Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 07:49 AM EDT

PDB ID	:	4L3X
Title	:	Nitrite complex of TvNiR, first middle dose data set
Authors	:	Trofimov, A.A.; Polyakov, K.M.; Lazarenko, V.A.; Popov, A.N.; Tikhonova, T.V.; Tikhonov, A.V.; Popov, V.O.
Deposited on	:	2013-06-07
Resolution	:	1.85 Å(reported)

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

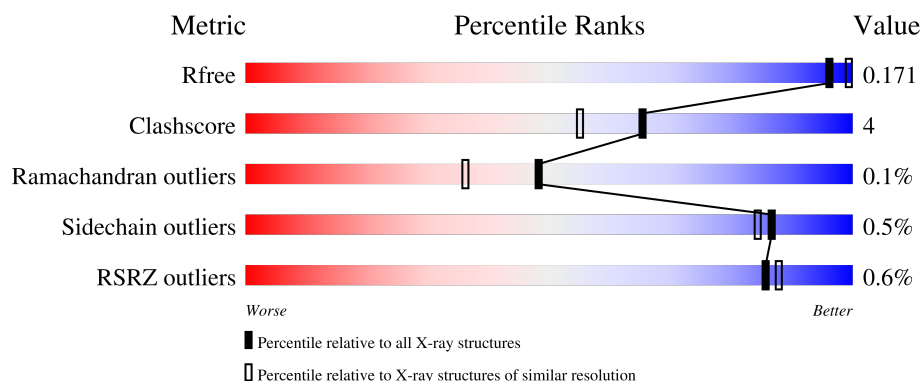|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.171
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		0.5%
RSRZ outliers		0.6%

Worse → *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	520	95% ... 5%
1	B	520	95% ... 5%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 10387 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 Eight-heme nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	18	0
			4176	2588	758	796	34			
1	B	520	Total	C	N	O	S	0	16	0
			4179	2591	759	795	34			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	524	VAL	-	expression tag	UNP L0DSL2
B	524	VAL	-	expression tag	UNP L0DSL2

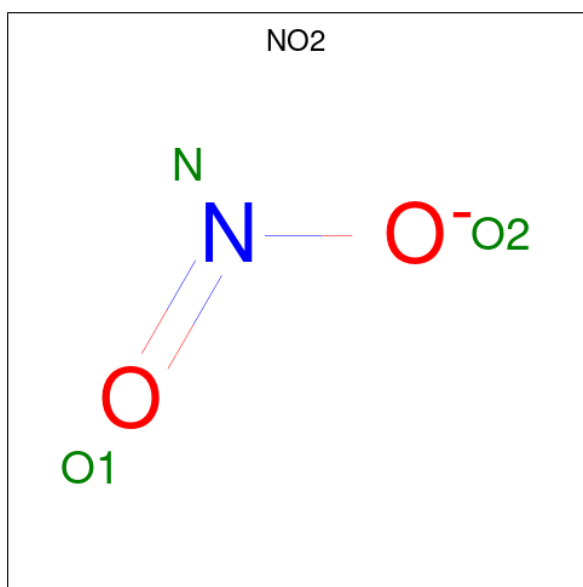- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).
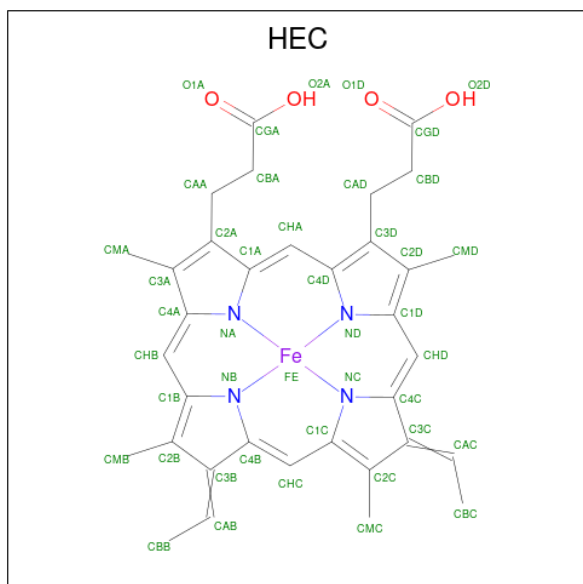
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	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
			38	31	1	4	2		
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	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	1
			47	36	1	4	6		
2	B	1	Total	C	Fe	N	O	0	0
			39	32	1	4	2		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

• Molecule 3 is NITRITE ION (three-letter code: NO2) (formula: NO_2).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 3	N 1	O 2	0	0
3	A	1	Total 3	N 1	O 2	0	0
3	A	1	Total 3	N 1	O 2	0	0
3	B	1	Total 3	N 1	O 2	0	0
3	B	1	Total 3	N 1	O 2	0	0
3	B	1	Total 3	N 1	O 2	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Ca 2	0	0
4	B	2	Total 2	Ca 2	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).

MPD

O4
OH
C1
C5
C4(S)
C2
CM
C3
OH
O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 8	C 6	O 2	0	0
5	B	1	Total 8	C 6	O 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3
OH O3
C1 C2
HO
O1
OH
O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 7	C 3	O 4	0	1
6	A	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 7	C 3	O 4	0	1
6	B	1	Total 7	C 3	O 4	0	1
6	B	1	Total 6	C 3	O 3	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
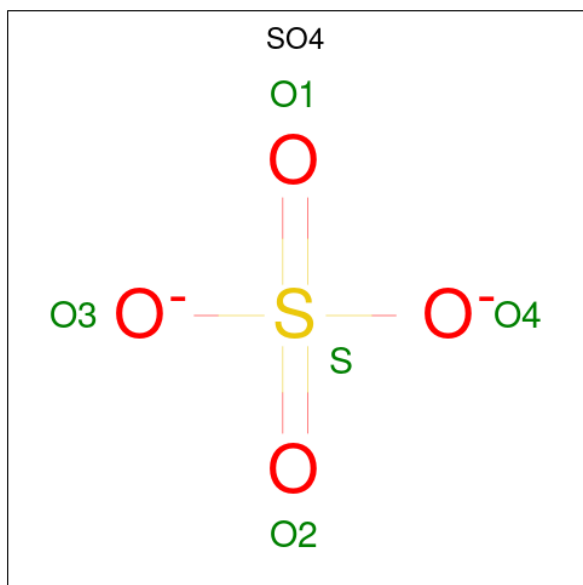
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 5	O 4	S 1	0	0
7	B	1	Total 5	O 4	S 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	631	Total 631	O 631	0	0
8	B	637	Total 637	O 637	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: Eight-heme nitrite reductase

Chain A:

• Molecule 1: Eight-heme nitrite reductase

Chain B:
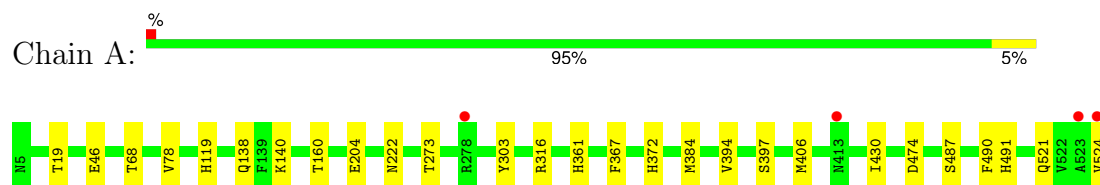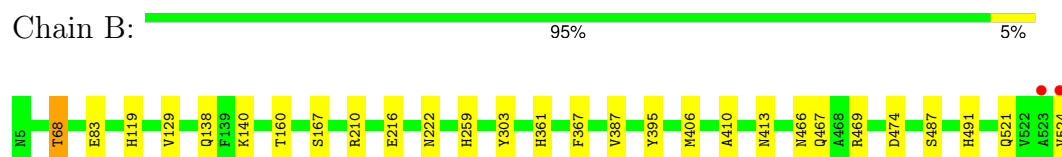
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	194.85Å 194.85Å 194.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.06 – 1.85 29.06 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.06-1.85) 99.4 (29.06-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.153 , 0.170 0.153 , 0.171	Depositor DCC
R_{free} test set	10425 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	13.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.049 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10387	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, MPD, NO2, HEC, CA

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	0.73	0/4381	0.75	0/5944
1	B	0.74	1/4369 (0.0%)	0.76	1/5928 (0.0%)
All	All	0.73	1/8750 (0.0%)	0.75	1/11872 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	GLU	CD-OE1	5.07	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	210	ARG	NE-CZ-NH1	5.29	122.94	120.30

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	4176	0	3879	24	0
1	B	4179	0	3892	27	0
2	A	339	0	236	9	0
2	B	344	0	214	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	9	0	0	0	0
3	B	9	0	0	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	8	0	14	0	0
5	B	8	0	14	3	0
6	A	20	0	18	0	0
6	B	13	0	12	0	0
7	A	5	0	0	1	0
7	B	5	0	0	1	0
8	A	631	0	0	14	0
8	B	637	0	0	14	0
All	All	10387	0	8279	64	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 4.

All (64) 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:259[B]:HIS:HD2	8:B:958:HOH:O	0.81	1.15
1:B:138[B]:GLN:CD	8:B:1142:HOH:O	1.84	1.13
1:B:138[B]:GLN:NE2	8:B:1142:HOH:O	1.80	1.12
1:B:138[B]:GLN:OE1	8:B:1142:HOH:O	1.65	1.11
1:A:222[A]:ASN:ND2	8:A:1116:HOH:O	1.88	1.05
7:B:615:SO4:O1	8:B:1229:HOH:O	1.76	1.02
7:A:616:SO4:O3	8:A:1202:HOH:O	1.80	0.99
1:B:222[B]:ASN:ND2	8:B:1143:HOH:O	1.95	0.99
1:B:259[B]:HIS:CD2	8:B:958:HOH:O	1.66	0.91
1:A:204:GLU:OE2	8:A:1075:HOH:O	1.92	0.87
1:B:222[A]:ASN:OD1	8:B:1168:HOH:O	1.94	0.84
1:B:68[A]:THR:HG21	8:B:726:HOH:O	1.81	0.80
2:A:605:HEC:HMC1	2:A:605:HEC:HBC3	1.65	0.78
3:B:616:NO2:N	8:B:1152:HOH:O	2.18	0.75
1:A:222[B]:ASN:OD1	8:A:1141:HOH:O	2.03	0.74
1:B:474[A]:ASP:OD2	8:B:1133:HOH:O	2.04	0.74
1:A:474[B]:ASP:OD1	8:A:1106:HOH:O	2.04	0.73
1:B:138[B]:GLN:NE2	5:B:612:MPD:H32	2.06	0.70
1:A:521:GLN:O	1:A:524:VAL:HG22	1.92	0.69
1:A:19[B]:THR:HG23	8:A:1247:HOH:O	1.92	0.69
2:B:605:HEC:HMC1	2:B:605:HEC:HBC3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:606:HEC:HMC1	2:A:606:HEC:HBC3	1.79	0.65
1:A:68[A]:THR:OG1	2:B:607:HEC:HBD1	1.96	0.64
1:A:160[B]:THR:HG21	8:A:1257:HOH:O	1.99	0.62
2:B:603:HEC:HMA3	2:B:604[B]:HEC:HBA2	1.81	0.62
2:B:606:HEC:HMC1	2:B:606:HEC:HBC3	1.83	0.60
1:A:140:LYS:HG2	1:A:160[B]:THR:HG23	1.84	0.59
1:A:273[B]:THR:HG21	8:A:1158:HOH:O	2.04	0.57
1:B:413:ASN:HB2	8:B:1253:HOH:O	2.06	0.56
1:B:361:HIS:NE2	3:B:609:NO2:O2	2.33	0.54
1:B:413:ASN:ND2	8:B:1158:HOH:O	2.41	0.53
1:B:138[B]:GLN:HE21	5:B:612:MPD:H32	1.72	0.53
1:A:68[A]:THR:HG1	2:B:607:HEC:HBD1	1.72	0.52
1:A:140:LYS:HG2	1:A:160[B]:THR:CG2	2.40	0.52
1:A:46:GLU:HG3	8:A:1254:HOH:O	2.11	0.51
1:A:394[B]:VAL:HG12	8:A:955:HOH:O	2.11	0.50
1:B:303:TYR:CE2	2:B:601:HEC:HMC2	2.46	0.50
1:B:140:LYS:HG2	1:B:160[B]:THR:HG23	1.94	0.49
1:A:303:TYR:CE2	2:A:601:HEC:HMC2	2.48	0.49
1:B:521:GLN:O	1:B:524:VAL:HG22	2.13	0.48
1:B:138[B]:GLN:NE2	5:B:612:MPD:C3	2.77	0.48
1:A:367:PHE:CZ	2:A:604:HEC:HMC2	2.50	0.47
1:A:138:GLN:HG2	8:A:1115:HOH:O	2.15	0.47
1:B:129:VAL:HG11	2:B:601:HEC:HMA1	1.97	0.46
2:A:604:HEC:HBC3	2:A:604:HEC:HMC1	1.97	0.46
1:A:384:MET:HB2	1:A:397:SER:O	2.15	0.46
1:A:487:SER:HB3	1:A:491:HIS:CE1	2.51	0.46
1:B:387[A]:VAL:HG21	1:B:395:TYR:CE1	2.52	0.45
2:B:606:HEC:HHA	2:B:606:HEC:HBD2	1.98	0.45
1:B:466:ASN:ND2	1:B:469:ARG:HH11	2.15	0.44
1:B:487:SER:HB3	1:B:491:HIS:CE1	2.53	0.44
1:B:410:ALA:O	2:B:605:HEC:HMC3	2.18	0.44
1:A:372:HIS:HB2	8:A:1119:HOH:O	2.19	0.42
2:A:608:HEC:HBC3	2:A:608:HEC:HMC1	2.00	0.42
1:A:68[B]:THR:HG21	8:A:1330:HOH:O	2.19	0.42
2:A:606:HEC:HHA	2:A:606:HEC:HBD2	2.02	0.42
1:B:167:SER:HB2	1:B:216[B]:GLU:HG2	2.02	0.42
1:A:119:HIS:CD2	2:A:603:HEC:ND	2.88	0.41
1:B:467[B]:GLN:HG2	8:B:996:HOH:O	2.19	0.41
1:A:430:ILE:HG21	1:A:490:PHE:HA	2.03	0.41
1:B:119:HIS:CD2	2:B:603:HEC:ND	2.89	0.41
2:A:605:HEC:HAA1	8:A:1285:HOH:O	2.22	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	536/520 (103%)	510 (95%)	25 (5%)	1 (0%)	44	32
1	B	534/520 (103%)	510 (96%)	24 (4%)	0	100	100
All	All	1070/1040 (103%)	1020 (95%)	49 (5%)	1 (0%)	48	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	HIS

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	456/439 (104%)	454 (100%)	2 (0%)	89	88
1	B	454/439 (103%)	451 (99%)	3 (1%)	81	78
All	All	910/878 (104%)	905 (100%)	5 (0%)	86	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	ARG
1	A	406	MET

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Res	Type
1	B	68[A]	THR
1	B	68[B]	THR
1	B	406	MET

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

Mol	Chain	Res	Type
1	A	138	GLN
1	A	388	GLN
1	B	388	GLN
1	B	413	ASN
1	B	466	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 39 ligands modelled in this entry, 4 are monoatomic - leaving 35 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	B	604[A]	-	32,50,50	1.91	10 (31%)	30,82,82	3.05	10 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	HEC	A	607	1	32,50,50	1.79	9 (28%)	30,82,82	2.51	10 (33%)
2	HEC	B	605	1	28,46,50	2.25	10 (35%)	27,77,82	2.91	10 (37%)
5	MPD	A	612	-	7,7,7	0.75	0	9,10,10	0.79	0
2	HEC	B	607	1	32,50,50	1.91	7 (21%)	30,82,82	2.47	9 (30%)
7	SO4	B	615	-	4,4,4	0.66	0	6,6,6	0.44	0
2	HEC	A	603	4,1	32,50,50	1.92	11 (34%)	30,82,82	3.21	14 (46%)
3	NO2	B	609	2	1,2,2	0.13	0	0,1,1	-	-
6	GOL	A	613[B]	-	5,5,5	0.64	0	5,5,5	0.55	0
2	HEC	B	602	1	32,50,50	1.78	8 (25%)	30,82,82	2.83	11 (36%)
3	NO2	A	617	-	1,2,2	0.02	0	0,1,1	-	-
6	GOL	A	613[A]	-	5,5,5	0.59	0	5,5,5	0.43	0
2	HEC	B	606	1	32,50,50	2.23	9 (28%)	30,82,82	2.50	9 (30%)
3	NO2	B	616	-	1,2,2	0.07	0	0,1,1	-	-
6	GOL	A	614	-	5,5,5	0.59	0	5,5,5	0.43	0
2	HEC	A	601	3,1,8	32,50,50	1.77	8 (25%)	30,82,82	2.41	8 (26%)
2	HEC	B	608	1	32,50,50	2.25	10 (31%)	30,82,82	3.15	12 (40%)
6	GOL	A	615[B]	-	5,5,5	0.45	0	5,5,5	0.51	0
2	HEC	A	606	1	32,50,50	2.16	10 (31%)	30,82,82	2.92	9 (30%)
7	SO4	A	616	-	4,4,4	0.42	0	6,6,6	0.33	0
6	GOL	A	615[A]	-	5,5,5	0.41	0	5,5,5	0.54	0
5	MPD	B	612	-	7,7,7	0.70	0	9,10,10	1.07	0
3	NO2	B	617	-	1,2,2	0.16	0	0,1,1	-	-
6	GOL	B	613[B]	-	5,5,5	0.66	0	5,5,5	0.62	0
2	HEC	B	603	4,1	32,50,50	1.88	7 (21%)	30,82,82	3.05	11 (36%)
2	HEC	A	608	1	32,50,50	2.04	10 (31%)	30,82,82	2.60	11 (36%)
2	HEC	A	602	1	32,50,50	2.10	8 (25%)	30,82,82	2.84	11 (36%)
3	NO2	A	609	2	1,2,2	0.24	0	0,1,1	-	-
2	HEC	A	605	1	27,45,50	3.09	11 (40%)	24,75,82	2.90	10 (41%)
6	GOL	B	613[A]	-	5,5,5	0.64	0	5,5,5	0.34	0
6	GOL	B	614	-	5,5,5	0.50	0	5,5,5	0.49	0
3	NO2	A	618	-	1,2,2	0.06	0	0,1,1	-	-
2	HEC	A	604	1	32,50,50	1.83	7 (21%)	30,82,82	3.00	11 (36%)
2	HEC	B	604[B]	4	32,50,50	1.87	10 (31%)	30,82,82	3.08	10 (33%)
2	HEC	B	601	3,1,8	32,50,50	2.12	8 (25%)	30,82,82	2.70	9 (30%)

