



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:05 AM EDT

PDB ID : 1Z1N / pdb_00001z1n
Title : Crystal Structure of the sixteen heme cytochrome from *Desulfovibrio gigas*
Authors : Santos-Silva, T.; Dias, J.M.; Romao, M.J.
Deposited on : 2005-03-04
Resolution : 2.10 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 : 2022.3.0, CSD as543be (2022)
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

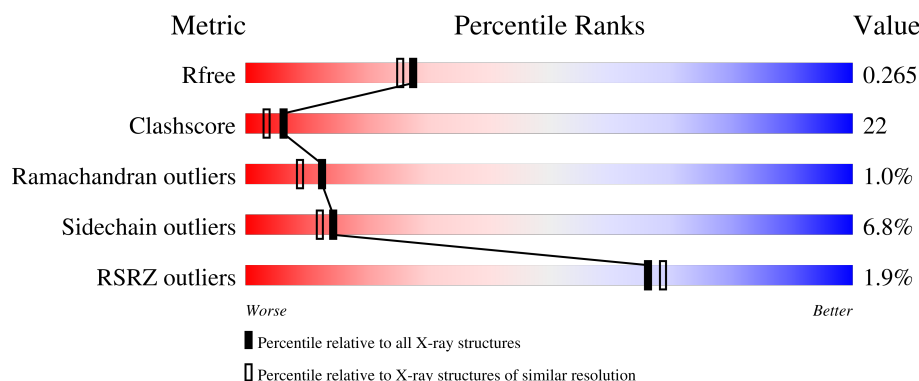
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

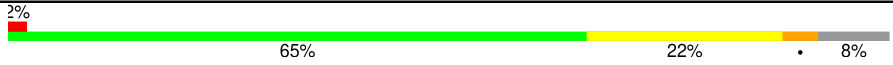
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	X	560	
2	A	2	

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	NAG	A	1	X	-	-	-
5	GOL	X	722	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4998 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 sixteen heme cytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	516	Total	C	N	O	S	0	0	0
			3837	2355	703	739	40			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-allopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.

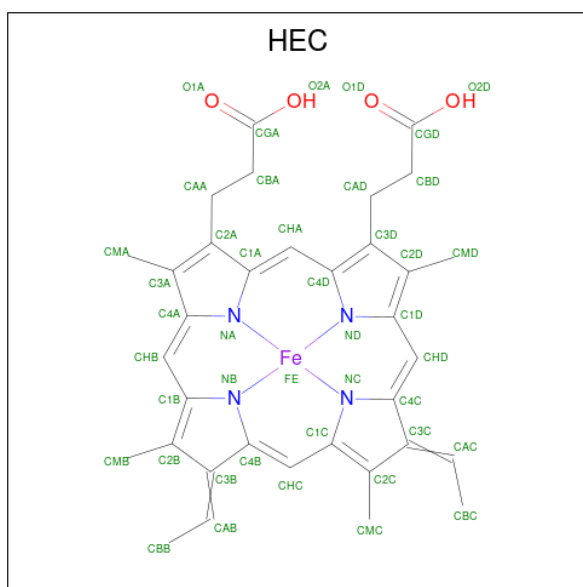


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	3	Total	Zn	0	0
			3	3		

- Molecule 4 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).

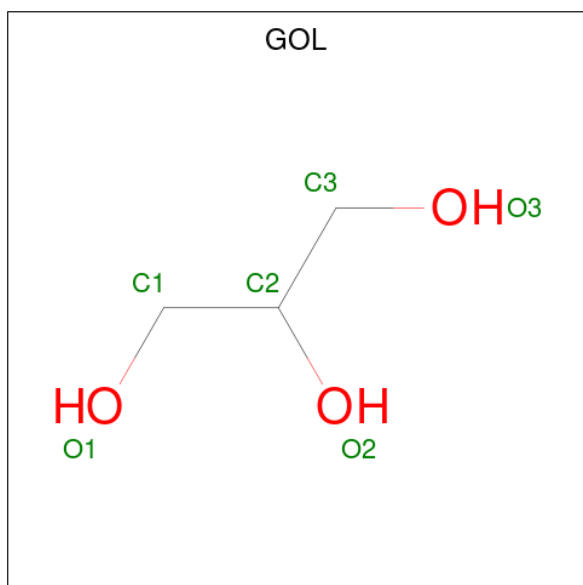
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	X	1	Total C O 6 3 3	0	0
5	X	1	Total C O 6 3 3	0	0
5	X	1	Total C O 6 3 3	0	0
5	X	1	Total C O 6 3 3	0	0
5	X	1	Total C O 6 3 3	0	0

