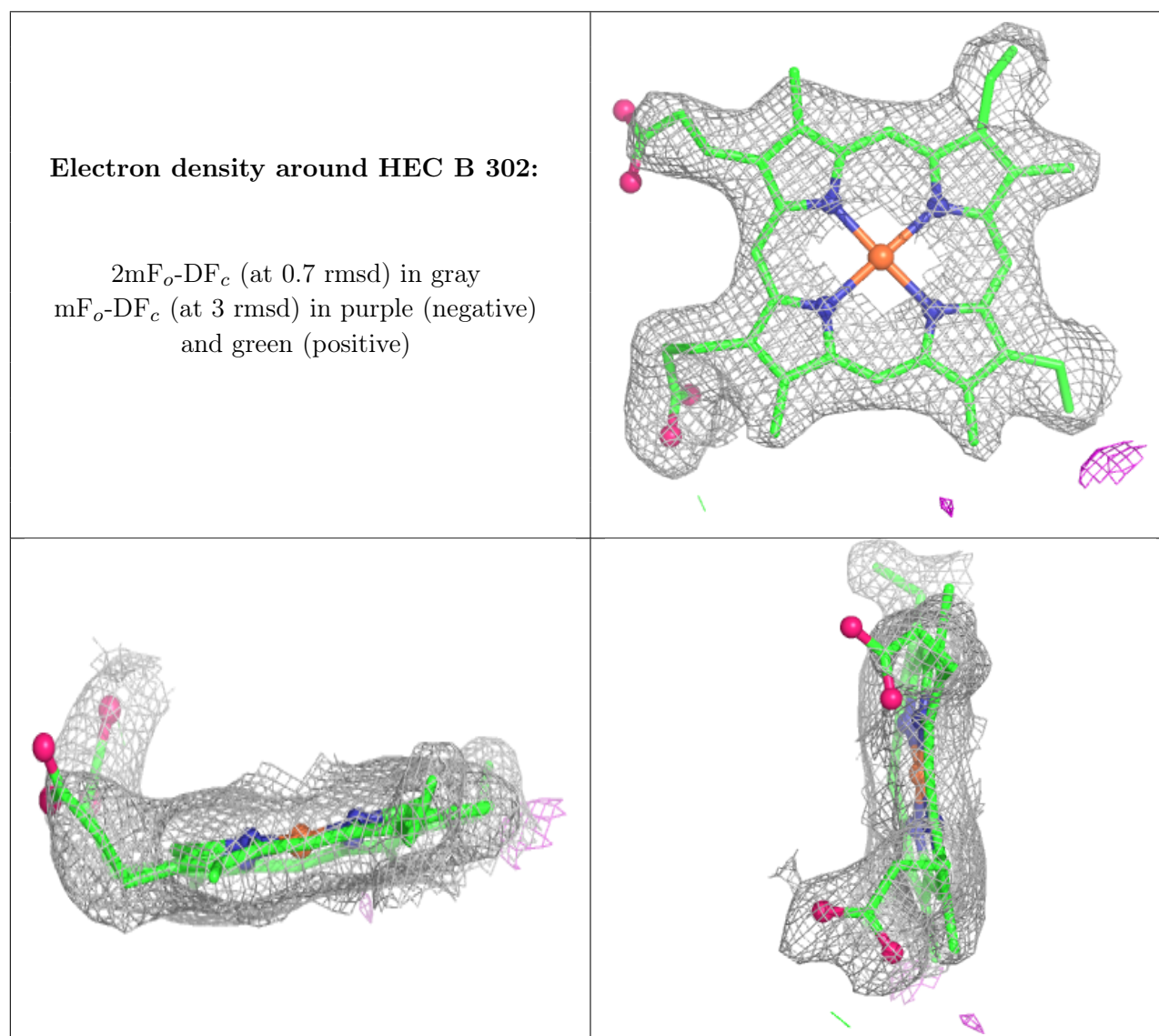
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	B	308	1/1	0.95	0.07	84,84,84,84	0
2	HEC	B	302	43/43	0.97	0.08	41,49,75,97	0
2	HEC	A	304	43/43	0.98	0.06	29,32,47,64	0
2	HEC	A	305	43/43	0.98	0.06	26,32,47,50	0
2	HEC	A	306	43/43	0.98	0.07	26,32,63,86	0
2	HEC	A	307	43/43	0.98	0.06	25,33,46,57	0
2	HEC	B	301	43/43	0.98	0.06	36,38,61,91	0
2	HEC	A	301	43/43	0.98	0.07	29,39,61,80	0
2	HEC	B	303	43/43	0.98	0.06	33,38,44,48	0