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	B	604[A]	-	-	2/10/54/54	-
2	HEC	A	607	1	-	1/10/54/54	-
2	HEC	B	605	1	-	0/5/49/54	-
5	MPD	A	612	-	-	0/5/5/5	-
2	HEC	B	607	1	-	4/10/54/54	-
2	HEC	A	603	4,1	-	0/10/54/54	-
6	GOL	A	613[B]	-	-	0/4/4/4	-
2	HEC	B	602	1	-	3/10/54/54	-
6	GOL	A	613[A]	-	-	0/4/4/4	-
2	HEC	B	606	1	-	2/10/54/54	-
6	GOL	A	614	-	-	0/4/4/4	-
2	HEC	A	601	3,1,8	-	2/10/54/54	-
2	HEC	B	608	1	-	4/10/54/54	-
6	GOL	A	615[B]	-	-	4/4/4/4	-
2	HEC	A	606	1	-	3/10/54/54	-
6	GOL	A	615[A]	-	-	4/4/4/4	-
5	MPD	B	612	-	-	0/5/5/5	-
6	GOL	B	613[B]	-	-	0/4/4/4	-
2	HEC	B	603	4,1	-	0/10/54/54	-
2	HEC	A	608	1	-	4/10/54/54	-
2	HEC	A	602	1	-	4/10/54/54	-
6	GOL	B	613[A]	-	-	0/4/4/4	-
2	HEC	A	605	1	-	0/5/49/54	-
6	GOL	B	614	-	-	0/4/4/4	-
2	HEC	A	604	1	-	2/10/54/54	-
2	HEC	B	604[B]	4	-	0/10/54/54	-
2	HEC	B	601	3,1,8	-	2/10/54/54	-

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	605	HEC	C3D-C4D	9.56	1.50	1.39
2	B	601	HEC	C2B-C3B	7.17	1.48	1.40
2	A	602	HEC	C3C-C2C	6.51	1.48	1.40
2	B	607	HEC	C3C-C2C	6.34	1.47	1.40
2	A	606	HEC	C2B-C3B	6.20	1.47	1.40
2	B	606	HEC	C3C-C2C	6.18	1.47	1.40
2	B	608	HEC	C2B-C3B	6.04	1.47	1.40
2	B	606	HEC	C2B-C3B	6.04	1.47	1.40
2	A	606	HEC	C3C-C2C	5.93	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	608	HEC	C3C-C2C	5.88	1.47	1.40
2	A	608	HEC	C3C-C2C	5.68	1.47	1.40
2	A	604	HEC	C3C-C2C	5.42	1.46	1.40
2	B	605	HEC	C3C-C2C	5.32	1.46	1.40
2	A	605	HEC	C2B-C3B	5.31	1.46	1.40
2	A	603	HEC	C3C-C2C	5.30	1.46	1.40
2	B	601	HEC	C3C-C2C	5.24	1.46	1.40
2	A	607	HEC	C2B-C3B	5.10	1.46	1.40
2	B	604[A]	HEC	C3C-C2C	5.04	1.46	1.40
2	B	604[B]	HEC	C3C-C2C	5.04	1.46	1.40
2	B	603	HEC	C3C-C2C	5.01	1.46	1.40
2	A	605	HEC	C3C-C2C	4.98	1.46	1.40
2	B	603	HEC	C2B-C3B	4.98	1.46	1.40
2	B	602	HEC	C3C-C2C	4.91	1.46	1.40
2	A	602	HEC	C2B-C3B	4.87	1.46	1.40
2	B	608	HEC	C3C-C4C	4.66	1.51	1.43
2	A	605	HEC	C3D-C2D	4.36	1.50	1.38
2	A	601	HEC	C3C-C2C	4.29	1.45	1.40
2	A	605	HEC	C3C-C4C	4.15	1.50	1.43
2	A	607	HEC	C3C-C2C	4.14	1.45	1.40
2	B	605	HEC	C3C-C4C	4.13	1.50	1.43
2	A	603	HEC	C2B-C3B	4.11	1.45	1.40
2	A	608	HEC	C2B-C3B	4.11	1.45	1.40
2	B	602	HEC	C2B-C3B	4.00	1.45	1.40
2	A	601	HEC	C2B-C3B	3.96	1.45	1.40
2	B	605	HEC	C2A-C3A	3.80	1.48	1.37
2	A	605	HEC	C2A-C1A	3.71	1.50	1.42
2	A	605	HEC	C2A-C3A	3.68	1.48	1.37
2	A	604	HEC	C2B-C3B	3.67	1.44	1.40
2	B	607	HEC	C2B-C3B	3.65	1.44	1.40
2	B	605	HEC	C2B-C3B	3.52	1.44	1.40
2	B	606	HEC	C4B-C3B	3.43	1.49	1.43
2	B	605	HEC	C2A-C1A	3.38	1.50	1.42
2	B	605	HEC	C3A-C4A	3.36	1.50	1.42
2	A	606	HEC	C4B-C3B	3.33	1.49	1.43
2	B	604[A]	HEC	C2B-C3B	3.32	1.44	1.40
2	B	604[B]	HEC	C2B-C3B	3.32	1.44	1.40
2	A	605	HEC	C3A-C4A	3.28	1.49	1.42
2	B	603	HEC	C3D-C2D	3.26	1.47	1.37
2	A	603	HEC	C3D-C2D	3.26	1.47	1.37
2	B	604[A]	HEC	C2A-C3A	3.23	1.47	1.37
2	B	604[B]	HEC	C2A-C3A	3.23	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEC	C3D-C2D	3.21	1.47	1.37
2	B	606	HEC	C3C-C4C	3.21	1.48	1.43
2	A	608	HEC	C3C-C4C	3.20	1.48	1.43
2	B	607	HEC	C4B-C3B	3.20	1.48	1.43
2	A	602	HEC	O2D-CGD	-3.18	1.20	1.30
2	A	606	HEC	C3C-C4C	3.11	1.48	1.43
2	A	608	HEC	C2A-C3A	3.11	1.46	1.37
2	A	608	HEC	C4B-C3B	3.11	1.48	1.43
2	B	604[A]	HEC	C3A-C4A	3.07	1.49	1.42
2	B	604[B]	HEC	C3A-C4A	3.07	1.49	1.42
2	B	605	HEC	C4D-CHA	3.05	1.49	1.41
2	B	602	HEC	C2A-C1A	3.05	1.49	1.42
2	A	604	HEC	C2A-C3A	3.04	1.46	1.37
2	B	606	HEC	C2A-C1A	3.00	1.49	1.42
2	B	608	HEC	C2A-C3A	2.99	1.46	1.37
2	A	602	HEC	C3D-C2D	2.99	1.46	1.37
2	B	605	HEC	C1D-CHD	2.98	1.49	1.41
2	B	608	HEC	C3D-C2D	2.98	1.46	1.37
2	B	601	HEC	C2A-C1A	2.97	1.49	1.42
2	B	606	HEC	C3A-C4A	2.93	1.49	1.42
2	B	606	HEC	C3D-C2D	2.91	1.46	1.37
2	A	607	HEC	C2A-C3A	2.88	1.46	1.37
2	A	606	HEC	C2A-C3A	2.88	1.46	1.37
2	A	605	HEC	C1D-CHD	2.86	1.49	1.41
2	A	608	HEC	C3D-C2D	2.86	1.46	1.37
2	A	602	HEC	C2A-C3A	2.86	1.46	1.37
2	A	601	HEC	C2A-C1A	2.85	1.48	1.42
2	A	605	HEC	C4D-CHA	2.84	1.49	1.44
2	A	603	HEC	C2A-C1A	2.83	1.48	1.42
2	A	602	HEC	C2A-C1A	2.82	1.48	1.42
2	A	602	HEC	C3C-C4C	2.82	1.48	1.43
2	A	601	HEC	C2A-C3A	2.81	1.46	1.37
2	B	602	HEC	O2D-CGD	-2.78	1.21	1.30
2	A	603	HEC	C3C-C4C	2.77	1.48	1.43
2	B	608	HEC	C4B-C3B	2.76	1.48	1.43
2	B	603	HEC	C2A-C1A	2.73	1.48	1.42
2	A	608	HEC	C2A-C1A	2.72	1.48	1.42
2	B	605	HEC	C4B-C3B	2.67	1.47	1.43
2	B	602	HEC	C2A-C3A	2.66	1.45	1.37
2	A	606	HEC	C3D-C2D	2.65	1.45	1.37
2	B	601	HEC	C2A-C3A	2.63	1.45	1.37
2	B	604[A]	HEC	C3D-C2D	2.61	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	604[B]	HEC	C3D-C2D	2.61	1.45	1.37
2	A	601	HEC	C3D-C2D	2.60	1.45	1.37
2	B	604[A]	HEC	C4B-C3B	2.59	1.47	1.43
2	B	604[B]	HEC	C4B-C3B	2.59	1.47	1.43
2	B	607	HEC	C2A-C3A	2.58	1.45	1.37
2	B	603	HEC	C2A-C3A	2.58	1.45	1.37
2	A	606	HEC	C3A-C4A	2.54	1.48	1.42
2	B	606	HEC	C2A-C3A	2.54	1.45	1.37
2	B	604[A]	HEC	C3C-C4C	2.53	1.47	1.43
2	B	604[B]	HEC	C3C-C4C	2.53	1.47	1.43
2	B	608	HEC	C2A-C1A	2.52	1.48	1.42
2	B	601	HEC	C3C-C4C	2.50	1.47	1.43
2	A	608	HEC	C3A-C4A	2.50	1.48	1.42
2	B	605	HEC	C3D-C2D	2.49	1.50	1.41
2	A	607	HEC	C3D-C2D	2.48	1.45	1.37
2	A	604	HEC	C2A-C1A	2.45	1.48	1.42
2	B	608	HEC	C3A-C4A	2.45	1.48	1.42
2	A	604	HEC	C3C-C4C	2.44	1.47	1.43
2	B	604[A]	HEC	C2A-C1A	2.42	1.47	1.42
2	B	604[B]	HEC	C2A-C1A	2.42	1.47	1.42
2	A	608	HEC	C1C-CHC	2.40	1.47	1.41
2	A	604	HEC	C4B-C3B	2.40	1.47	1.43
2	B	602	HEC	C3D-C2D	2.40	1.44	1.37
2	B	601	HEC	C3A-C4A	2.39	1.47	1.42
2	B	607	HEC	C3D-C2D	2.39	1.44	1.37
2	A	605	HEC	C4B-C3B	2.37	1.47	1.43
2	A	607	HEC	C2A-C1A	2.37	1.47	1.42
2	B	603	HEC	CBA-CGA	2.36	1.56	1.50
2	A	601	HEC	C3A-C4A	2.35	1.47	1.42
2	A	603	HEC	C2A-C3A	2.33	1.44	1.37
2	B	608	HEC	C1C-CHC	2.33	1.47	1.41
2	A	608	HEC	C4D-CHA	2.32	1.47	1.41
2	B	607	HEC	C1B-CHB	2.31	1.47	1.41
2	A	607	HEC	C3C-C4C	2.30	1.47	1.43
2	B	608	HEC	C1D-CHD	2.28	1.47	1.41
2	B	607	HEC	C1C-CHC	2.28	1.47	1.41
2	B	606	HEC	C1B-CHB	2.28	1.47	1.41
2	B	602	HEC	C3C-C4C	2.24	1.47	1.43
2	A	607	HEC	C3A-C4A	2.21	1.47	1.42
2	B	604[A]	HEC	C4D-ND	-2.20	1.31	1.36
2	B	604[B]	HEC	C4D-ND	-2.20	1.31	1.36
2	A	603	HEC	C3A-C4A	2.17	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	604[A]	HEC	C1C-CHC	2.14	1.46	1.41
2	B	604[B]	HEC	C1C-CHC	2.14	1.46	1.41
2	A	601	HEC	C3C-C4C	2.13	1.46	1.43
2	A	603	HEC	C1C-CHC	2.13	1.46	1.41
2	A	607	HEC	C1D-CHD	2.12	1.46	1.41
2	A	603	HEC	C4D-CHA	2.10	1.46	1.41
2	B	603	HEC	C4D-CHA	2.09	1.46	1.41
2	A	604	HEC	C3A-C4A	2.09	1.47	1.42
2	A	606	HEC	C2A-C1A	2.08	1.47	1.42
2	B	602	HEC	C3A-C4A	2.08	1.47	1.42
2	A	601	HEC	C1B-CHB	2.08	1.46	1.41
2	A	606	HEC	C1C-CHC	2.05	1.46	1.41
2	A	607	HEC	C1B-CHB	2.04	1.46	1.41
2	A	603	HEC	C4B-C3B	2.03	1.46	1.43
2	B	601	HEC	O2D-CGD	-2.03	1.24	1.30
2	A	603	HEC	C1B-CHB	2.01	1.46	1.41
2	A	602	HEC	C3A-C4A	2.01	1.47	1.42
2	A	606	HEC	C4D-CHA	2.00	1.46	1.41