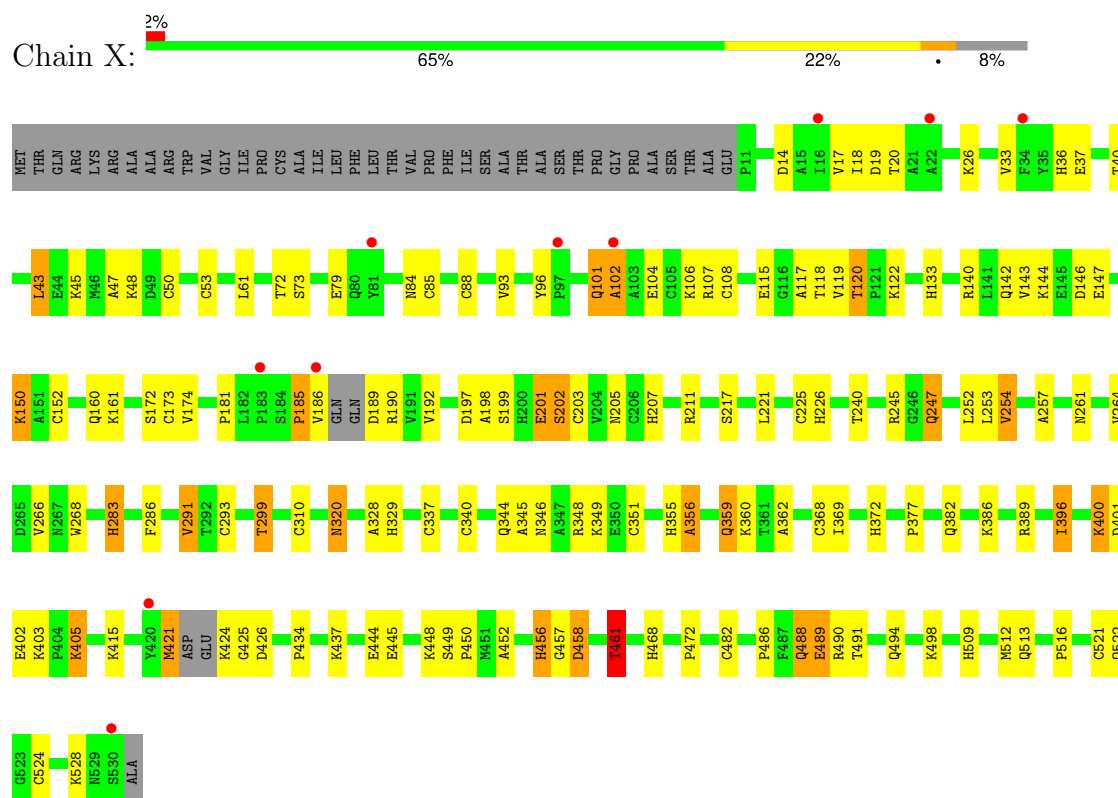
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	X	412	Total O 412 412	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: sixteen heme cytochrome



- Molecule 2: 2-acetamido-2-deoxy-beta-D-allopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.89Å 90.80Å 83.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 25.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (25.00-2.10) 98.1 (25.00-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.194 , 0.260 0.204 , 0.265	Depositor DCC
R_{free} test set	1979 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4998	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ZN, GOL, NAA, 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	X	1.25	15/3925 (0.4%)	1.28	22/5326 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	252	LEU	CA-C	-6.61	1.44	1.52
1	X	372	HIS	CA-C	-6.37	1.44	1.52
1	X	328	ALA	CA-CB	-6.19	1.44	1.53
1	X	355	HIS	CA-C	-6.08	1.44	1.52
1	X	266	VAL	CA-CB	5.98	1.61	1.54
1	X	264	VAL	CA-CB	5.82	1.62	1.54
1	X	449	SER	C-O	-5.80	1.17	1.24
1	X	452	ALA	C-O	5.66	1.30	1.24
1	X	257	ALA	CA-CB	5.49	1.60	1.53
1	X	452	ALA	CA-CB	5.38	1.61	1.53
1	X	450	PRO	CA-C	5.27	1.60	1.52
1	X	286	PHE	N-CA	5.24	1.52	1.46
1	X	396	ILE	N-CA	5.24	1.52	1.46
1	X	172	SER	N-CA	-5.20	1.39	1.46
1	X	247	GLN	N-CA	5.08	1.52	1.45