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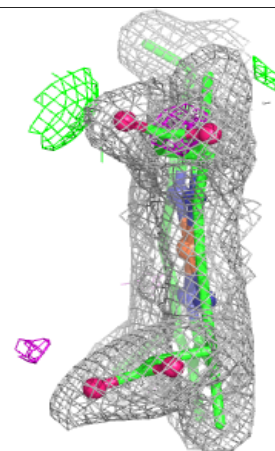
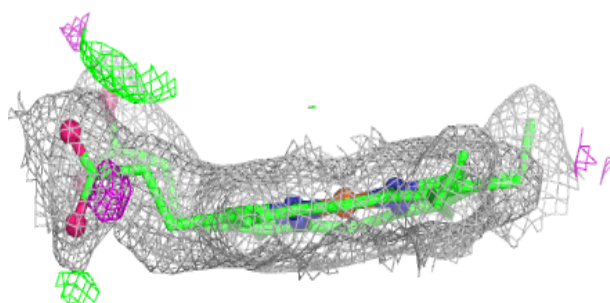
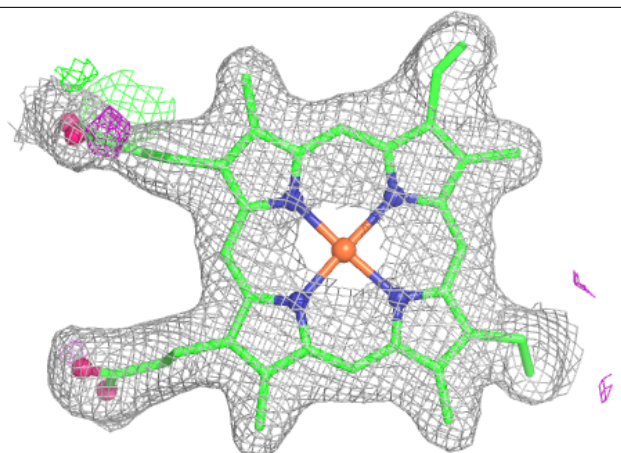
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEC	B	304	43/43	0.98	0.07	30,37,47,55	0
2	HEC	B	305	43/43	0.98	0.07	35,43,60,73	0
2	HEC	B	306	43/43	0.98	0.06	31,34,55,60	0
2	HEC	B	307	43/43	0.98	0.09	33,37,64,96	0
2	HEC	A	302	43/43	0.98	0.07	27,35,65,89	0
3	CA	A	308	1/1	0.99	0.02	39,39,39,39	0
2	HEC	A	303	43/43	0.99	0.05	27,30,40,48	0
4	MG	B	309	1/1	0.99	0.02	38,38,38,38	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.



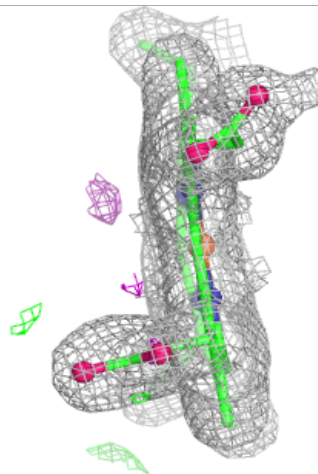
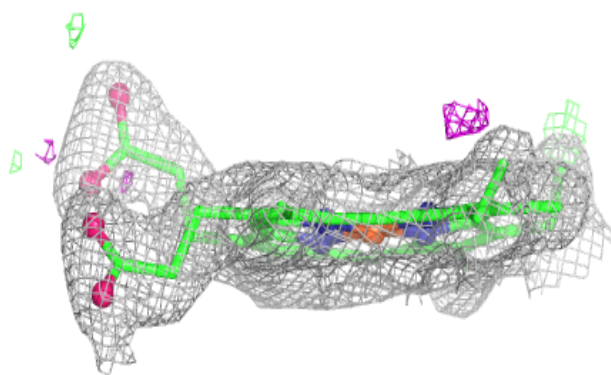
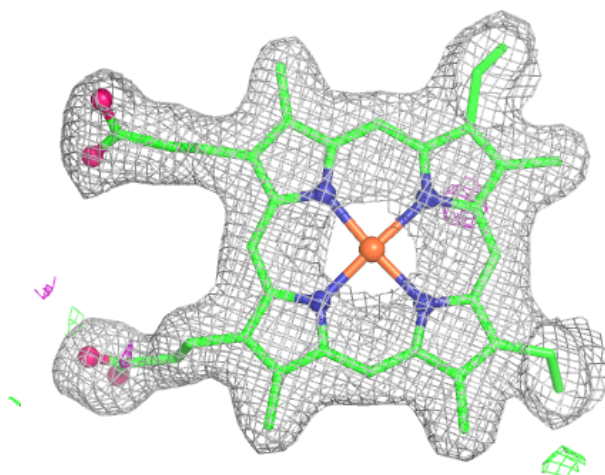
Electron density around HEC A 304:

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



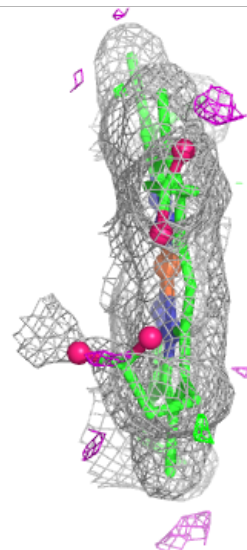
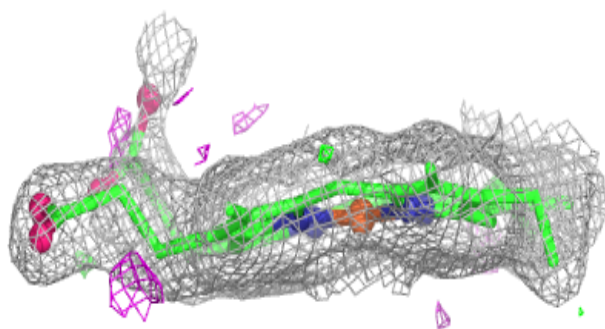
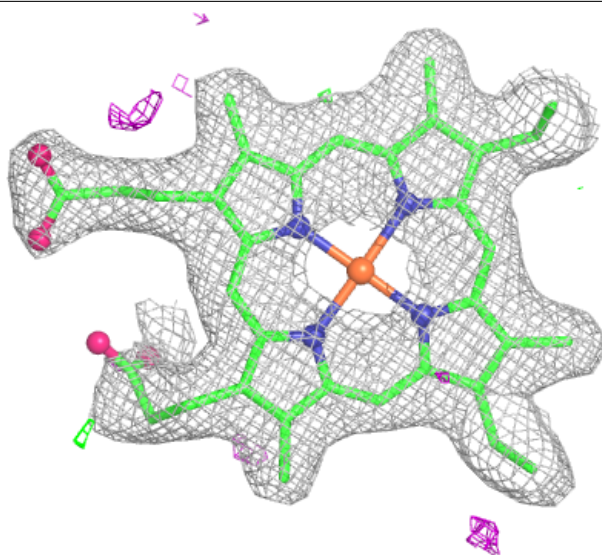
Electron density around HEC A 305:

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



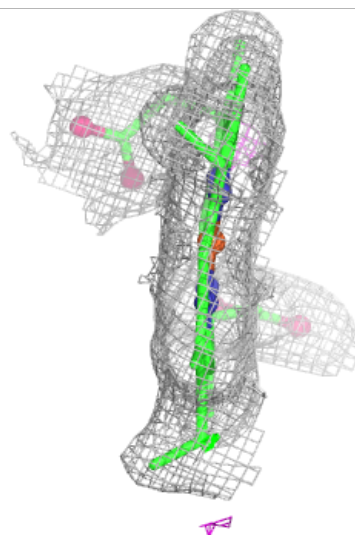
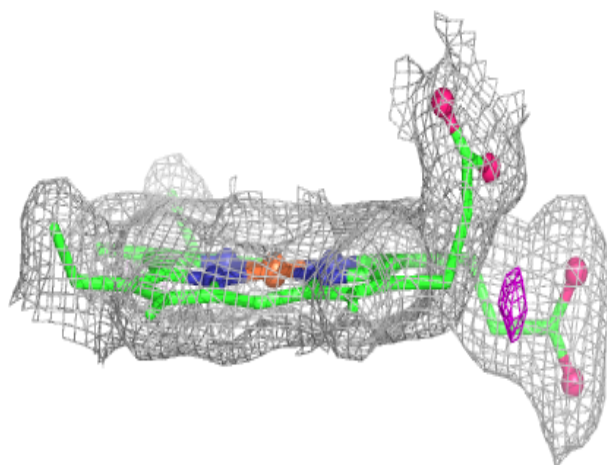
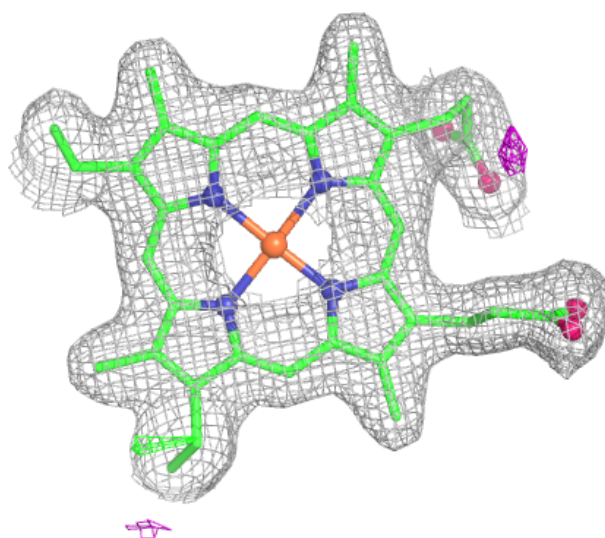
Electron density around HEC A 306:

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



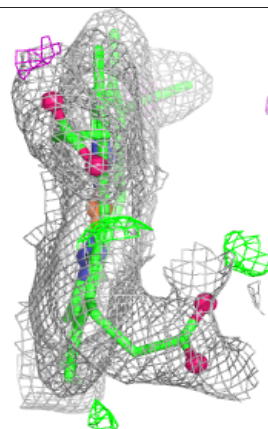
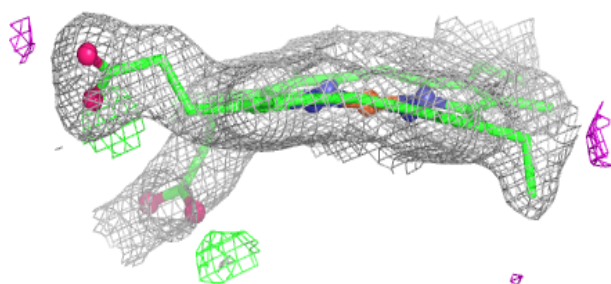
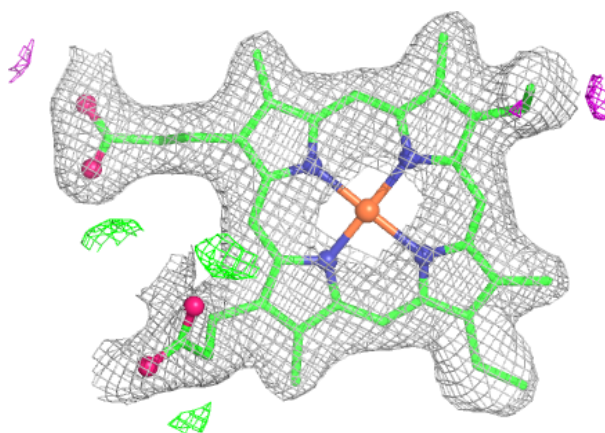
Electron density around HEC A 307:

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



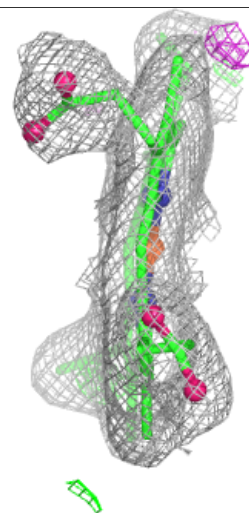
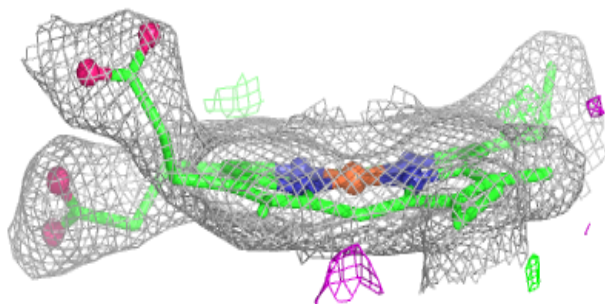
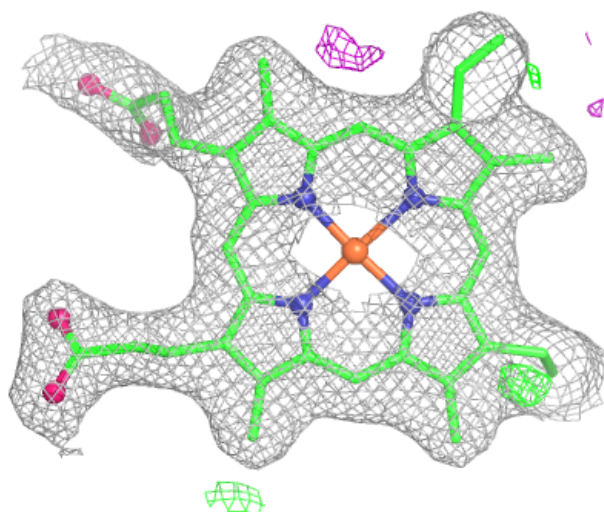
Electron density around HEC B 301:

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



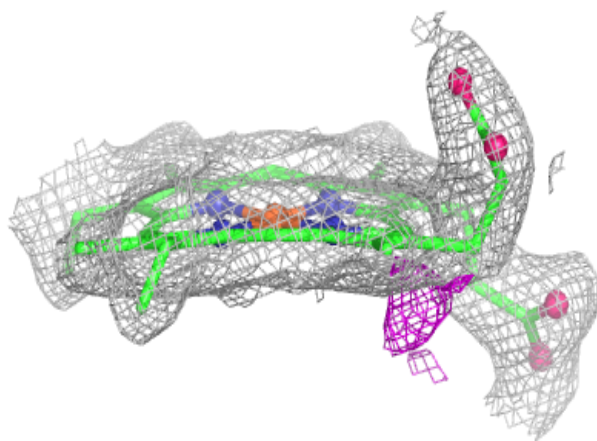
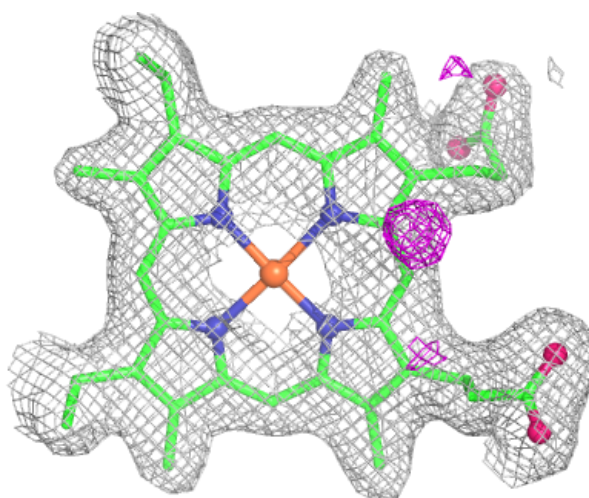
Electron density around HEC A 301:

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



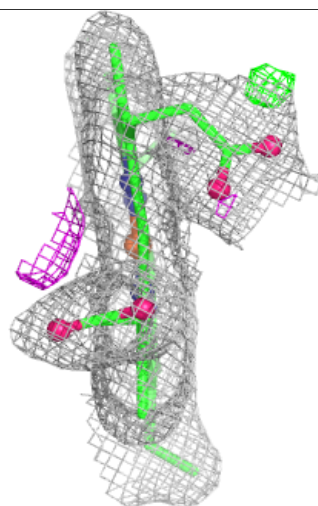
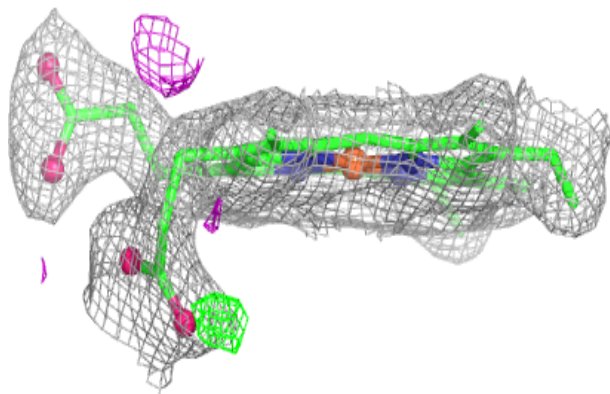
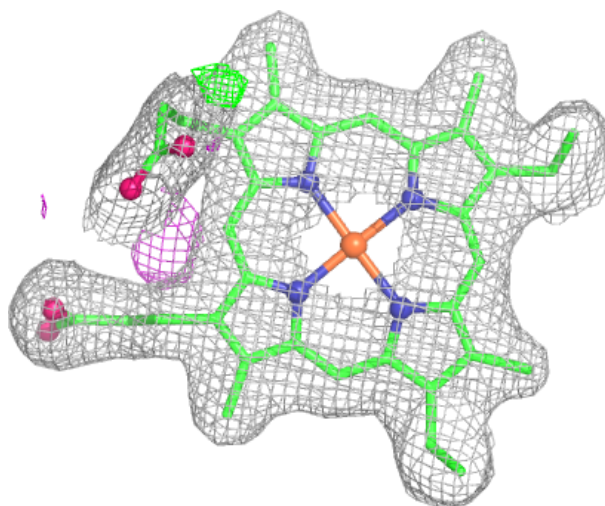
Electron density around HEC B 303:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



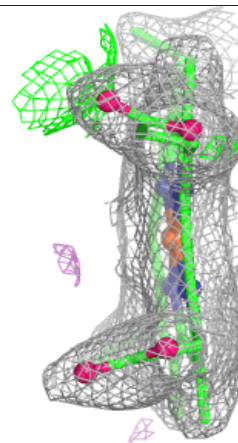
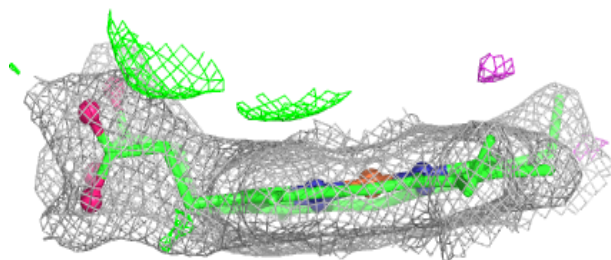
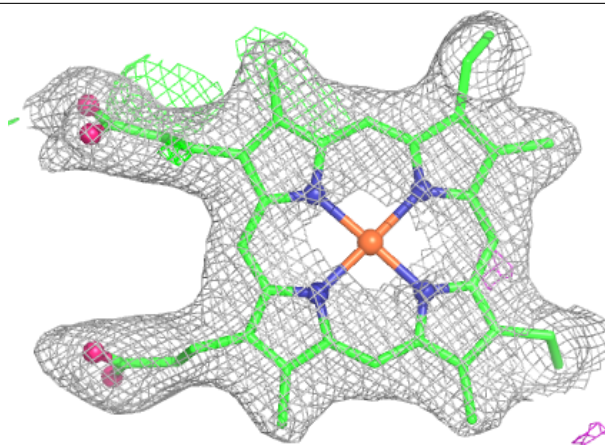
Electron density around HEC B 304:

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



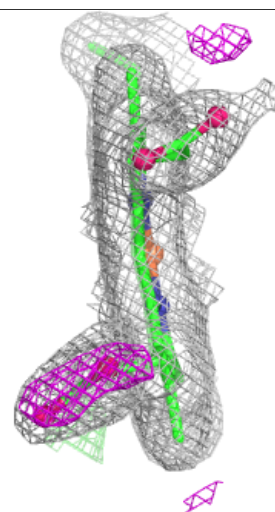
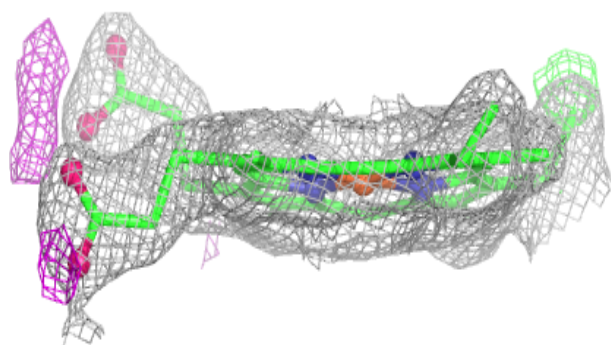
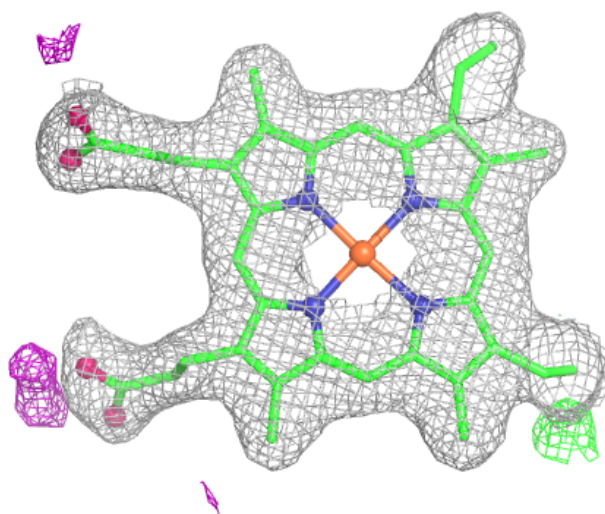
Electron density around HEC B 305:

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



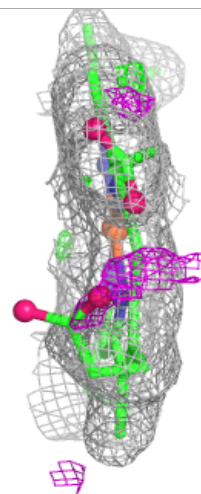
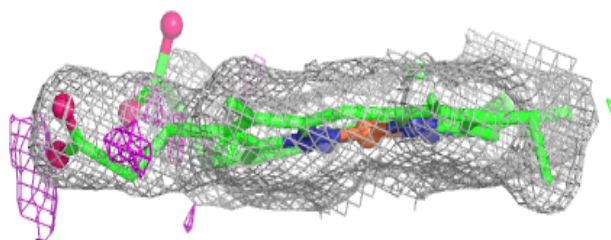
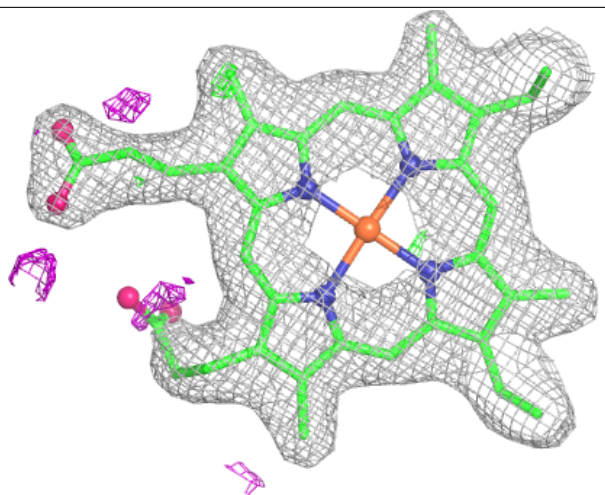
Electron density around HEC B 306:

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



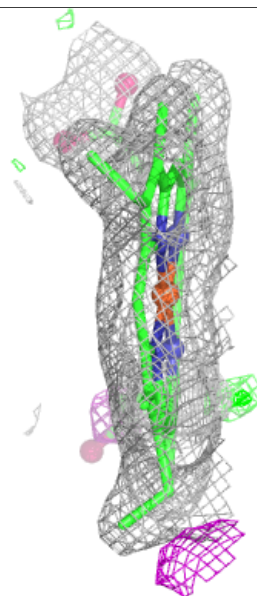
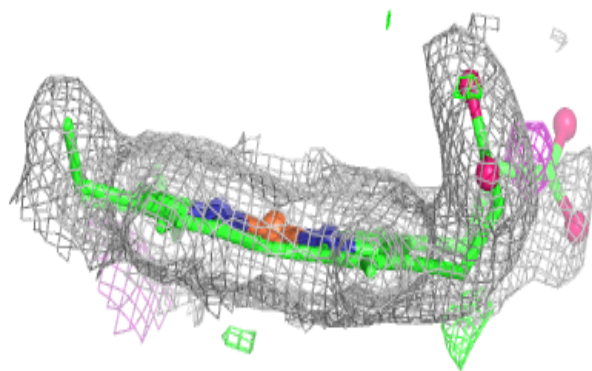
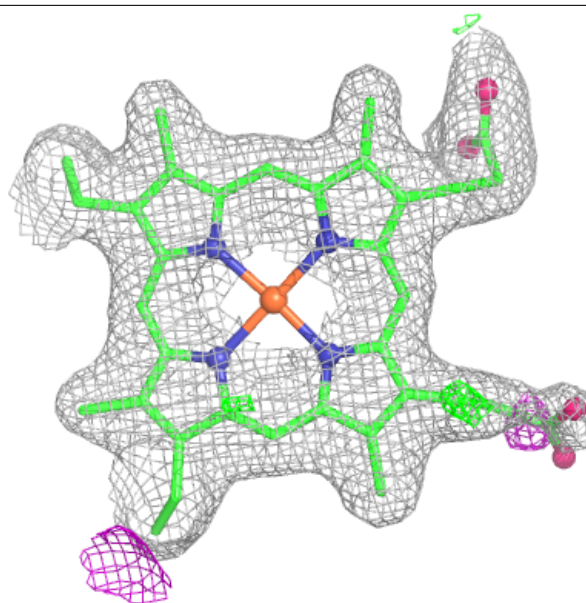
Electron density around HEC B 307:

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



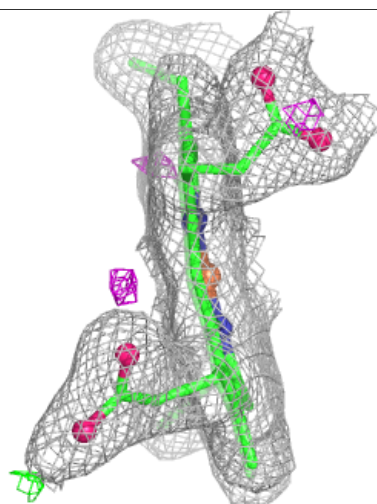
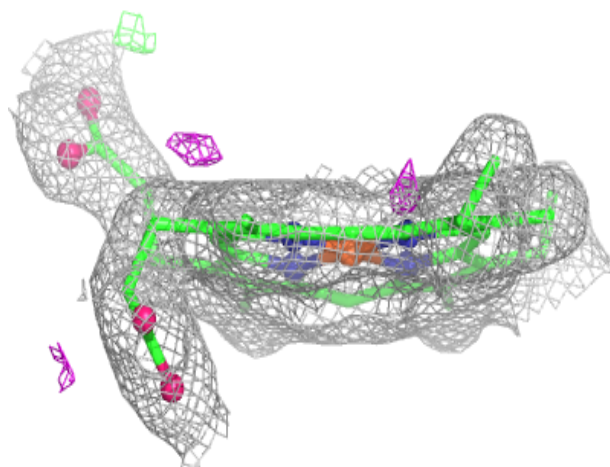
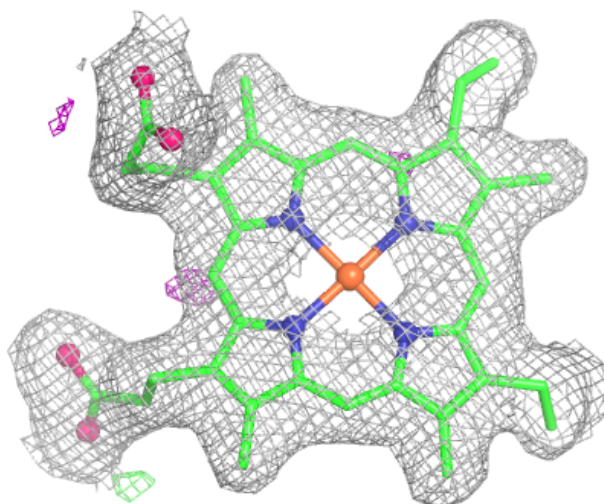
Electron density around HEC A 302:

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



Electron density around HEC A 303:

$2mF_o-DF_c$ (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.