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	HEC	CBB-CAB-C3B	-8.92	106.62	127.49
2	A	604	HEC	CBA-CAA-C2A	-8.79	98.07	112.55
2	B	604[A]	HEC	CBB-CAB-C3B	-8.36	107.92	127.49
2	B	604[B]	HEC	CBB-CAB-C3B	-8.36	107.92	127.49
2	B	603	HEC	CBB-CAB-C3B	-7.87	109.08	127.49
2	B	601	HEC	CBB-CAB-C3B	-7.80	109.24	127.49
2	A	603	HEC	CBB-CAB-C3B	-7.62	109.65	127.49
2	A	602	HEC	CBB-CAB-C3B	-7.58	109.74	127.49
2	B	608	HEC	CBB-CAB-C3B	-7.52	109.90	127.49
2	B	608	HEC	CMC-C2C-C3C	7.28	134.38	125.82
2	A	604	HEC	CBB-CAB-C3B	-7.08	110.92	127.49
2	A	606	HEC	CBB-CAB-C3B	-6.90	111.35	127.49
2	A	606	HEC	C1D-C2D-C3D	-6.78	102.28	107.00
2	A	602	HEC	C1D-C2D-C3D	-6.78	102.28	107.00
2	A	607	HEC	CBB-CAB-C3B	-6.71	111.79	127.49
2	B	604[A]	HEC	C1D-C2D-C3D	-6.70	102.34	107.00
2	B	604[B]	HEC	C1D-C2D-C3D	-6.70	102.34	107.00
2	B	607	HEC	CBB-CAB-C3B	-6.52	112.23	127.49
2	B	603	HEC	C1D-C2D-C3D	-6.49	102.48	107.00
2	B	605	HEC	CMC-C2C-C3C	6.47	133.43	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEC	CBB-CAB-C3B	-6.42	112.47	127.49
2	B	602	HEC	C1D-C2D-C3D	-6.35	102.58	107.00
2	B	601	HEC	C1D-C2D-C3D	-6.34	102.58	107.00
2	A	608	HEC	CBC-CAC-C3C	-6.20	112.99	127.49
2	B	606	HEC	C1D-C2D-C3D	-6.17	102.70	107.00
2	A	606	HEC	CBC-CAC-C3C	-6.17	113.06	127.49
2	A	605	HEC	CBB-CAB-C3B	-6.12	113.18	127.49
2	B	605	HEC	CBA-CAA-C2A	-6.11	102.48	112.55
2	A	603	HEC	CMC-C2C-C3C	6.08	132.97	125.82
2	A	603	HEC	CMB-C2B-C3B	6.05	132.93	125.82
2	A	603	HEC	CBC-CAC-C3C	-5.94	113.58	127.49
2	B	603	HEC	CBC-CAC-C3C	-5.91	113.67	127.49
2	A	604	HEC	C1D-C2D-C3D	-5.90	102.89	107.00
2	B	608	HEC	CBC-CAC-C3C	-5.86	113.77	127.49
2	B	604[B]	HEC	CBA-CAA-C2A	-5.79	103.00	112.55
2	A	608	HEC	CMC-C2C-C3C	5.73	132.56	125.82
2	B	601	HEC	CMB-C2B-C3B	5.73	132.55	125.82
2	B	604[A]	HEC	CBD-CAD-C3D	-5.52	103.27	112.54
2	B	604[B]	HEC	CBD-CAD-C3D	-5.52	103.27	112.54
2	A	605	HEC	CBA-CAA-C2A	-5.50	103.48	112.55
2	A	608	HEC	CBB-CAB-C3B	-5.49	114.63	127.49
2	A	606	HEC	CMC-C2C-C3C	5.43	132.21	125.82
2	A	605	HEC	C4D-C3D-C2D	-5.37	102.31	106.34
2	A	603	HEC	C1D-C2D-C3D	-5.37	103.26	107.00
2	B	606	HEC	CBB-CAB-C3B	-5.35	114.96	127.49
2	B	608	HEC	CBA-CAA-C2A	-5.30	103.81	112.55
2	B	604[A]	HEC	CBA-CAA-C2A	-5.29	103.84	112.55
2	A	608	HEC	C1D-C2D-C3D	-5.28	103.32	107.00
2	A	604	HEC	CBD-CAD-C3D	-5.25	103.71	112.54
2	B	608	HEC	C1D-C2D-C3D	-5.25	103.34	107.00
2	B	605	HEC	CBB-CAB-C3B	-5.24	115.24	127.49
2	A	601	HEC	C1D-C2D-C3D	-5.23	103.36	107.00
2	A	603	HEC	CBA-CAA-C2A	-5.20	103.97	112.55
2	B	605	HEC	CMB-C2B-C3B	5.16	131.89	125.82
2	A	605	HEC	CBC-CAC-C3C	-5.15	115.44	127.49
2	B	607	HEC	C1D-C2D-C3D	-5.14	103.42	107.00
2	A	607	HEC	CBA-CAA-C2A	-5.12	104.10	112.55
2	A	605	HEC	CMB-C2B-C3B	5.12	131.84	125.82
2	B	607	HEC	CBA-CAA-C2A	-5.07	104.20	112.55
2	B	606	HEC	CBC-CAC-C3C	-5.00	115.79	127.49
2	B	605	HEC	CBC-CAC-C3C	-4.94	115.93	127.49
2	A	602	HEC	CBC-CAC-C3C	-4.93	115.95	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	604[A]	HEC	CBC-CAC-C3C	-4.93	115.95	127.49
2	B	604[B]	HEC	CBC-CAC-C3C	-4.93	115.95	127.49
2	B	603	HEC	CBD-CAD-C3D	-4.90	104.30	112.54
2	B	605	HEC	C4D-C3D-C2D	-4.79	102.47	106.92
2	B	604[A]	HEC	CMC-C2C-C3C	4.76	131.42	125.82
2	B	604[B]	HEC	CMC-C2C-C3C	4.76	131.42	125.82
2	A	604	HEC	CBC-CAC-C3C	-4.75	116.36	127.49
2	A	607	HEC	C1D-C2D-C3D	-4.72	103.71	107.00
2	B	607	HEC	CMC-C2C-C3C	4.67	131.31	125.82
2	A	606	HEC	CMB-C2B-C3B	4.62	131.25	125.82
2	A	601	HEC	CMC-C2C-C3C	4.57	131.19	125.82
2	B	602	HEC	CMC-C2C-C3C	4.56	131.18	125.82
2	B	608	HEC	CBD-CAD-C3D	-4.51	104.95	112.54
2	B	604[A]	HEC	CMB-C2B-C3B	4.51	131.13	125.82
2	B	604[B]	HEC	CMB-C2B-C3B	4.51	131.13	125.82
2	B	603	HEC	CMC-C2C-C3C	4.50	131.12	125.82
2	A	602	HEC	CMB-C2B-C3B	4.48	131.09	125.82
2	A	606	HEC	CBA-CAA-C2A	-4.43	105.25	112.55
2	A	601	HEC	CBC-CAC-C3C	-4.41	117.18	127.49
2	B	603	HEC	CBA-CAA-C2A	-4.38	105.33	112.55
2	A	607	HEC	CBC-CAC-C3C	-4.34	117.33	127.49
2	B	606	HEC	CAA-CBA-CGA	-4.33	102.18	113.83
2	A	603	HEC	CBD-CAD-C3D	-4.32	105.28	112.54
2	B	601	HEC	CBC-CAC-C3C	-4.31	117.41	127.49
2	B	603	HEC	CMB-C2B-C3B	4.24	130.81	125.82
2	A	607	HEC	CMB-C2B-C3B	4.23	130.80	125.82
2	A	602	HEC	CMC-C2C-C3C	4.23	130.79	125.82
2	B	606	HEC	CMB-C2B-C3B	4.19	130.74	125.82
2	B	602	HEC	CBC-CAC-C3C	-4.12	117.85	127.49
2	B	606	HEC	CMC-C2C-C3C	4.00	130.52	125.82
2	A	605	HEC	CMC-C2C-C3C	3.96	130.47	125.82
2	B	602	HEC	CMB-C2B-C3B	3.96	130.47	125.82
2	B	607	HEC	CBC-CAC-C3C	-3.94	118.26	127.49
2	A	606	HEC	CAA-CBA-CGA	-3.82	103.54	113.83
2	A	601	HEC	CMB-C2B-C3B	3.74	130.22	125.82
2	B	605	HEC	C1D-C2D-C3D	-3.71	103.47	106.92
2	A	602	HEC	CAD-CBD-CGD	-3.61	104.12	113.83
2	B	608	HEC	CMA-C3A-C2A	3.57	131.68	124.94
2	A	601	HEC	CBA-CAA-C2A	-3.55	106.69	112.55
2	B	608	HEC	CMB-C2B-C3B	3.51	129.95	125.82
2	B	602	HEC	CAD-CBD-CGD	-3.47	104.49	113.83
2	A	602	HEC	C4C-C3C-C2C	-3.42	102.67	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	HEC	CMC-C2C-C3C	3.41	129.83	125.82
2	B	601	HEC	CBD-CAD-C3D	-3.27	107.04	112.54
2	A	604	HEC	CMB-C2B-C3B	3.25	129.64	125.82
2	B	603	HEC	CMD-C2D-C3D	3.23	131.03	124.94
2	B	601	HEC	CMD-C2D-C3D	3.21	131.00	124.94
2	A	607	HEC	CMC-C2C-C3C	3.21	129.59	125.82
2	A	602	HEC	CAA-CBA-CGA	-3.20	105.21	113.83
2	A	603	HEC	CMA-C3A-C2A	3.16	130.90	124.94
2	A	608	HEC	CBD-CAD-C3D	-3.14	107.26	112.54
2	B	608	HEC	CMC-C2C-C1C	-3.09	123.92	128.46
2	B	602	HEC	C4C-C3C-C2C	-2.97	103.15	106.35
2	A	607	HEC	C3C-C4C-NC	2.95	116.51	110.94
2	B	605	HEC	O1A-CGA-CBA	-2.93	113.79	123.09
2	B	606	HEC	C2B-C3B-C4B	-2.92	103.19	106.35
2	A	607	HEC	CAD-CBD-CGD	-2.92	105.95	113.83
2	A	608	HEC	CMB-C2B-C3B	2.90	129.22	125.82
2	A	605	HEC	O1A-CGA-CBA	-2.87	113.98	123.09
2	A	607	HEC	CBD-CAD-C3D	-2.87	107.72	112.54
2	B	602	HEC	CMA-C3A-C2A	2.85	130.32	124.94
2	B	603	HEC	CMA-C3A-C2A	2.85	130.32	124.94
2	A	605	HEC	C3D-C4D-ND	2.84	113.83	110.21
2	B	604[A]	HEC	C4C-C3C-C2C	-2.82	103.31	106.35
2	B	604[B]	HEC	C4C-C3C-C2C	-2.82	103.31	106.35
2	A	603	HEC	CMD-C2D-C3D	2.80	130.23	124.94
2	A	604	HEC	C4C-C3C-C2C	-2.78	103.36	106.35
2	A	607	HEC	C4C-C3C-C2C	-2.75	103.38	106.35
2	B	607	HEC	CAD-CBD-CGD	-2.73	106.47	113.83
2	A	601	HEC	CMA-C3A-C2A	2.69	130.02	124.94
2	A	604	HEC	CMC-C2C-C3C	2.56	128.84	125.82
2	B	602	HEC	CAA-CBA-CGA	-2.56	106.93	113.83
2	A	605	HEC	CMA-C3A-C2A	2.55	129.76	124.94
2	A	603	HEC	C4C-C3C-C2C	-2.51	103.64	106.35
2	A	608	HEC	C4C-C3C-C2C	-2.50	103.65	106.35
2	B	607	HEC	CMB-C2B-C3B	2.46	128.72	125.82
2	B	605	HEC	O2A-CGA-CBA	2.45	121.73	114.00
2	B	606	HEC	CBA-CAA-C2A	-2.44	108.53	112.55
2	B	606	HEC	C4C-C3C-C2C	-2.44	103.72	106.35
2	A	608	HEC	CAA-CBA-CGA	-2.40	107.38	113.83
2	B	607	HEC	CMA-C3A-C2A	2.38	129.43	124.94
2	A	604	HEC	CMA-C3A-C2A	2.36	129.39	124.94
2	B	603	HEC	C2B-C3B-C4B	-2.36	103.81	106.35
2	A	602	HEC	CMA-C3A-C2A	2.33	129.34	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	HEC	C3C-C4C-NC	2.30	115.29	110.94
2	B	605	HEC	CMD-C2D-C3D	2.30	129.50	124.69
2	B	608	HEC	C2B-C3B-C4B	-2.29	103.88	106.35
2	B	601	HEC	CBA-CAA-C2A	-2.29	108.78	112.55
2	A	606	HEC	C4C-C3C-C2C	-2.28	103.89	106.35
2	A	603	HEC	C3B-C4B-NB	2.25	115.19	110.94
2	A	602	HEC	O1A-CGA-CBA	-2.24	115.97	123.09
2	A	605	HEC	O2A-CGA-CBA	2.22	121.03	114.00
2	A	606	HEC	C2B-C3B-C4B	-2.21	103.96	106.35
2	A	608	HEC	CBA-CAA-C2A	-2.20	108.93	112.55
2	B	604[A]	HEC	C3C-C4C-NC	2.19	115.08	110.94
2	B	604[B]	HEC	C3C-C4C-NC	2.19	115.08	110.94
2	A	608	HEC	CMC-C2C-C1C	-2.19	125.25	128.46
2	B	602	HEC	CMD-C2D-C1D	2.18	131.64	128.46
2	B	607	HEC	CBD-CAD-C3D	-2.17	108.88	112.54
2	B	604[B]	HEC	O2A-CGA-CBA	2.15	120.79	114.00
2	B	602	HEC	C3C-C4C-NC	2.14	114.99	110.94
2	A	604	HEC	C2B-C3B-C4B	-2.13	104.05	106.35
2	A	601	HEC	CBD-CAD-C3D	-2.13	108.95	112.54
2	A	604	HEC	C3C-C4C-NC	2.13	114.97	110.94
2	A	603	HEC	CAA-CBA-CGA	-2.13	108.09	113.83
2	A	608	HEC	CAD-CBD-CGD	-2.12	108.11	113.83
2	A	603	HEC	CMB-C2B-C1B	-2.12	125.35	128.46
2	A	603	HEC	CMC-C2C-C1C	-2.10	125.38	128.46
2	B	608	HEC	O2D-CGD-CBD	2.09	120.61	114.00
2	B	604[A]	HEC	O2A-CGA-CBA	2.08	120.58	114.00
2	B	603	HEC	C3B-C4B-NB	2.07	114.85	110.94
2	B	601	HEC	C4C-C3C-C2C	-2.06	104.13	106.35
2	B	608	HEC	C4C-C3C-C2C	-2.05	104.14	106.35

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	615[A]	GOL	C1-C2-C3-O3
6	A	615[A]	GOL	O1-C1-C2-C3
6	A	615[B]	GOL	O1-C1-C2-C3
6	A	615[B]	GOL	C1-C2-C3-O3
6	A	615[B]	GOL	O2-C2-C3-O3
6	A	615[A]	GOL	O2-C2-C3-O3
6	A	615[A]	GOL	O1-C1-C2-O2
6	A	615[B]	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	604[A]	HEC	CAA-CBA-CGA-O1A
2	B	602	HEC	CAA-CBA-CGA-O1A
2	A	602	HEC	CAA-CBA-CGA-O1A
2	B	606	HEC	CAA-CBA-CGA-O1A
2	A	608	HEC	CAA-CBA-CGA-O1A
2	B	602	HEC	CAA-CBA-CGA-O2A
2	A	606	HEC	CAA-CBA-CGA-O2A
2	B	604[A]	HEC	CAA-CBA-CGA-O2A
2	B	601	HEC	CAA-CBA-CGA-O1A
2	B	601	HEC	CAA-CBA-CGA-O2A
2	A	606	HEC	CAA-CBA-CGA-O1A
2	A	602	HEC	CAA-CBA-CGA-O2A
2	A	604	HEC	CAA-CBA-CGA-O1A
2	A	608	HEC	CAD-CBD-CGD-O1D
2	A	601	HEC	CAA-CBA-CGA-O2A
2	A	608	HEC	CAD-CBD-CGD-O2D
2	A	602	HEC	CAD-CBD-CGD-O2D
2	A	601	HEC	CAA-CBA-CGA-O1A
2	B	608	HEC	CAD-CBD-CGD-O2D
2	B	607	HEC	CAD-CBD-CGD-O2D
2	B	606	HEC	CAA-CBA-CGA-O2A
2	B	607	HEC	CAA-CBA-CGA-O2A
2	A	604	HEC	CAA-CBA-CGA-O2A
2	A	608	HEC	CAA-CBA-CGA-O2A
2	A	602	HEC	CAD-CBD-CGD-O1D
2	B	608	HEC	CAD-CBD-CGD-O1D
2	B	607	HEC	CAD-CBD-CGD-O1D
2	B	608	HEC	CAA-CBA-CGA-O1A
2	B	608	HEC	CAA-CBA-CGA-O2A
2	B	602	HEC	CAD-CBD-CGD-O2D
2	A	607	HEC	CAD-CBD-CGD-O2D
2	B	607	HEC	CAA-CBA-CGA-O1A
2	A	606	HEC	C4D-C3D-CAD-CBD

There are no ring outliers.

17 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	605	HEC	2	0
2	B	607	HEC	2	0
7	B	615	SO4	1	0
2	A	603	HEC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	609	NO2	1	0
2	B	606	HEC	2	0
3	B	616	NO2	1	0
2	A	601	HEC	1	0
2	A	606	HEC	2	0
7	A	616	SO4	1	0
5	B	612	MPD	3	0
2	B	603	HEC	2	0
2	A	608	HEC	1	0
2	A	605	HEC	2	0
2	A	604	HEC	2	0
2	B	604[B]	HEC	1	0
2	B	601	HEC	2	0

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

Ligand HEC B 604 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC A 607

Bond lengths

Bond angles

Torsions

Rings
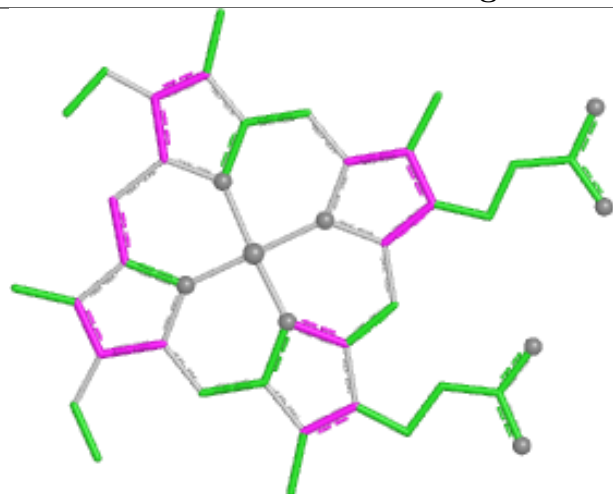
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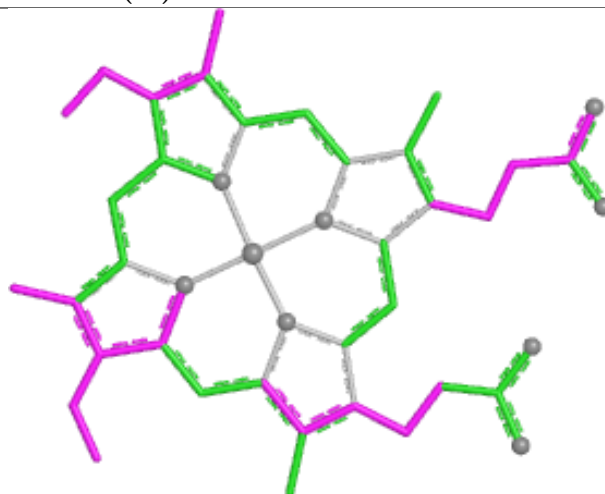
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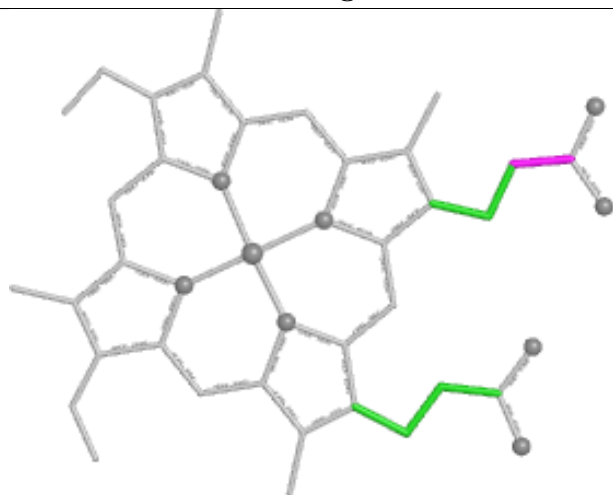
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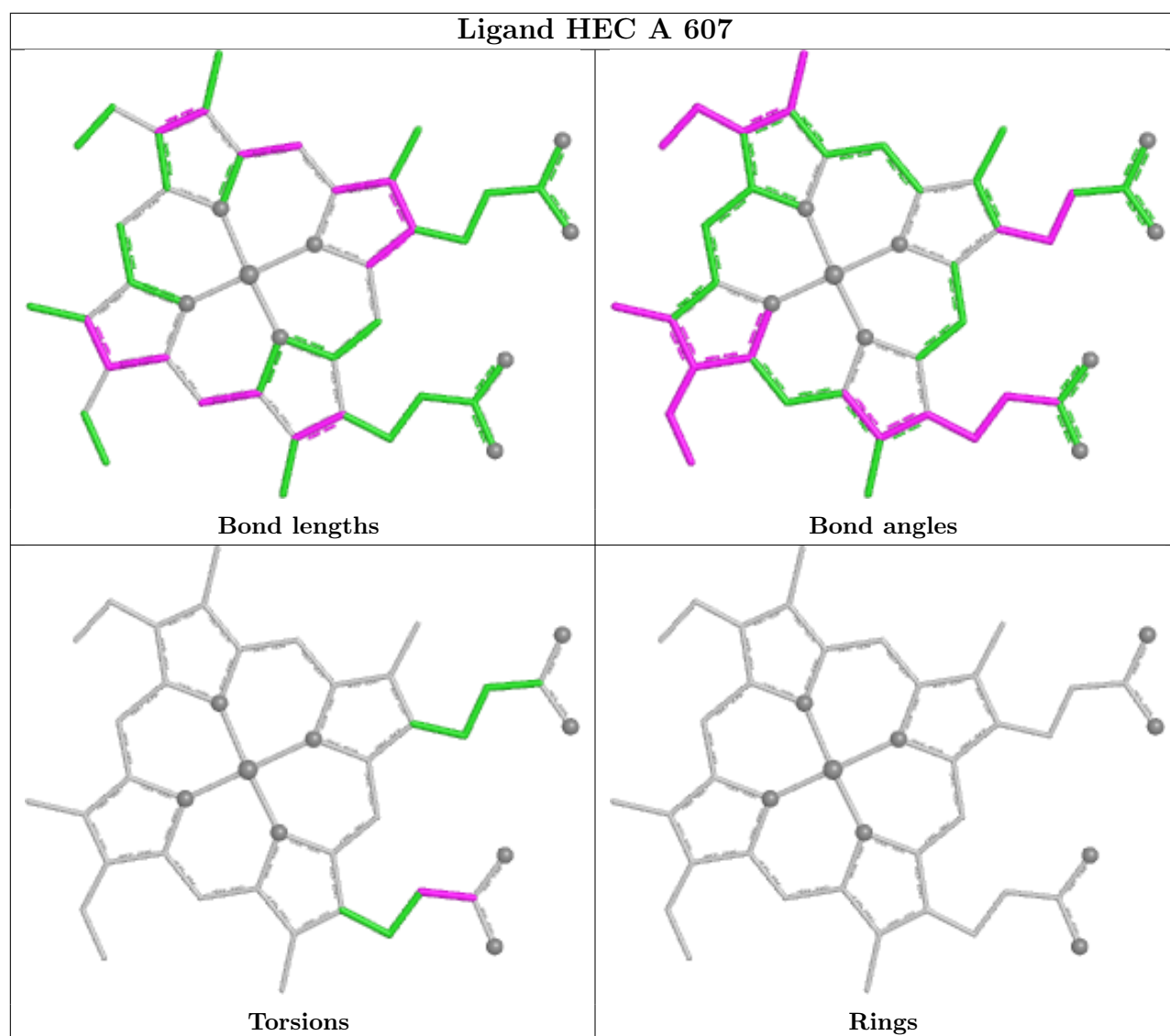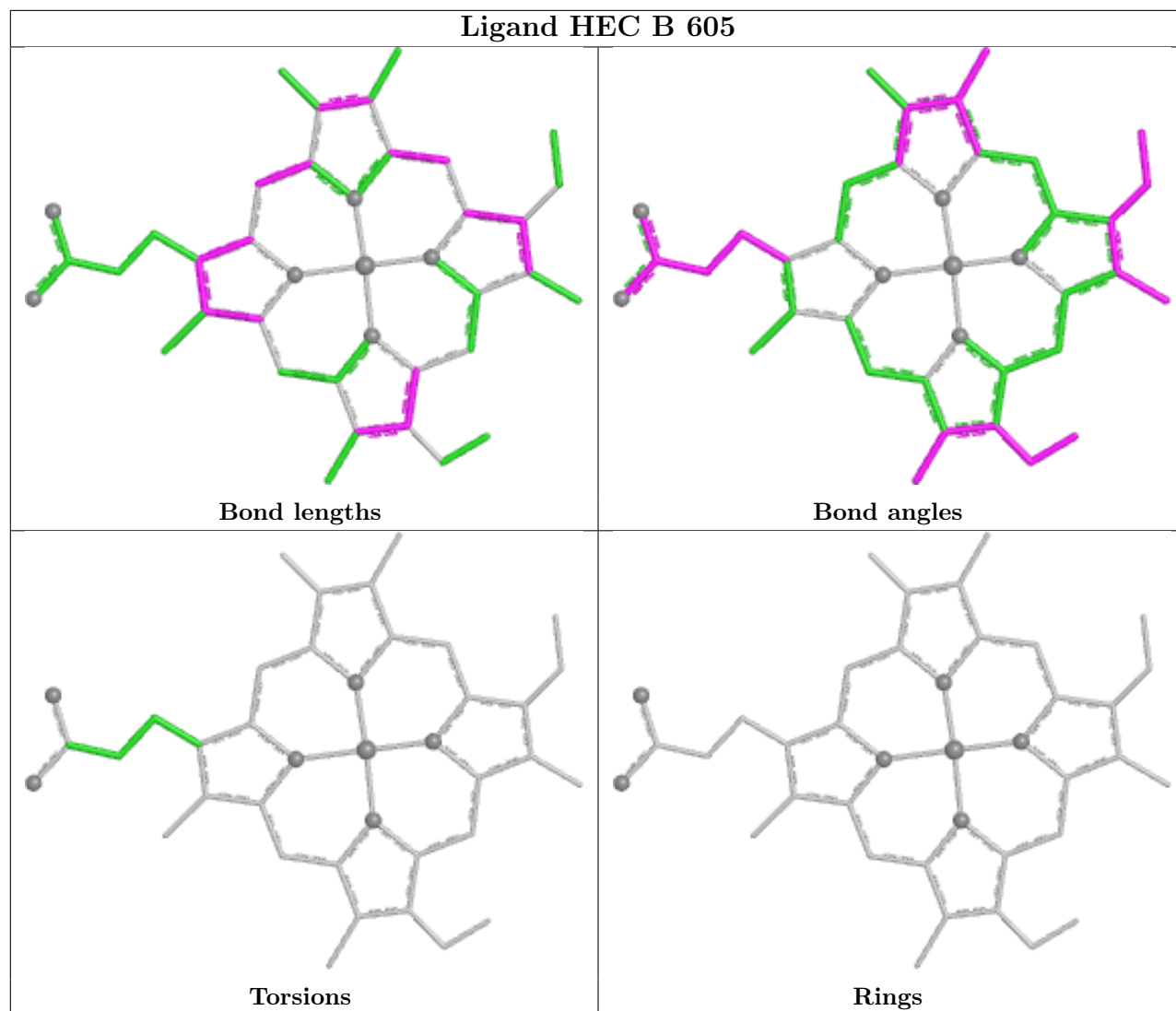
Torsions