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	291	VAL	CB-CA-C	-8.98	97.70	112.26
1	X	461	THR	N-CA-C	8.42	120.08	111.07
1	X	403	LYS	CA-C-N	-7.65	112.82	120.31
1	X	403	LYS	C-N-CA	-7.65	112.82	120.31
1	X	356	ALA	CA-C-N	-7.05	112.62	120.45
1	X	356	ALA	C-N-CA	-7.05	112.62	120.45
1	X	283	HIS	N-CA-C	6.59	119.29	111.71
1	X	457	GLY	N-CA-C	-6.29	98.27	113.18
1	X	254	VAL	CB-CA-C	-6.25	100.87	110.50
1	X	101	GLN	N-CA-C	6.17	121.33	113.55
1	X	240	THR	CA-C-N	-6.01	113.78	119.85
1	X	240	THR	C-N-CA	-6.01	113.78	119.85
1	X	201	GLU	N-CA-C	-5.60	105.17	111.28
1	X	197	ASP	N-CA-C	5.55	117.14	111.14
1	X	400	LYS	CB-CA-C	-5.53	101.22	110.56
1	X	291	VAL	CG1-CB-CG2	5.44	122.77	110.80
1	X	448	LYS	CD-CE-NZ	-5.43	94.53	111.90
1	X	389	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	X	425	GLY	N-CA-C	-5.30	107.93	115.30
1	X	456	HIS	N-CA-C	5.12	116.87	111.28
1	X	96	TYR	CA-C-N	5.08	124.77	119.64
1	X	96	TYR	C-N-CA	5.08	124.77	119.64

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	424	LYS	Peptide

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	X	3837	0	3662	162	1
2	A	28	0	25	1	0
3	X	3	0	0	0	0
4	X	688	0	495	104	1
5	X	30	0	40	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	X	412	0	0	27	1
All	All	4998	0	4222	184	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 22.