Rings

Ligand HEC B 607

Bond lengths

Bond angles

Torsions

Rings
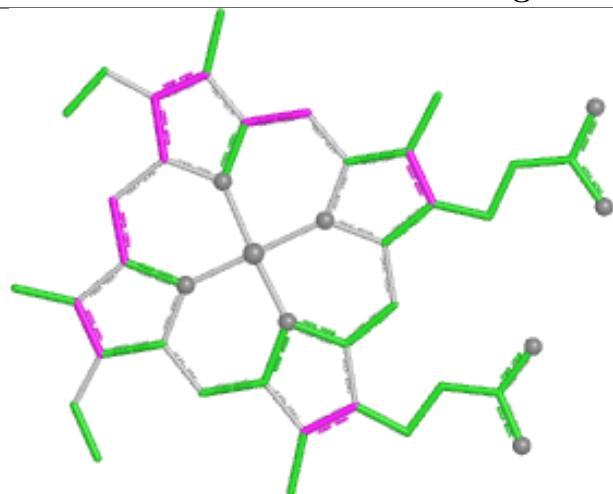
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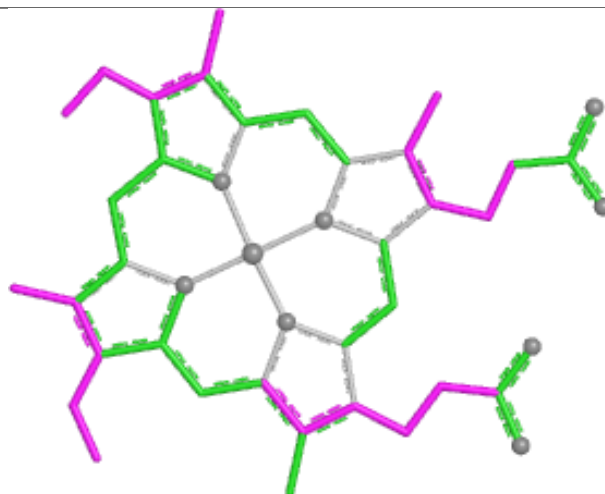
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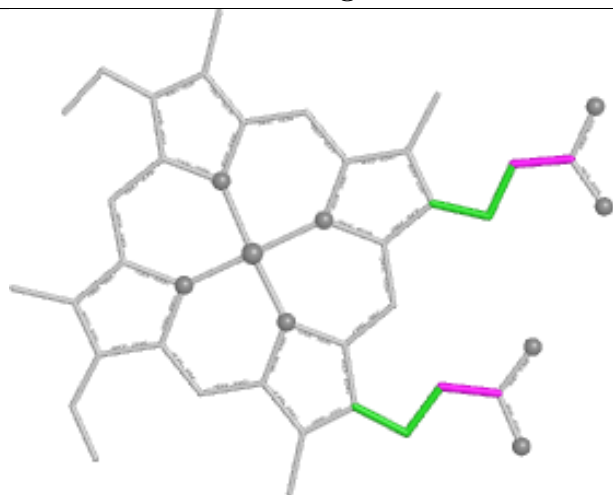
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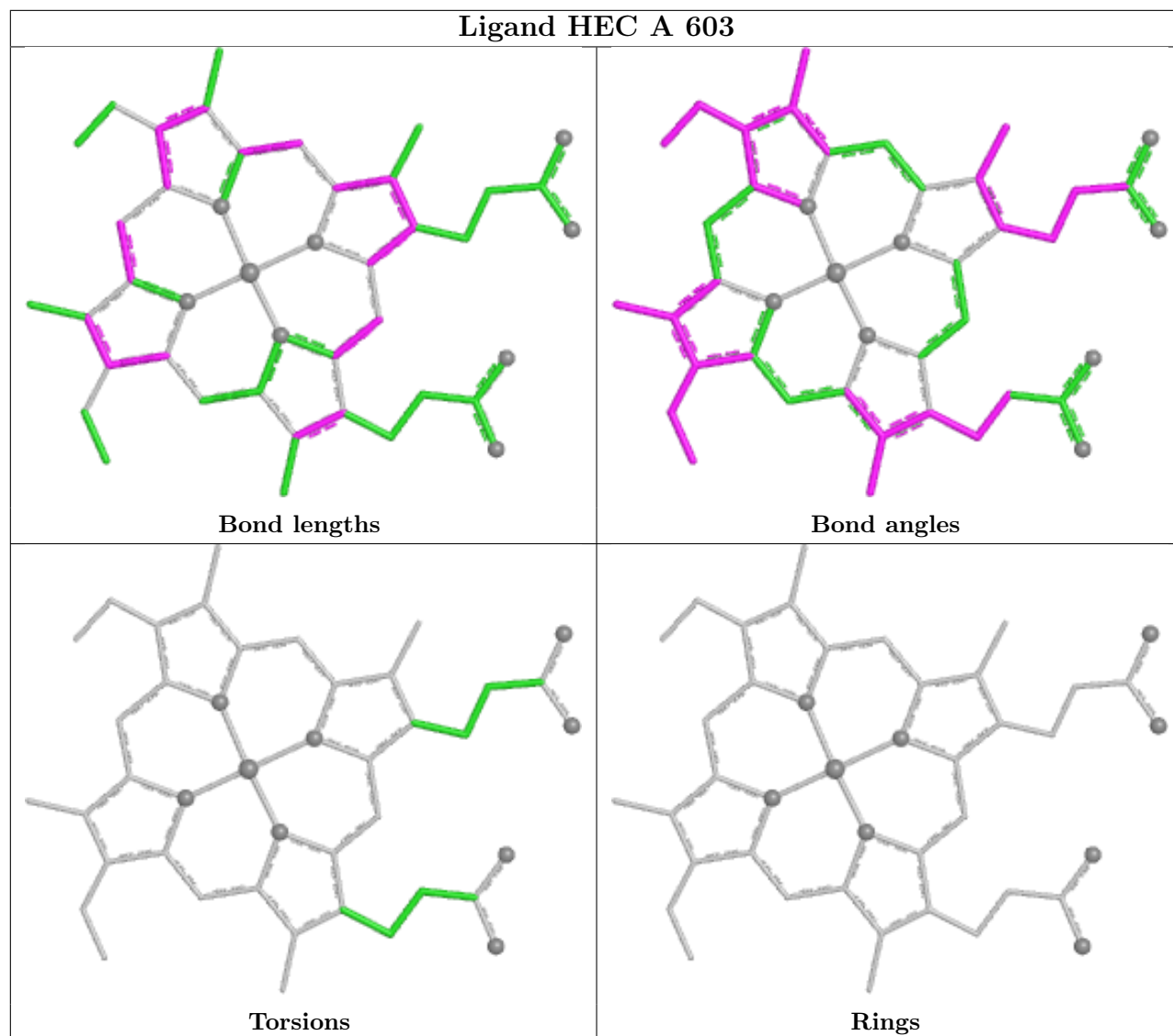
Torsions

Rings
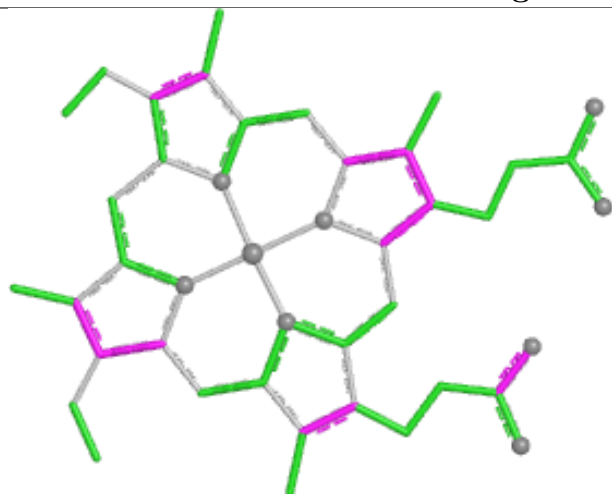
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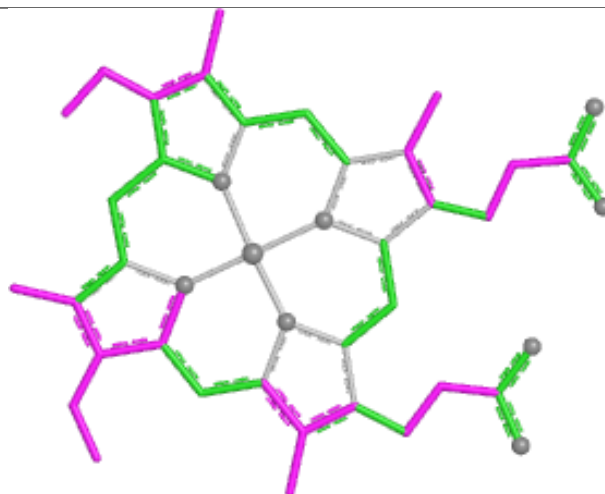
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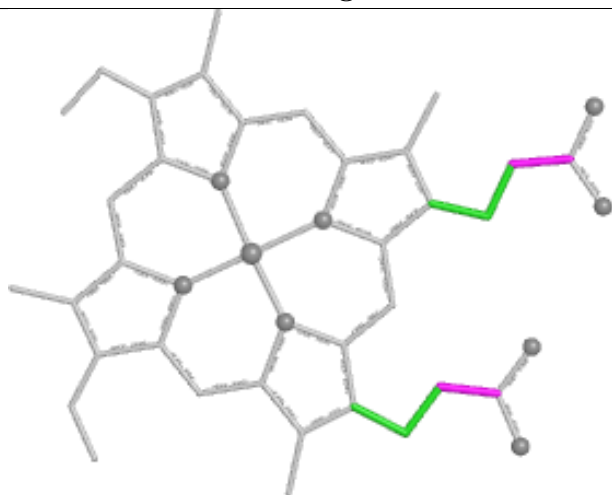
Torsions

Rings

Ligand HEC B 606

Bond lengths

Bond angles

Torsions

Rings
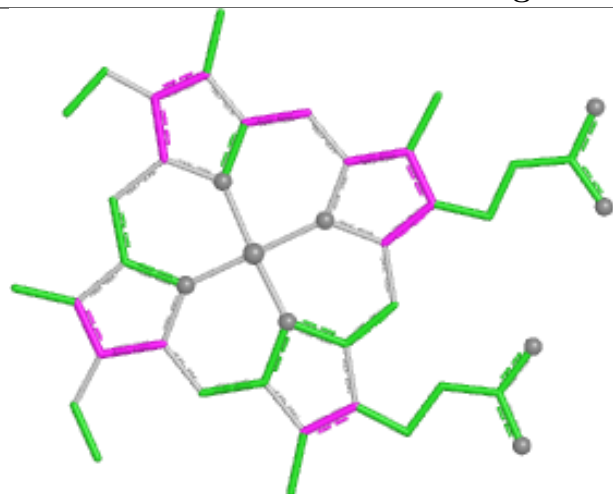
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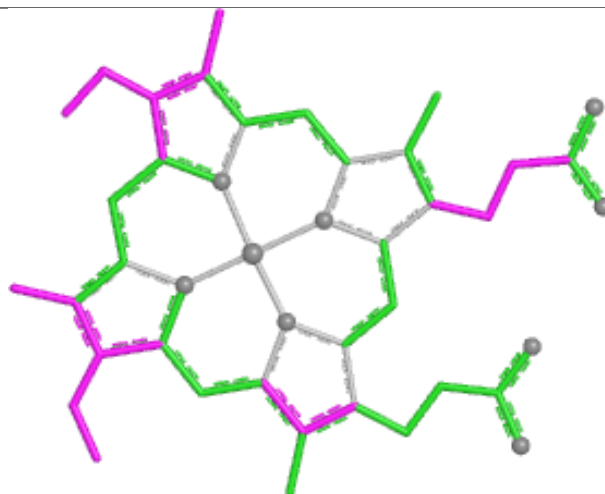
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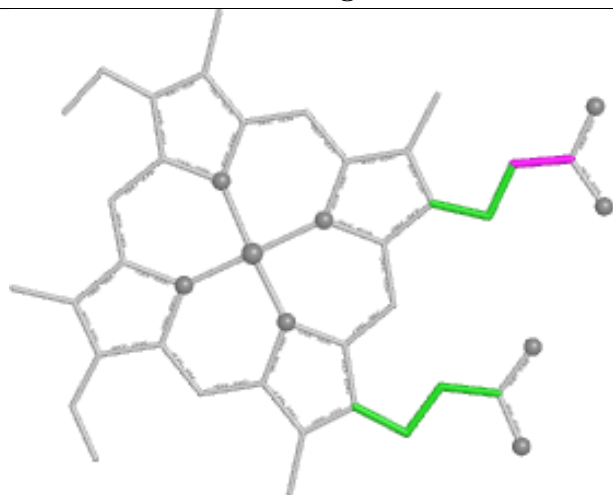
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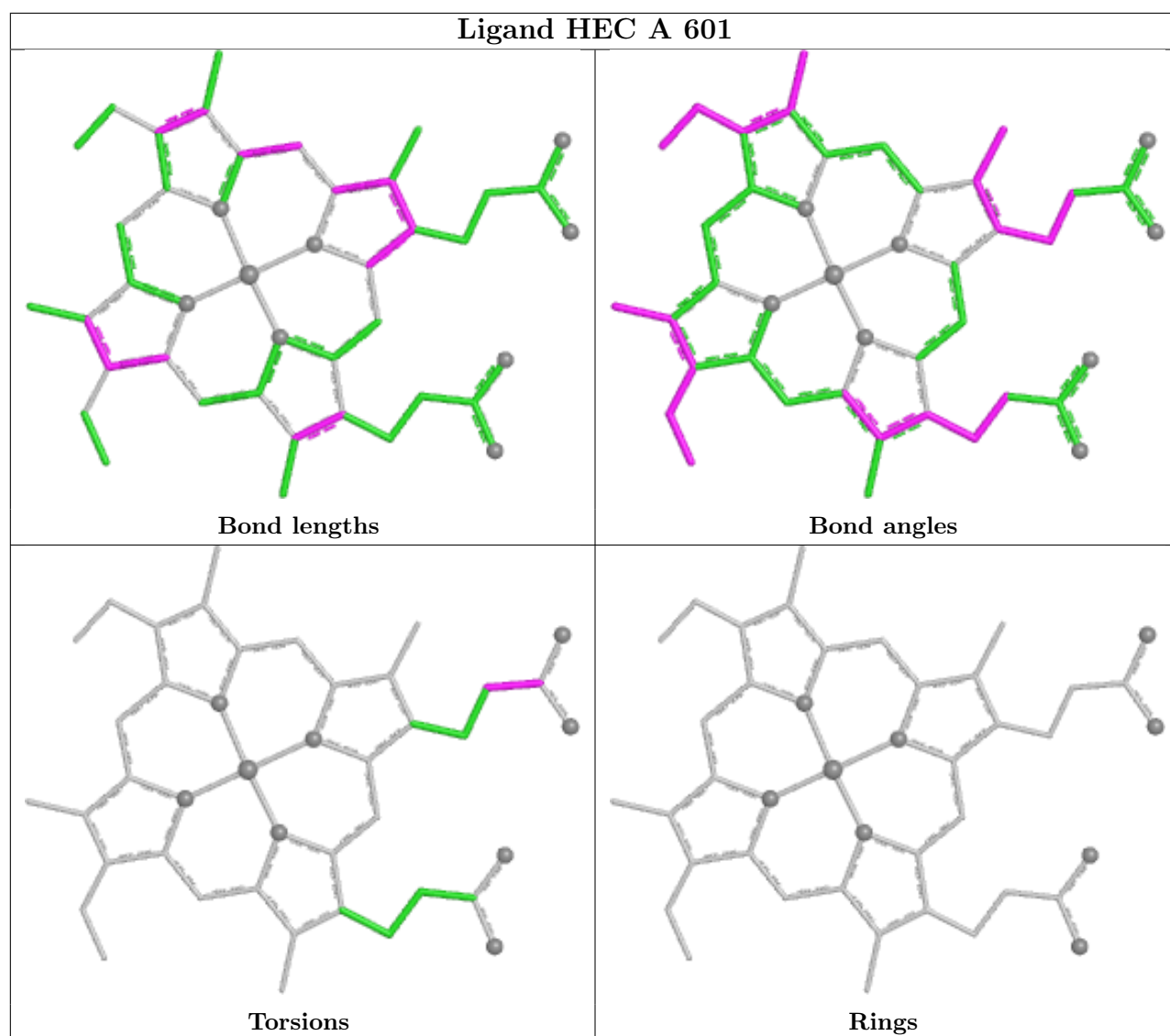
Torsions

Rings

Ligand HEC B 608

Bond lengths

Bond angles

Torsions

Rings
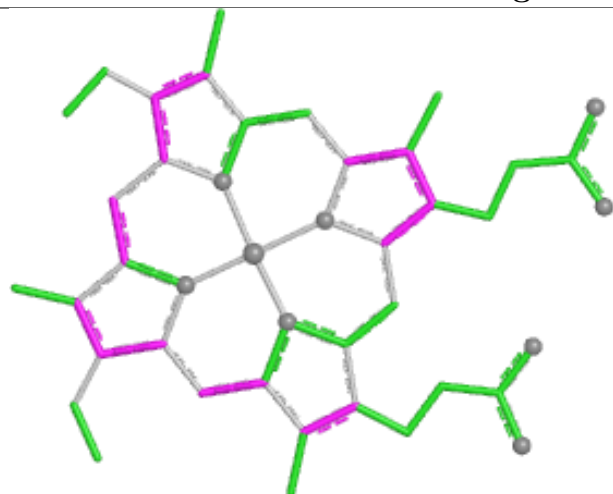
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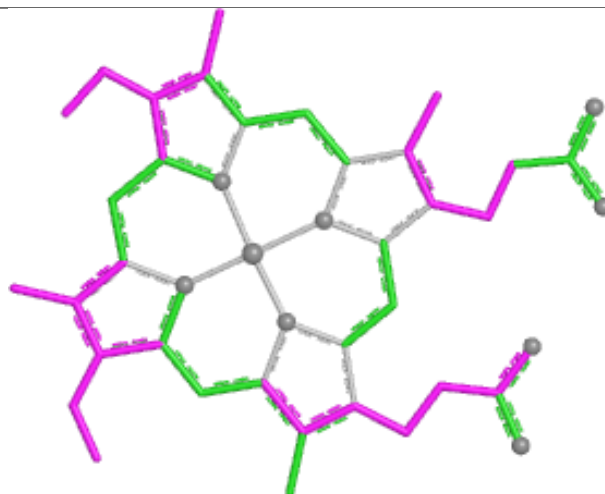
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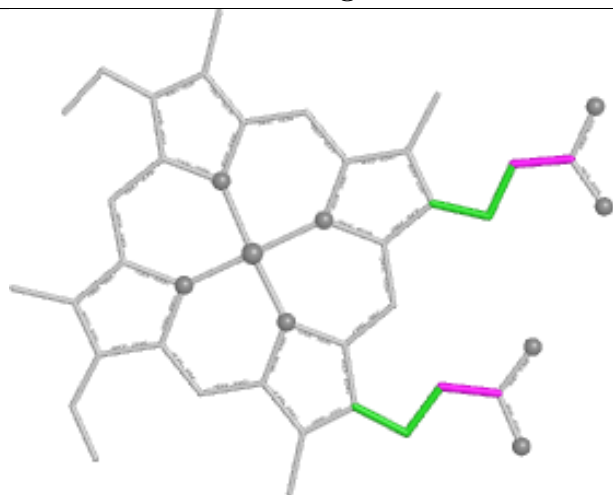
Bond angles
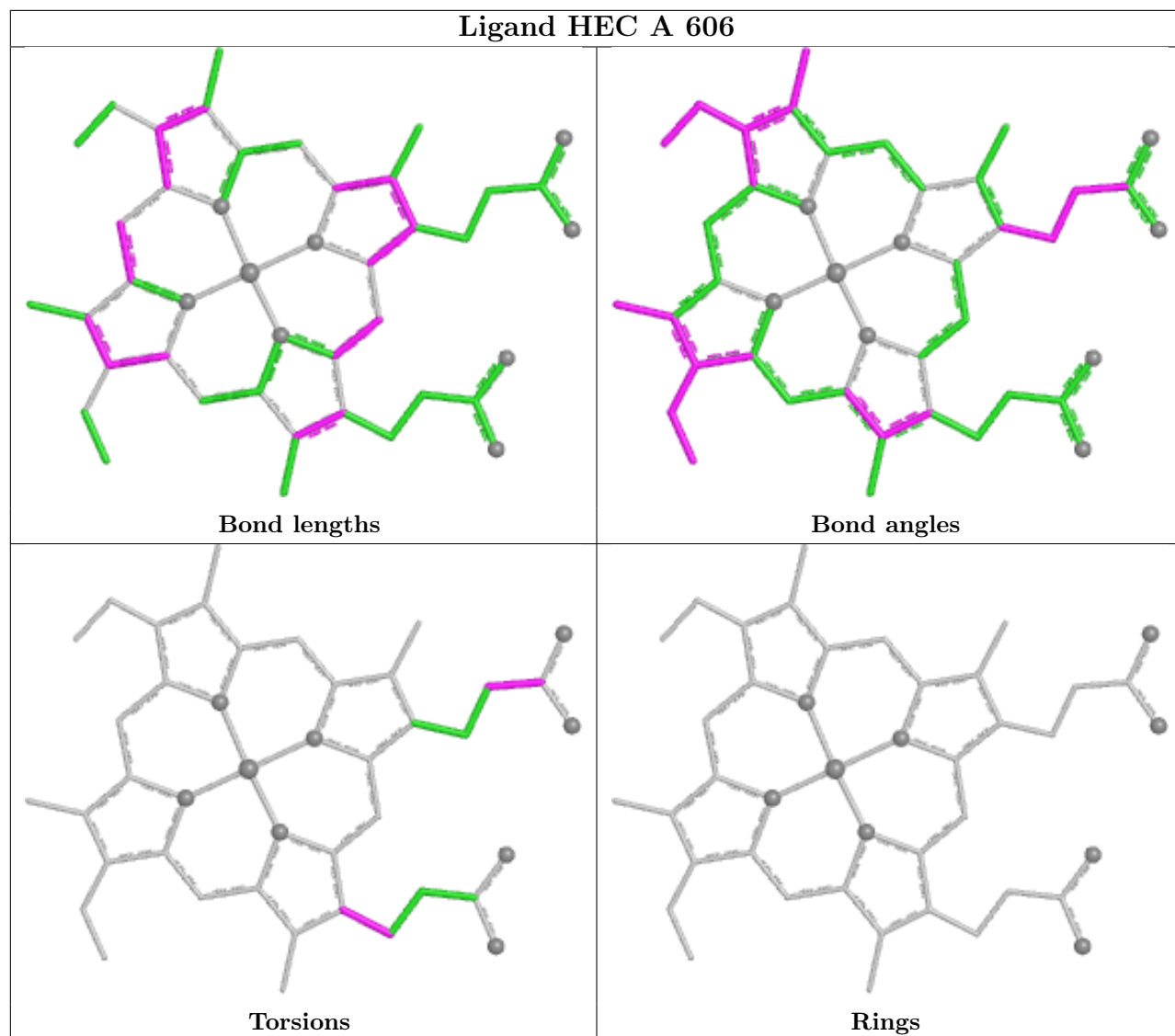
Torsions

Rings

Ligand HEC B 603

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC A 608

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC A 605

Bond lengths

Bond angles

Torsions

Rings
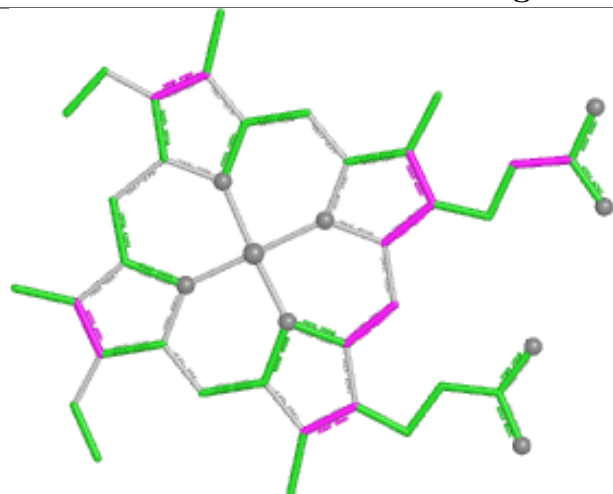
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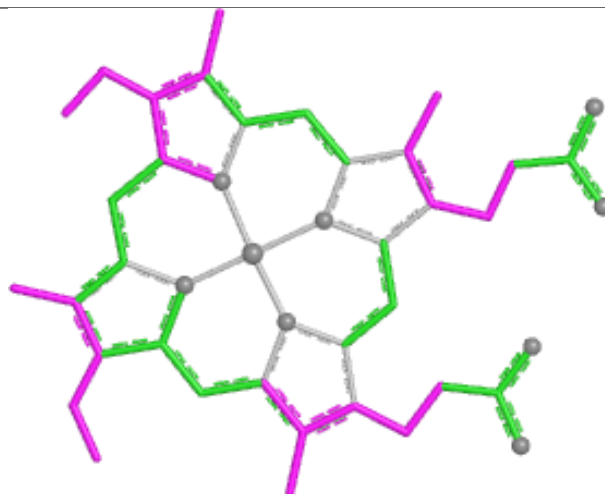
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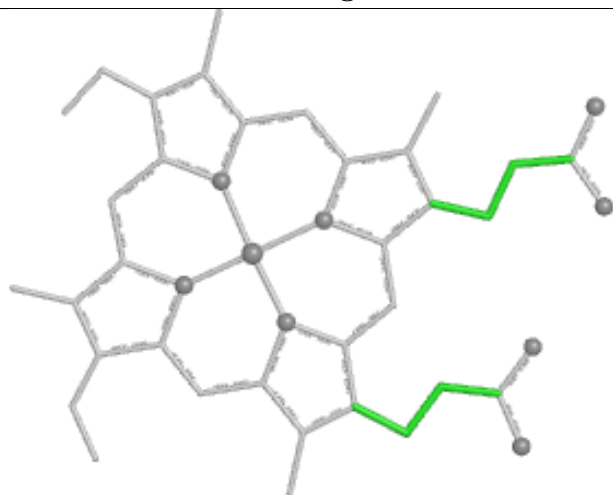
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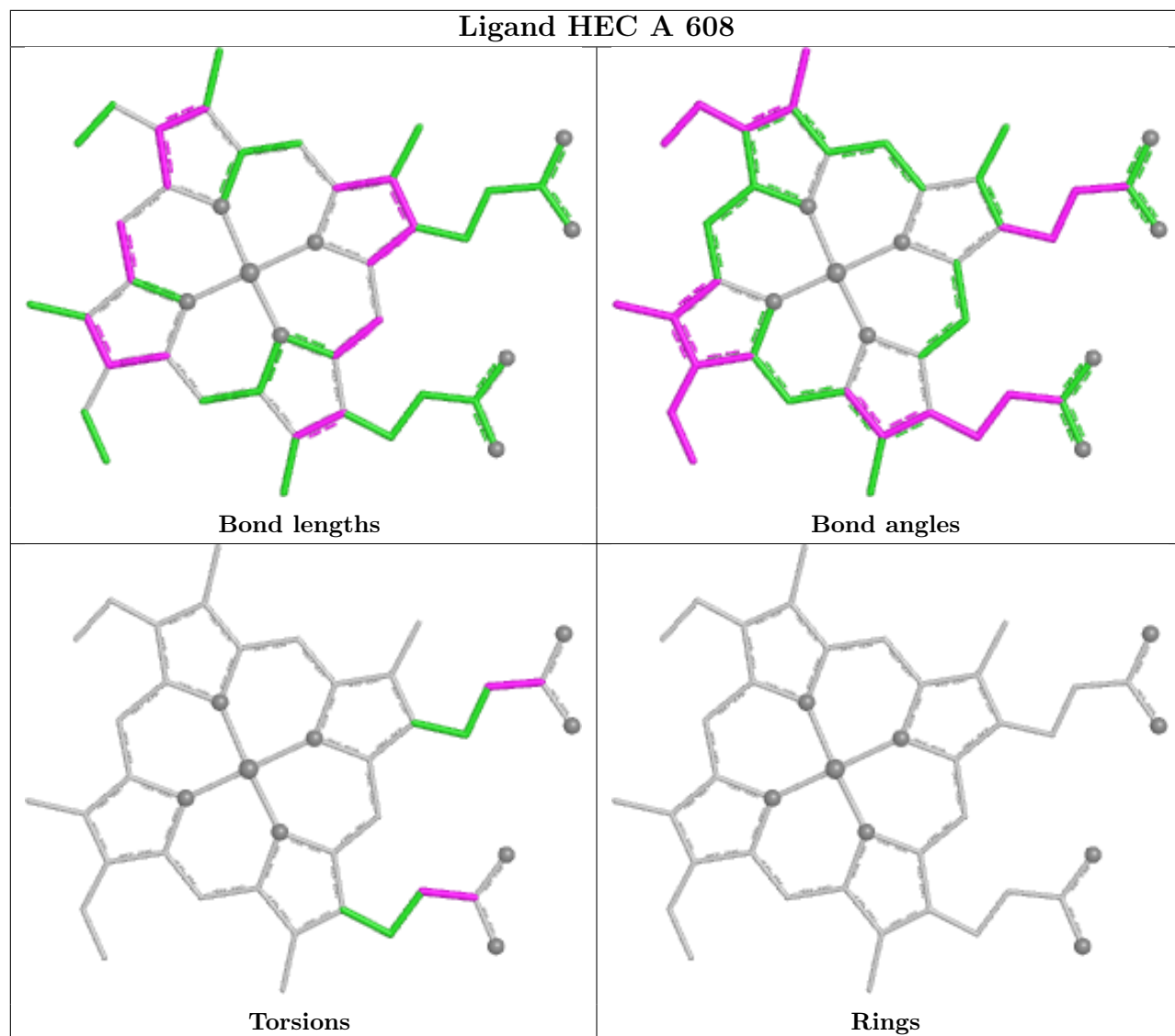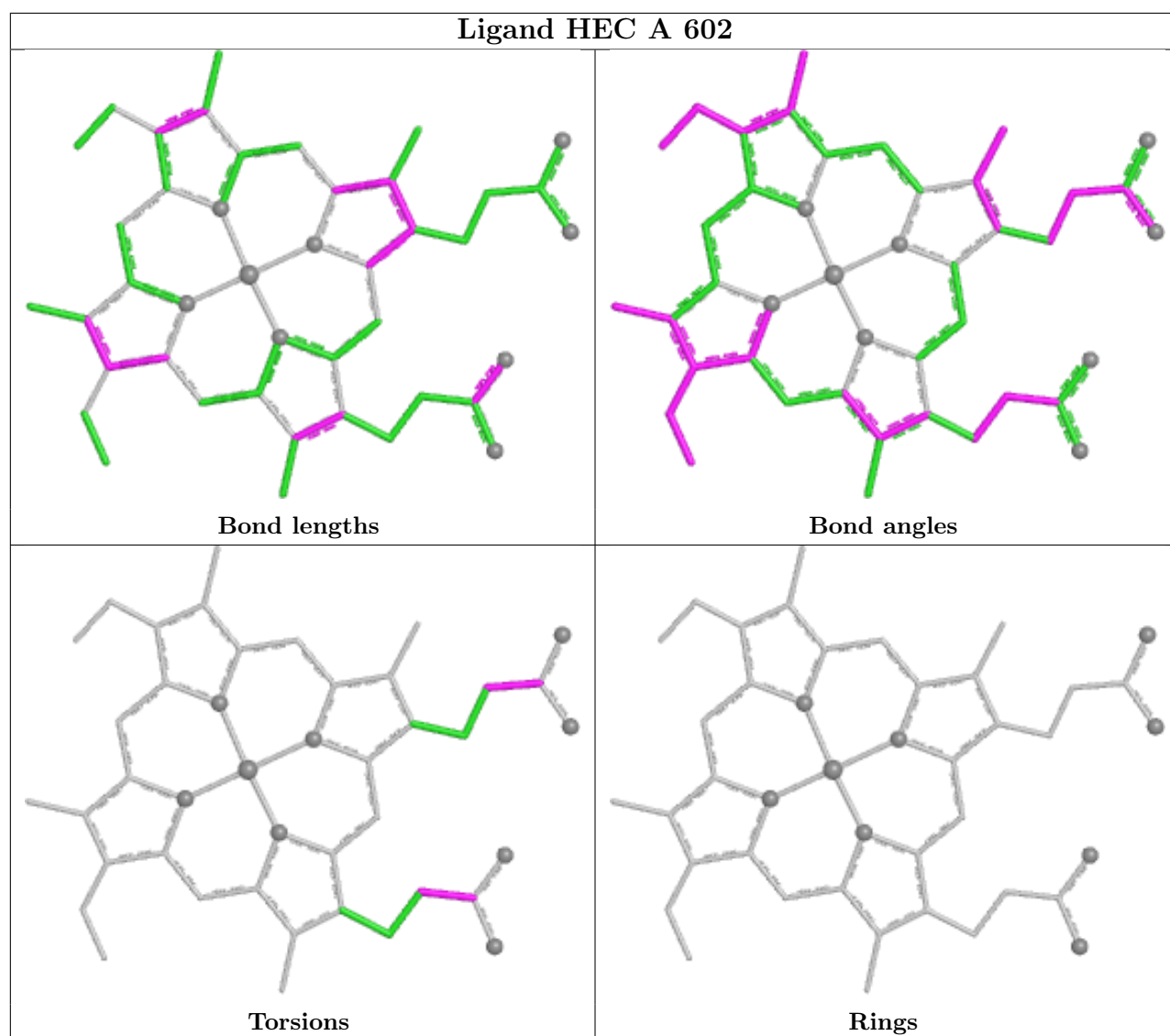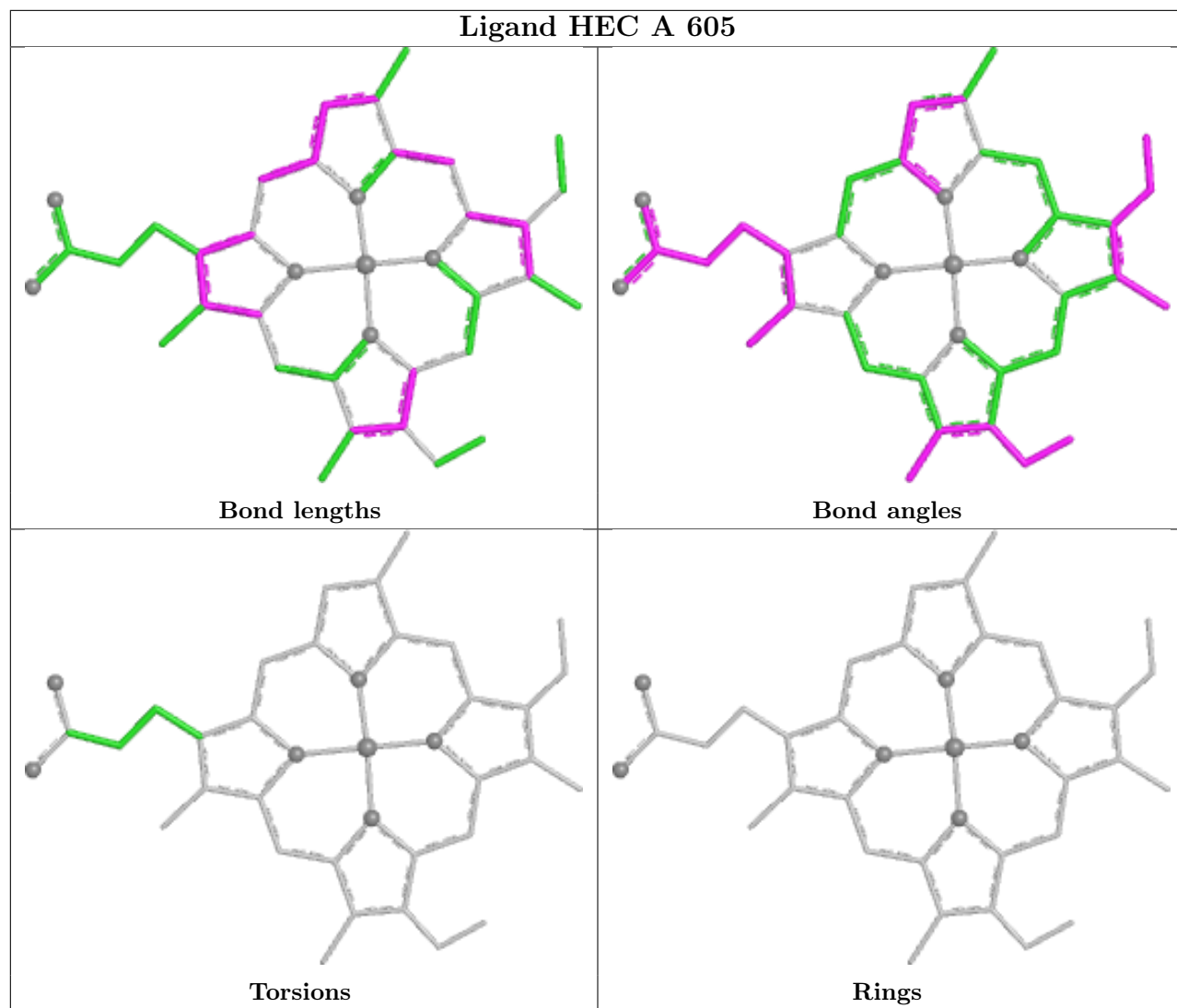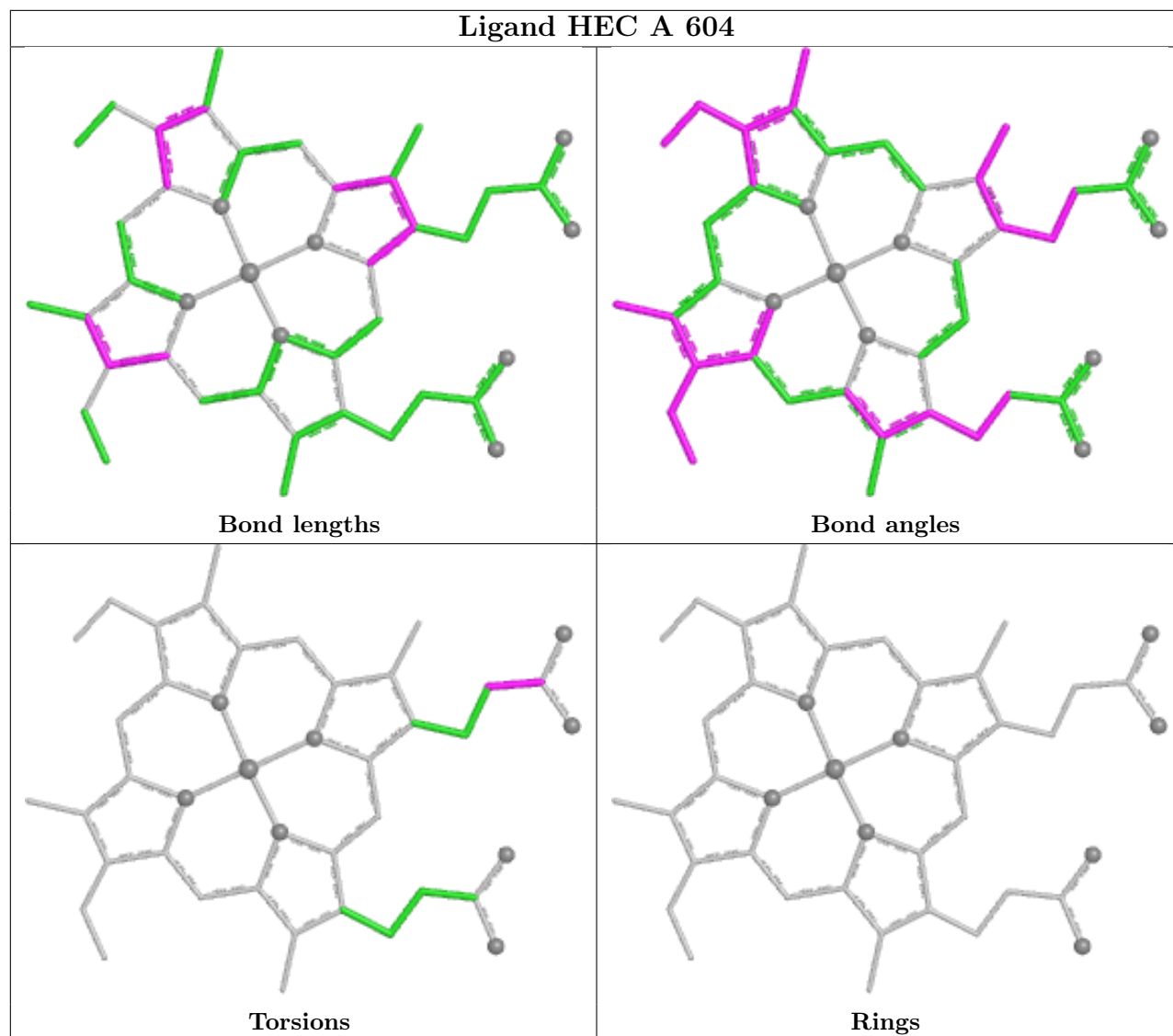
Torsions