All (184) 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:X:50:CYS:SG	4:X:704:HEC:HAB	1.37	1.63
1:X:152:CYS:SG	4:X:707:HEC:HAC	1.54	1.44
1:X:310:CYS:SG	4:X:712:HEC:CBC	2.04	1.44
1:X:524:CYS:SG	4:X:719:HEC:CAC	2.12	1.36
1:X:85:CYS:SG	4:X:705:HEC:CAB	2.14	1.35
1:X:88:CYS:SG	4:X:705:HEC:HAC	1.67	1.33
1:X:203:CYS:SG	4:X:709:HEC:HAB	1.69	1.33
1:X:293:CYS:SG	4:X:711:HEC:CAC	2.15	1.32
1:X:152:CYS:SG	4:X:707:HEC:CAC	2.24	1.25
1:X:50:CYS:SG	4:X:704:HEC:CAB	2.24	1.24
1:X:225:CYS:SG	4:X:710:HEC:CAC	2.27	1.23
1:X:53:CYS:SG	4:X:704:HEC:CAC	2.27	1.21
1:X:421:MET:O	6:X:801:HOH:O	1.61	1.19
1:X:521:CYS:SG	4:X:719:HEC:HAB	1.73	1.16
1:X:437:LYS:NZ	4:X:718:HEC:O1A	1.81	1.12
1:X:108:CYS:SG	4:X:706:HEC:CAC	2.37	1.11
1:X:85:CYS:SG	4:X:705:HEC:HAB	1.93	1.07
1:X:340:CYS:SG	4:X:713:HEC:HAC	1.90	1.06
1:X:401:ASP:O	6:X:803:HOH:O	1.75	1.05
1:X:482:CYS:SG	4:X:717:HEC:HAC	1.91	1.05
1:X:261:ASN:OD1	6:X:802:HOH:O	1.73	1.04
1:X:337:CYS:SG	4:X:713:HEC:HAB	2.00	1.00
1:X:108:CYS:SG	4:X:706:HEC:HAC	2.03	0.95
4:X:717:HEC:O1D	5:X:722:GOL:H32	1.65	0.95
1:X:53:CYS:SG	4:X:704:HEC:HAC	2.04	0.95
1:X:524:CYS:SG	4:X:719:HEC:CBC	2.55	0.94
1:X:120:THR:HG21	1:X:226:HIS:O	1.68	0.94
1:X:225:CYS:SG	4:X:710:HEC:HAC	2.13	0.89
1:X:186:VAL:HG22	1:X:189:ASP:HA	1.55	0.85
4:X:719:HEC:O2D	6:X:804:HOH:O	1.94	0.85
1:X:359:GLN:HE22	1:X:362:ALA:H	1.21	0.84
1:X:344:GLN:OE1	1:X:348:ARG:NH2	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:337:CYS:SG	4:X:713:HEC:CBB	2.67	0.82
1:X:84:ASN:O	6:X:805:HOH:O	1.99	0.80
1:X:253:LEU:HD21	4:X:711:HEC:HBD2	1.64	0.79
1:X:268:TRP:HE1	1:X:382:GLN:HE21	1.30	0.78
1:X:524:CYS:SG	4:X:719:HEC:C3C	2.71	0.78
1:X:293:CYS:SG	4:X:711:HEC:CBC	2.73	0.77
1:X:293:CYS:SG	4:X:711:HEC:HAC	2.23	0.77
1:X:524:CYS:SG	4:X:719:HEC:HBC3	2.26	0.76
1:X:310:CYS:SG	4:X:712:HEC:CAC	2.73	0.76
1:X:120:THR:CG2	1:X:226:HIS:O	2.34	0.76
1:X:37:GLU:OE2	6:X:806:HOH:O	2.03	0.76
1:X:115:GLU:O	1:X:118:THR:HG22	1.86	0.75
1:X:173:CYS:SG	4:X:708:HEC:CBB	2.77	0.73
1:X:340:CYS:SG	4:X:713:HEC:C3C	2.77	0.72
1:X:225:CYS:SG	4:X:710:HEC:C3C	2.77	0.71
1:X:37:GLU:CD	6:X:806:HOH:O	2.34	0.71
1:X:293:CYS:SG	4:X:711:HEC:C3C	2.79	0.70
4:X:709:HEC:CBC	4:X:709:HEC:HMC1	2.22	0.69
1:X:181:PRO:HB3	1:X:192:VAL:O	1.93	0.68
1:X:482:CYS:SG	4:X:717:HEC:C3C	2.81	0.68
1:X:482:CYS:SG	4:X:717:HEC:CBC	2.82	0.68
1:X:53:CYS:SG	4:X:704:HEC:C3C	2.82	0.68
1:X:14:ASP:CB	1:X:37:GLU:HG3	2.24	0.67
1:X:386:LYS:NZ	4:X:711:HEC:O2A	2.22	0.67
1:X:426:ASP:HB2	1:X:528:LYS:NZ	2.11	0.66
1:X:490:ARG:NH2	6:X:812:HOH:O	2.28	0.66
1:X:426:ASP:HB2	1:X:528:LYS:HZ1	1.61	0.66
1:X:405:LYS:HB2	6:X:1128:HOH:O	1.96	0.65
1:X:521:CYS:SG	4:X:719:HEC:C3B	2.84	0.65