Rings

Ligand HEC B 604 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC B 601
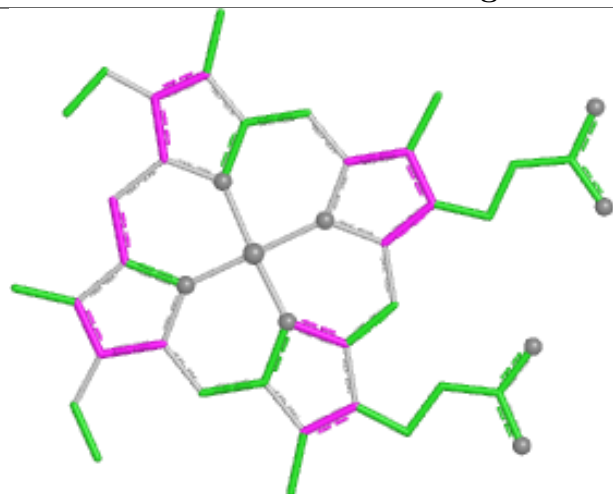
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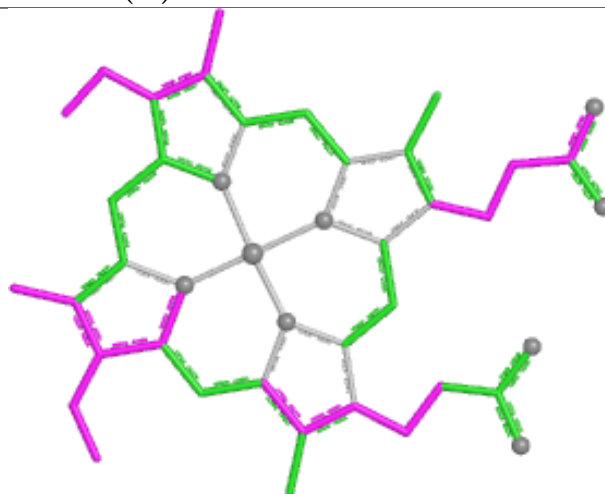
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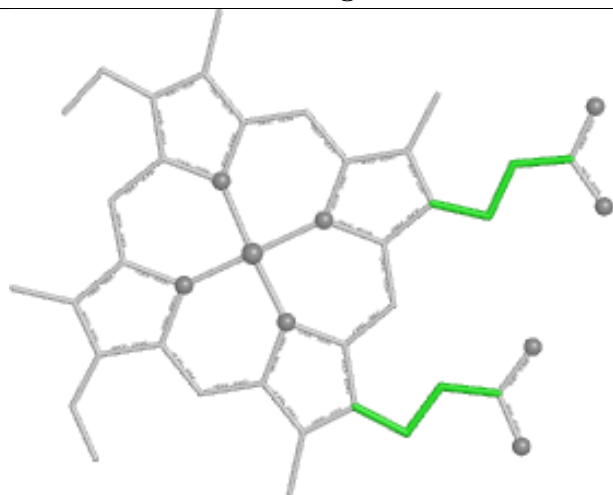
Torsions

Rings
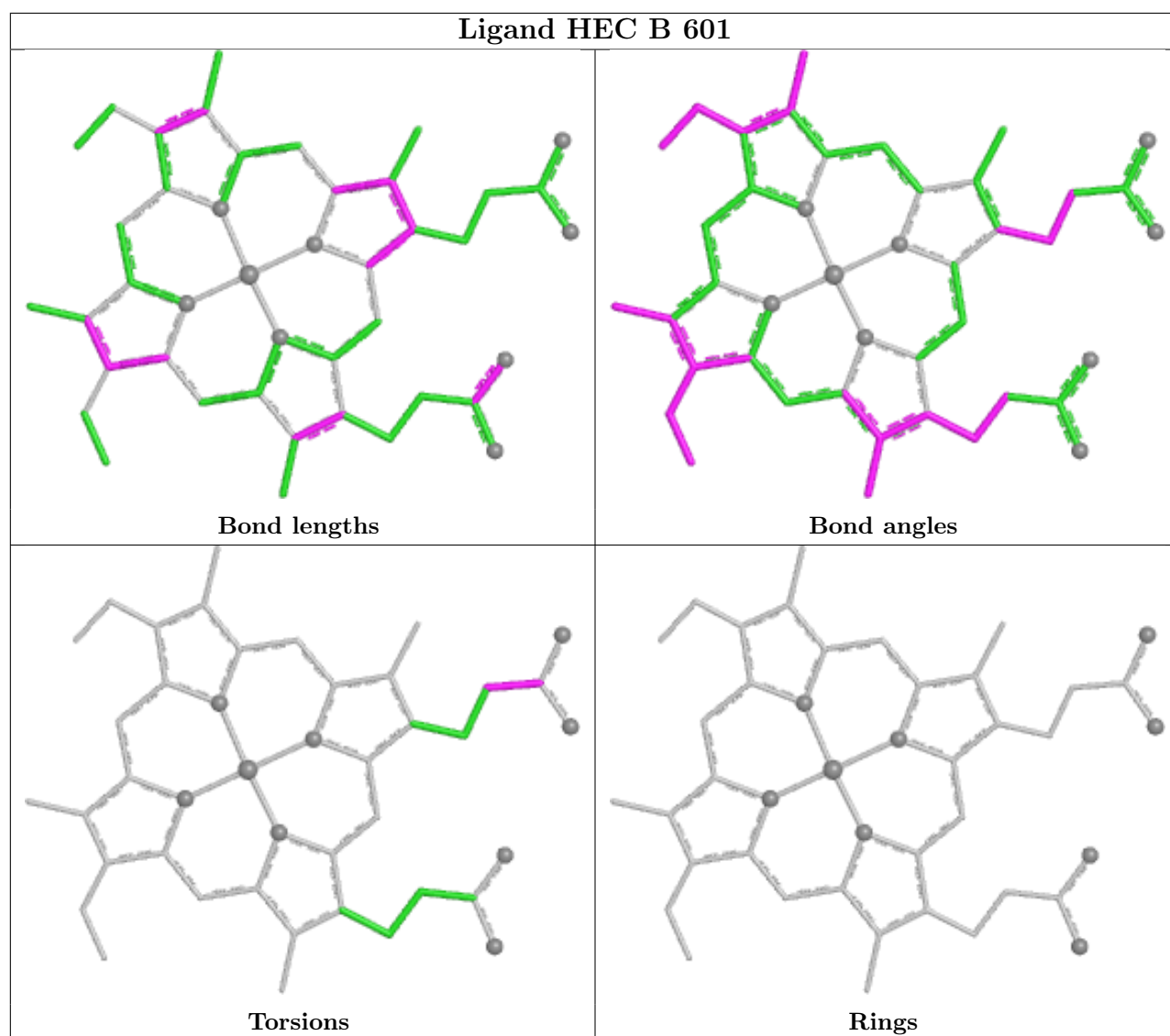
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	520/520 (100%)	-0.77	4 (0%)	82	85	8, 13, 25, 52	19 (3%)
1	B	520/520 (100%)	-0.85	2 (0%)	89	91	7, 11, 24, 48	16 (3%)
All	All	1040/1040 (100%)	-0.81	6 (0%)	85	88	7, 12, 24, 52	35 (3%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	524	VAL	4.9
1	A	524	VAL	3.8
1	B	523	ALA	2.4
1	A	523	ALA	2.4
1	A	278	ARG	2.2
1	A	413	ASN	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
6	GOL	A	615[A]	6/6	0.70	0.23	30,41,44,47	1
6	GOL	A	615[B]	6/6	0.70	0.23	31,41,44,47	1
5	MPD	A	612	8/8	0.91	0.13	17,20,23,24	0
7	SO4	B	615	5/5	0.91	0.12	16,16,18,18	5
7	SO4	A	616	5/5	0.93	0.12	22,22,23,24	5
5	MPD	B	612	8/8	0.94	0.10	17,19,20,20	0
6	GOL	B	613[B]	6/6	0.95	0.07	11,12,13,14	1
3	NO2	A	618	3/3	0.95	0.07	19,19,20,20	3
6	GOL	B	613[A]	6/6	0.95	0.07	10,12,12,13	1
2	HEC	B	605	39/43	0.96	0.12	17,23,37,42	0
2	HEC	A	605	38/43	0.96	0.13	19,26,39,42	0
6	GOL	A	613[A]	6/6	0.96	0.06	12,13,15,17	1
6	GOL	A	613[B]	6/6	0.96	0.06	13,14,16,17	1
3	NO2	B	617	3/3	0.96	0.07	11,11,11,12	3
3	NO2	B	609	3/3	0.97	0.08	10,10,10,10	3
6	GOL	A	614	6/6	0.97	0.09	17,21,22,22	0
6	GOL	B	614	6/6	0.97	0.08	13,18,20,21	0
3	NO2	B	616	3/3	0.97	0.06	16,16,17,17	3
3	NO2	A	609	3/3	0.97	0.07	12,12,13,14	3
3	NO2	A	617	3/3	0.98	0.04	15,15,15,15	3
4	CA	A	611	1/1	0.98	0.04	12,12,12,12	1
4	CA	B	611	1/1	0.98	0.03	10,10,10,10	1
2	HEC	A	608	43/43	0.99	0.05	10,12,15,18	0
2	HEC	B	601	43/43	0.99	0.04	7,8,8,9	0
2	HEC	B	602	43/43	0.99	0.05	7,8,15,21	0
2	HEC	B	603	43/43	0.99	0.04	6,6,7,9	0
2	HEC	B	604[A]	43/43	0.99	0.05	6,7,8,9	4
2	HEC	B	604[B]	43/43	0.99	0.05	6,7,9,10	4
2	HEC	A	602	43/43	0.99	0.05	8,9,15,20	0
2	HEC	B	606	43/43	0.99	0.04	9,10,12,13	0
2	HEC	B	607	43/43	0.99	0.05	8,9,19,29	0
2	HEC	B	608	43/43	0.99	0.06	10,14,17,20	0
2	HEC	A	603	43/43	0.99	0.04	7,8,9,10	0
2	HEC	A	604	43/43	0.99	0.05	7,9,11,17	0
2	HEC	A	601	43/43	0.99	0.04	8,9,10,10	0
2	HEC	A	606	43/43	0.99	0.04	9,10,11,12	0
2	HEC	A	607	43/43	0.99	0.06	9,10,21,33	0
4	CA	B	610	1/1	1.00	0.05	13,13,13,13	0
4	CA	A	610	1/1	1.00	0.05	14,14,14,14	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.
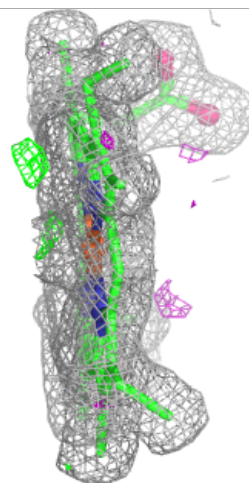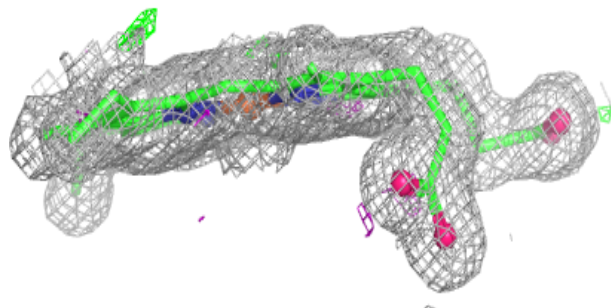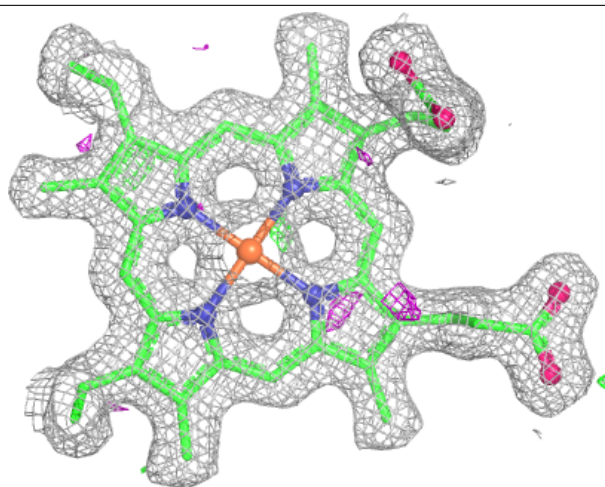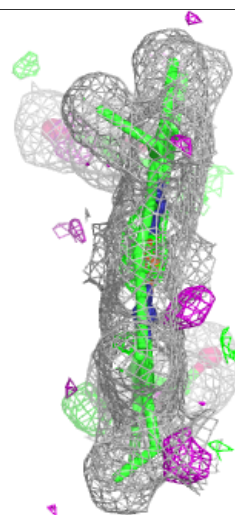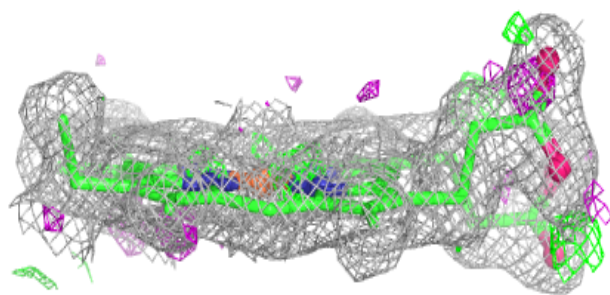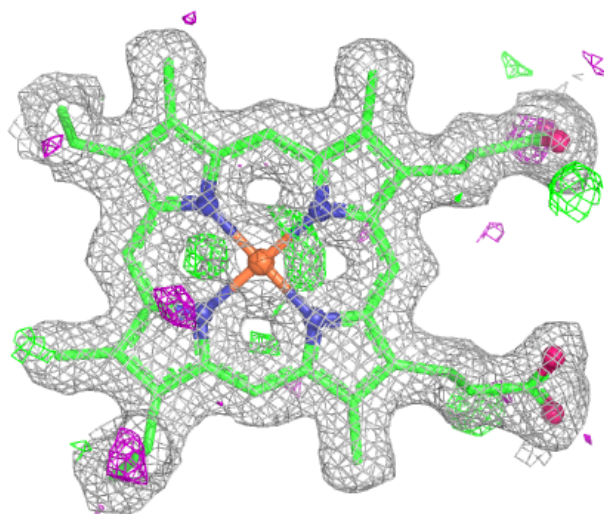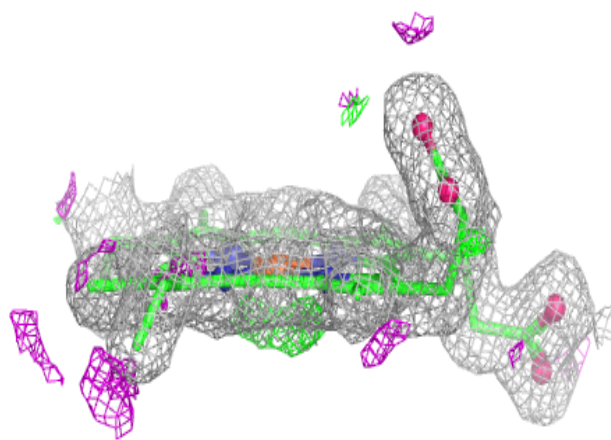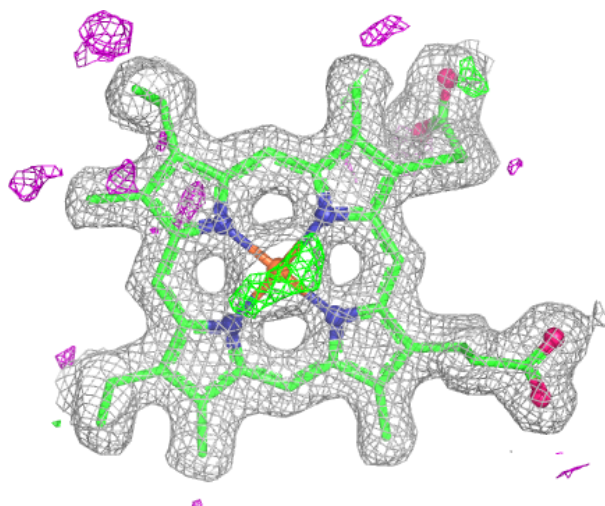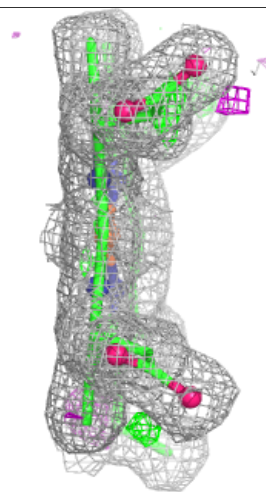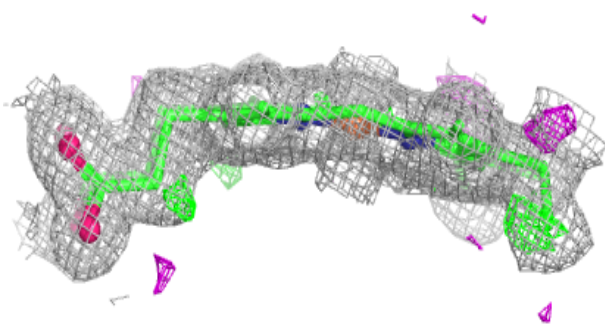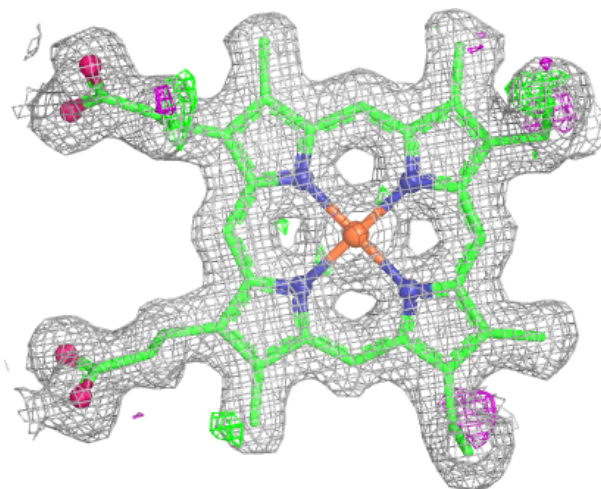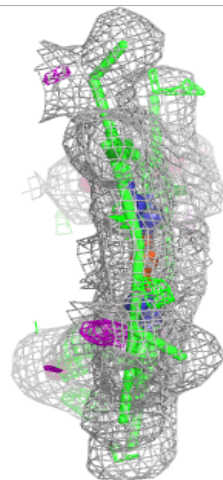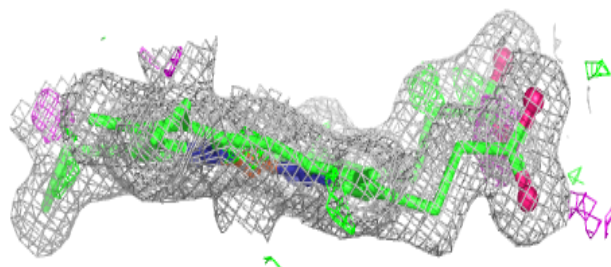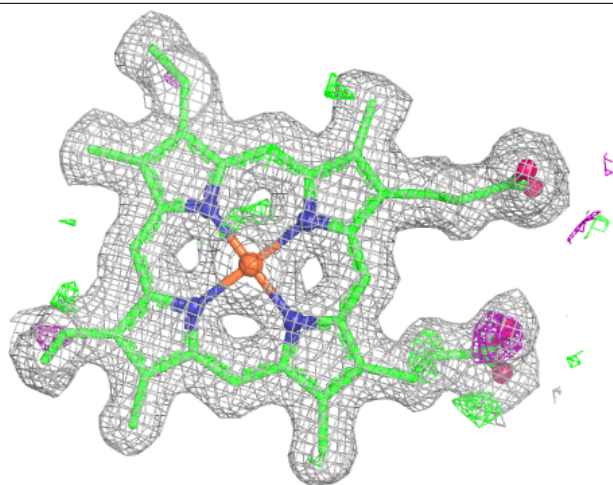
Electron density around HEC B 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
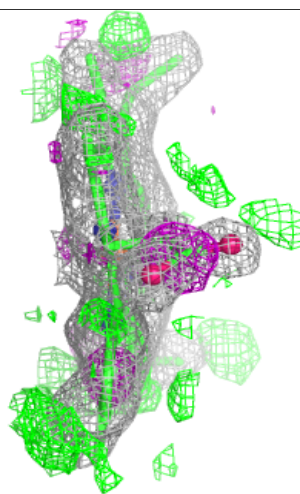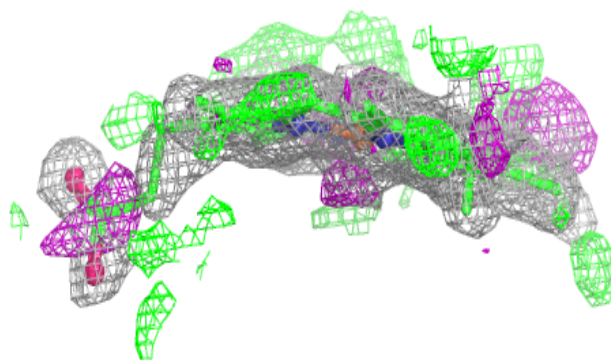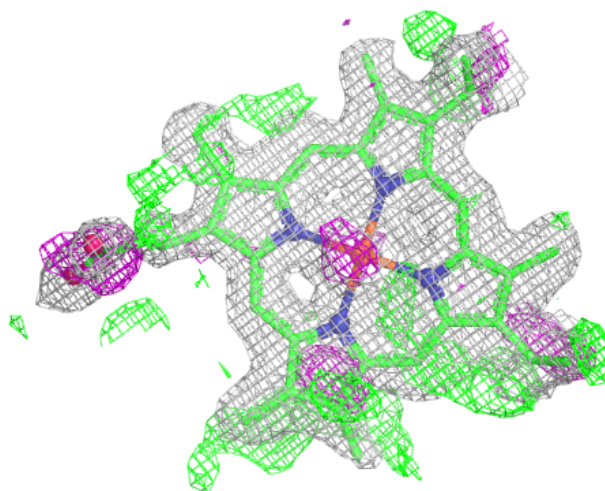
Electron density around HEC A 605:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
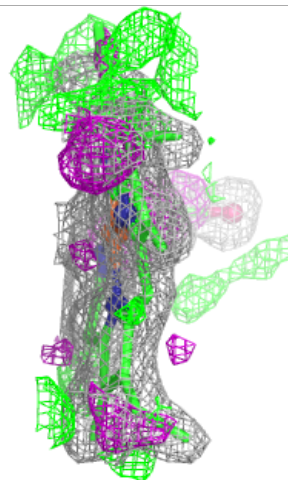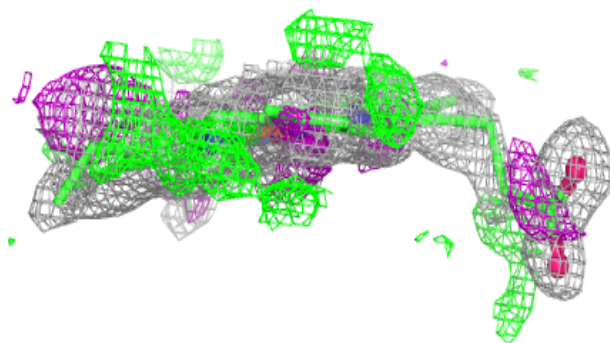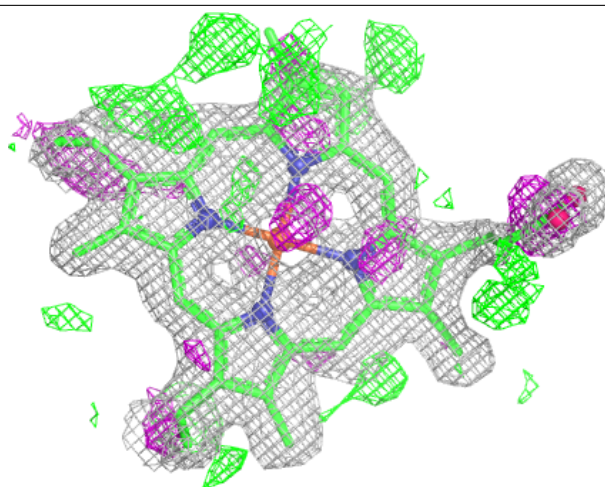
Electron density around HEC A 608:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
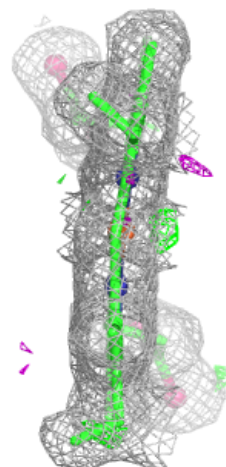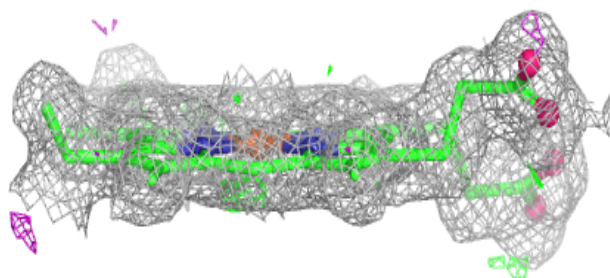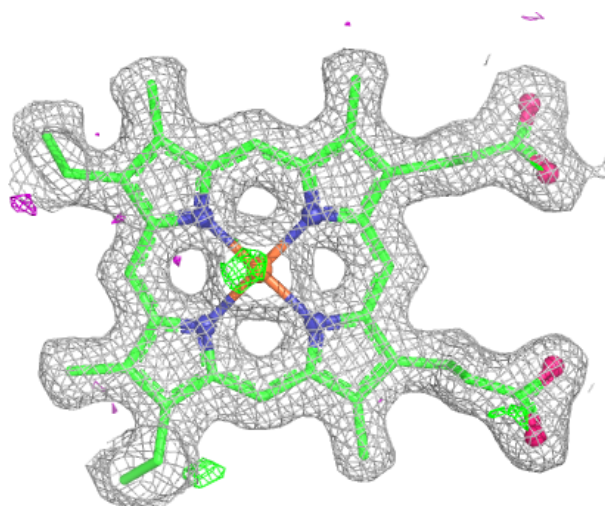
Electron density around HEC B 601:

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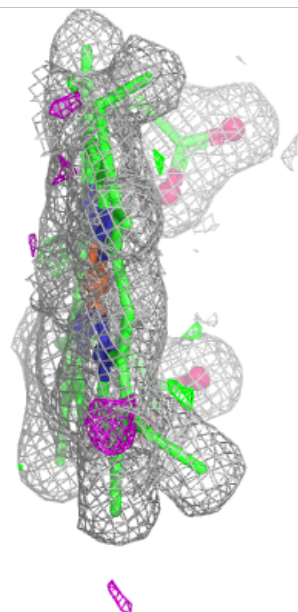$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
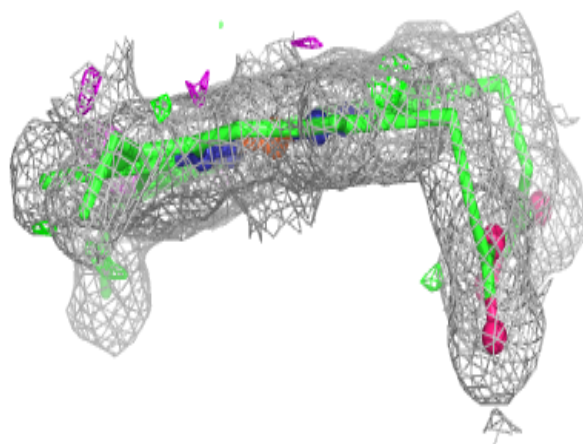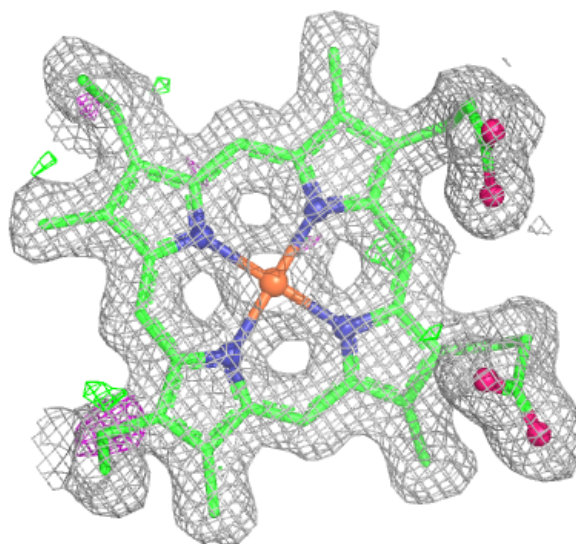and green (positive)
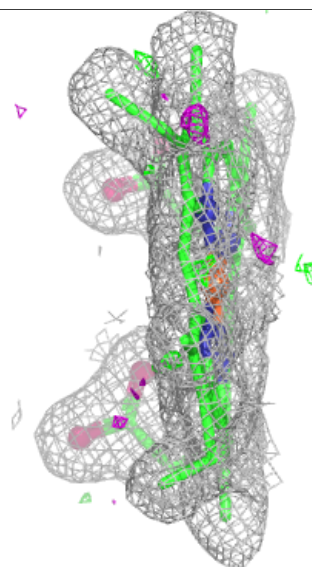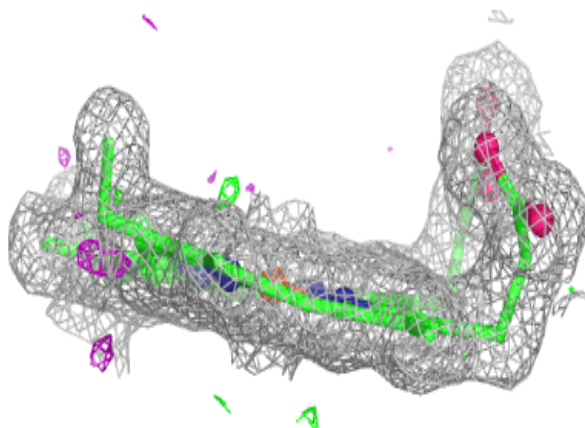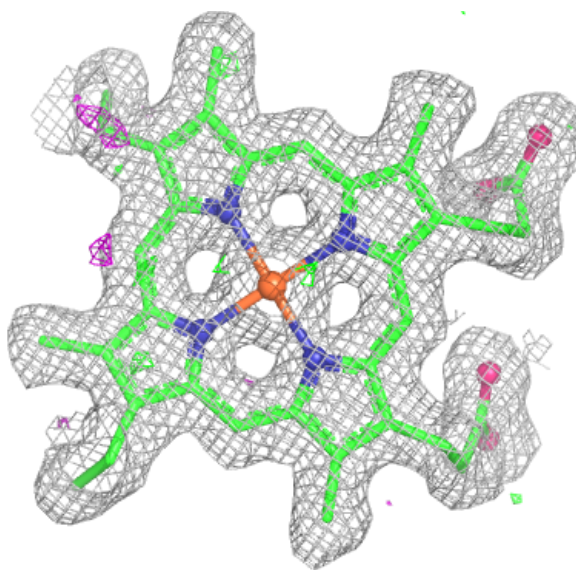
Electron density around HEC B 602:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
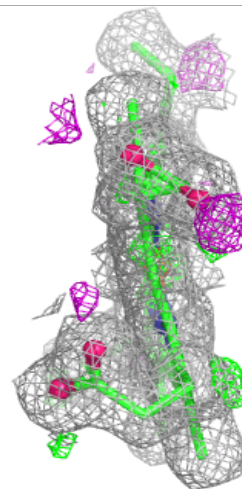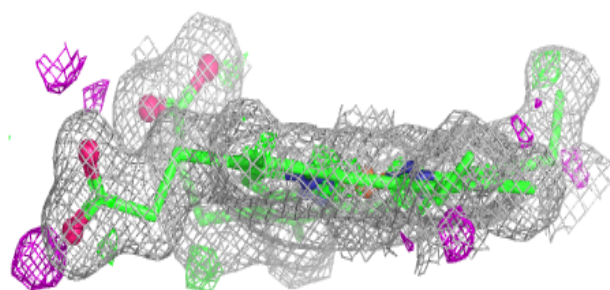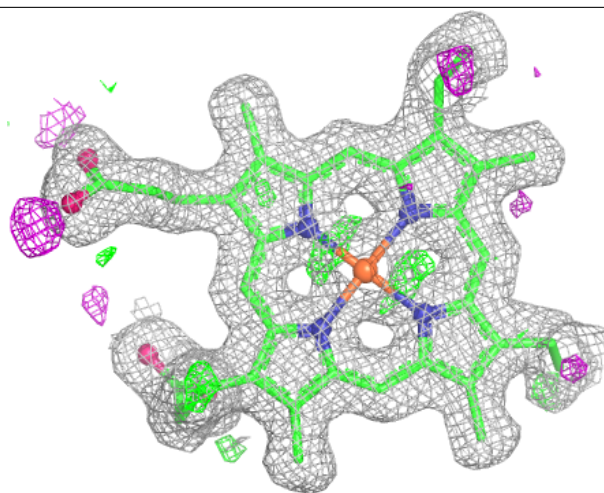
Electron density around HEC B 603:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
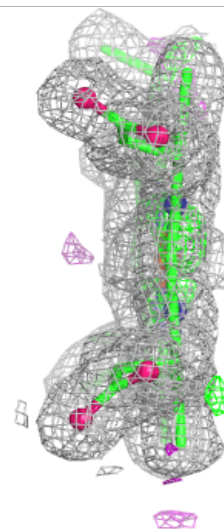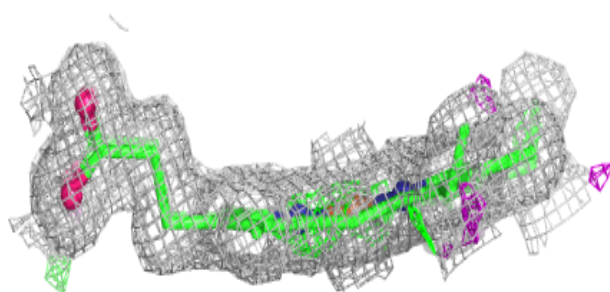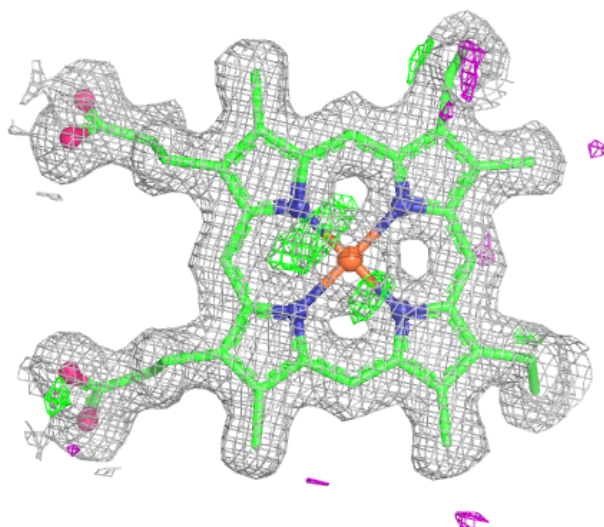
Electron density around HEC B 604 (A):

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
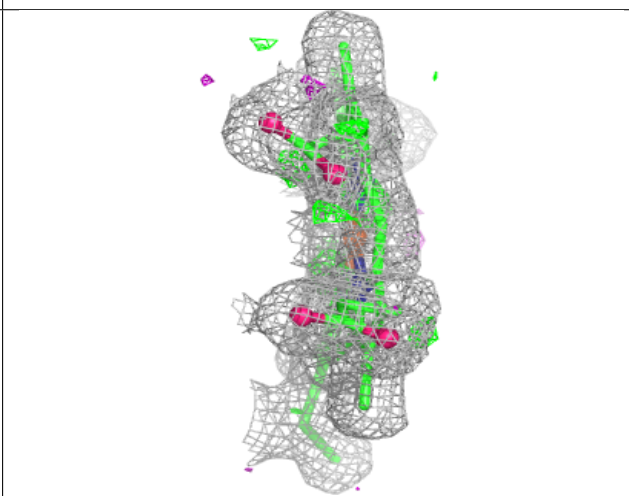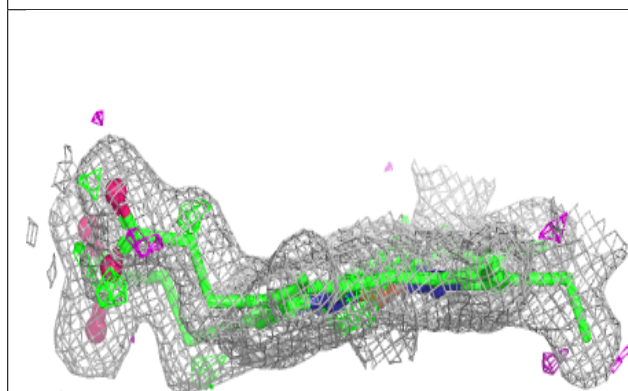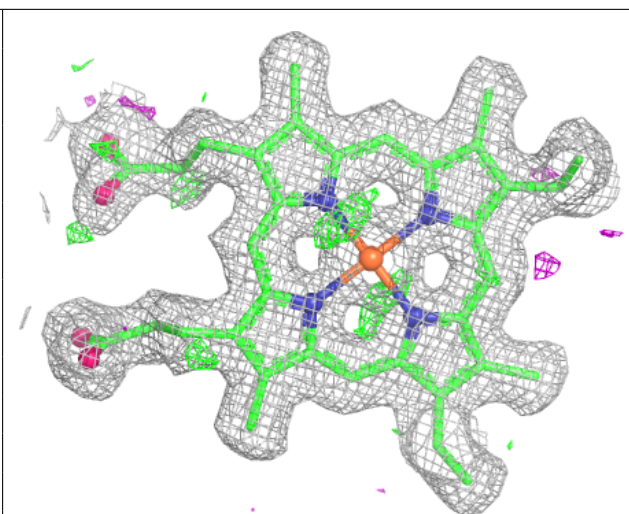
Electron density around HEC B 604 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
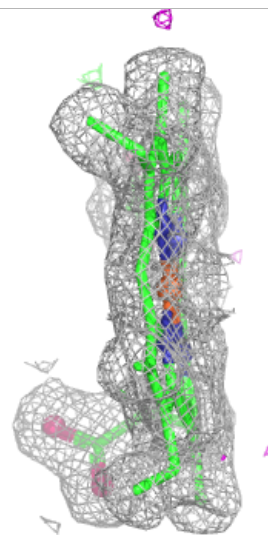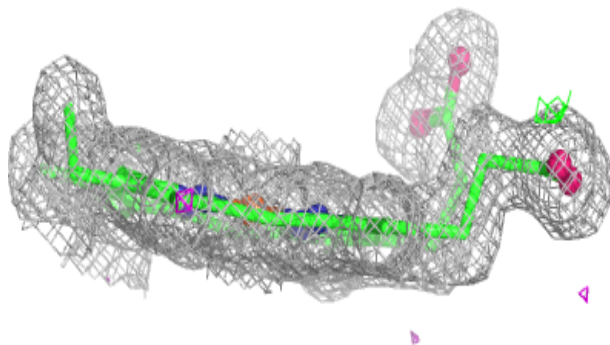and green (positive)
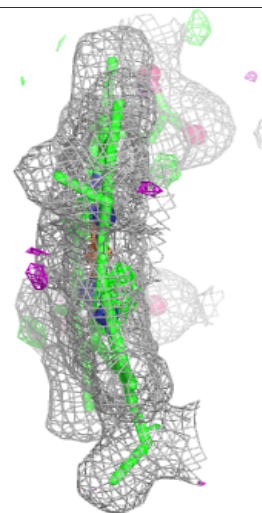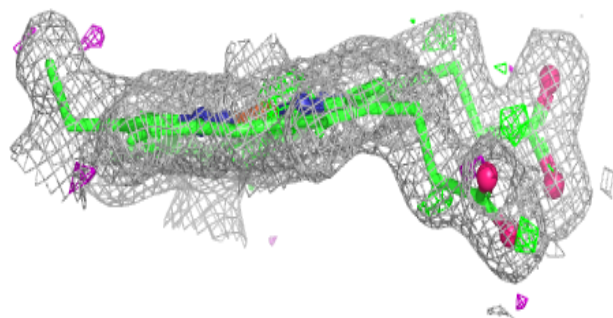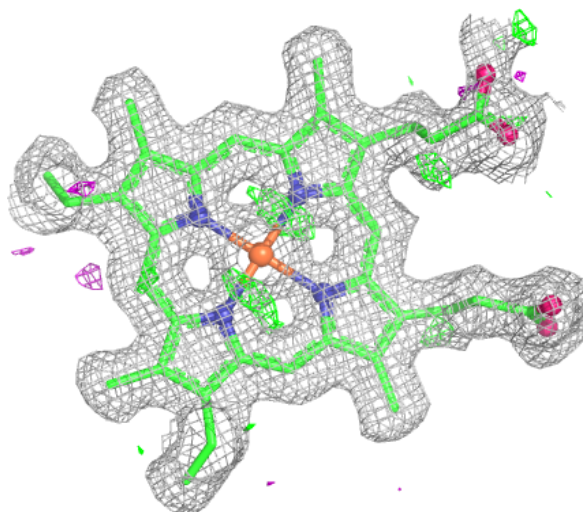
Electron density around HEC A 602:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
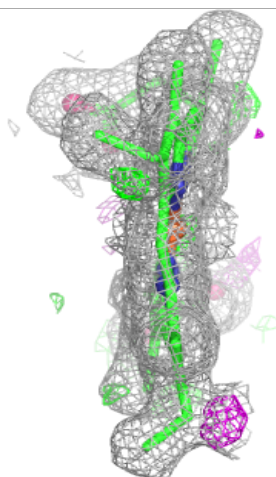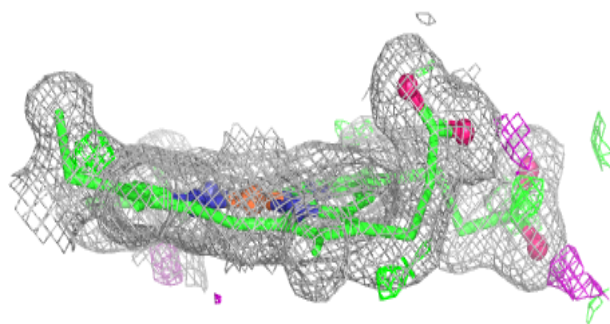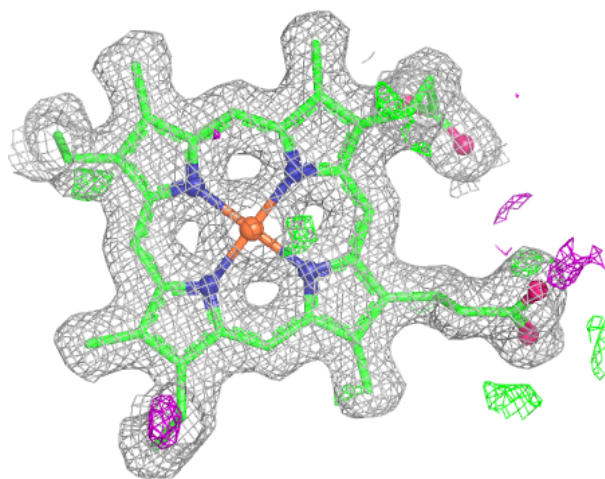
Electron density around HEC B 606:

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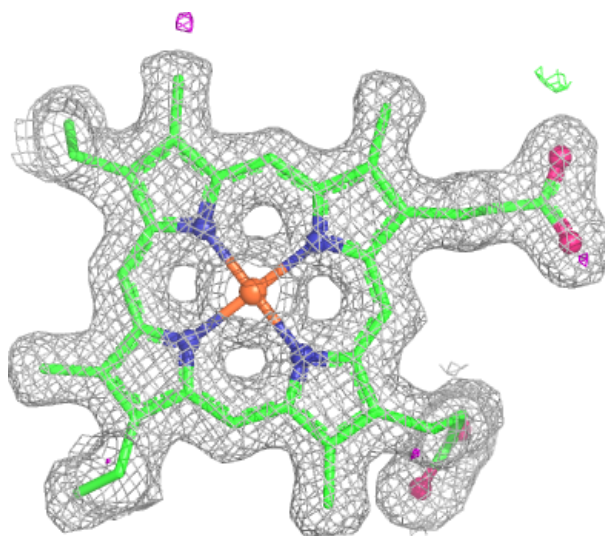and green (positive)

Electron density around HEC B 607:

$2mF_o$-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 608:

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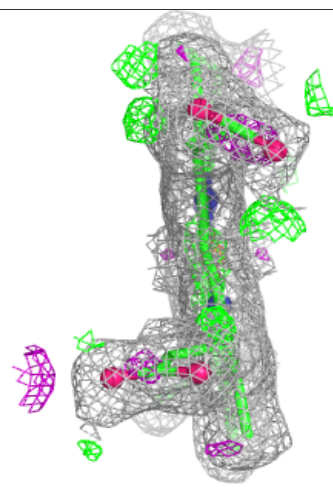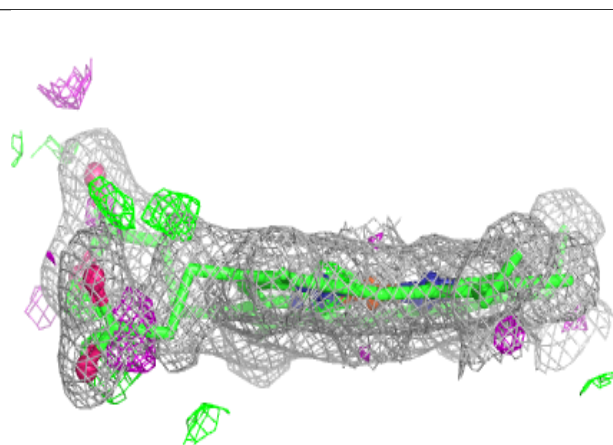and green (positive)

Electron density around HEC 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 HEC 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 HEC A 601:

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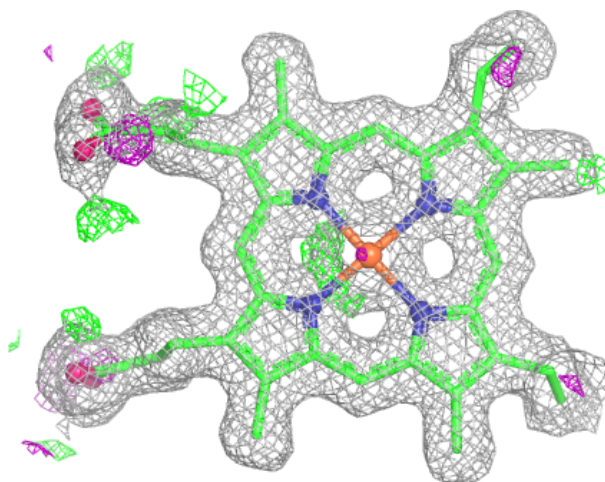and green (positive)

Electron density around HEC A 606:

$2mF_o$-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 607:

$2mF_o$-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 ⓘ

There are no such residues in this entry.