1:X:173:CYS:SG	4:X:708:HEC:C3B	2.84	0.63
1:X:88:CYS:HG	4:X:705:HEC:HAC	1.60	0.63
1:X:85:CYS:SG	4:X:705:HEC:C3B	2.87	0.63
4:X:716:HEC:O2A	6:X:807:HOH:O	2.14	0.62
1:X:337:CYS:SG	4:X:713:HEC:C3B	2.86	0.62
4:X:715:HEC:O1D	5:X:723:GOL:O2	2.17	0.62
4:X:718:HEC:CGA	6:X:808:HOH:O	2.47	0.62
4:X:717:HEC:HBC3	4:X:717:HEC:HMC1	1.80	0.62
1:X:359:GLN:NE2	1:X:362:ALA:H	1.93	0.62
1:X:50:CYS:HG	4:X:704:HEC:CAB	2.10	0.61
1:X:524:CYS:SG	4:X:719:HEC:HAC	2.31	0.60
1:X:101:GLN:O	1:X:102:ALA:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:104:GLU:HB3	1:X:107:ARG:HG3	1.83	0.60
1:X:36:HIS:HE1	4:X:704:HEC:NB	1.99	0.59
1:X:152:CYS:SG	4:X:707:HEC:C3C	2.91	0.59
1:X:198:ALA:O	1:X:202:SER:HB2	2.03	0.58
1:X:402:GLU:CA	6:X:803:HOH:O	2.52	0.58
1:X:402:GLU:HA	6:X:803:HOH:O	2.04	0.58
1:X:201:GLU:O	1:X:205:ASN:HB2	2.03	0.58
1:X:14:ASP:HB3	1:X:37:GLU:HG3	1.85	0.58
1:X:349:LYS:HE3	1:X:513:GLN:NE2	2.18	0.58
4:X:704:HEC:C3A	4:X:710:HEC:HBB2	2.34	0.58
1:X:261:ASN:N	6:X:802:HOH:O	2.37	0.57
1:X:458:ASP:O	1:X:461:THR:HG23	2.04	0.57
1:X:152:CYS:HG	4:X:707:HEC:CAC	2.17	0.57
1:X:437:LYS:HE3	4:X:718:HEC:O1D	2.04	0.57
1:X:207:HIS:O	1:X:211:ARG:HG3	2.05	0.57
1:X:437:LYS:HZ1	4:X:718:HEC:CGA	2.04	0.56
4:X:705:HEC:HMC3	4:X:705:HEC:HBC3	1.87	0.56
1:X:421:MET:CE	4:X:719:HEC:HAA2	2.37	0.55
1:X:434:PRO:HG3	4:X:718:HEC:HBA1	1.89	0.55
1:X:359:GLN:HE22	1:X:362:ALA:N	2.00	0.55
1:X:43:LEU:HD12	4:X:704:HEC:HMC1	1.89	0.54
1:X:486:PRO:HD2	1:X:489:GLU:HG3	1.89	0.54
1:X:400:LYS:O	1:X:402:GLU:N	2.40	0.54
1:X:117:ALA:HA	1:X:120:THR:HG22	1.89	0.54
1:X:120:THR:HG23	6:X:874:HOH:O	2.08	0.53
4:X:709:HEC:HMC1	4:X:709:HEC:HBC3	1.88	0.53
1:X:73:SER:HB3	6:X:1141:HOH:O	2.08	0.53
1:X:437:LYS:CE	4:X:718:HEC:O1A	2.56	0.53
4:X:718:HEC:O1A	6:X:808:HOH:O	2.19	0.53
1:X:340:CYS:SG	4:X:713:HEC:CBC	2.93	0.53
1:X:14:ASP:CG	1:X:37:GLU:HG3	2.33	0.53
1:X:348:ARG:NH1	6:X:814:HOH:O	2.29	0.52
1:X:120:THR:CG2	6:X:874:HOH:O	2.57	0.52
1:X:498:LYS:NZ	6:X:826:HOH:O	2.43	0.52
1:X:456:HIS:O	1:X:461:THR:HG21	2.08	0.51
4:X:717:HEC:O1D	5:X:722:GOL:C2	2.55	0.51
1:X:140:ARG:HD3	6:X:1148:HOH:O	2.11	0.51
1:X:143:VAL:HG21	1:X:147:GLU:HG2	1.92	0.50
1:X:40:THR:HG22	4:X:704:HEC:HBB2	1.93	0.50
1:X:150:LYS:O	6:X:809:HOH:O	2.19	0.50
4:X:705:HEC:HMC3	4:X:705:HEC:CBC	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:509:HIS:CE1	1:X:516:PRO:HD2	2.47	0.50
1:X:88:CYS:SG	4:X:705:HEC:C3C	2.95	0.50
1:X:421:MET:HE3	4:X:719:HEC:HAA2	1.93	0.50
1:X:79:GLU:HG3	6:X:948:HOH:O	2.12	0.49
4:X:717:HEC:O2D	5:X:722:GOL:H2	2.12	0.49
1:X:143:VAL:CG1	1:X:147:GLU:HB3	2.42	0.49
1:X:101:GLN:O	1:X:102:ALA:CB	2.61	0.49
1:X:329:HIS:HE1	4:X:715:HEC:C4A	2.26	0.49
1:X:174:VAL:HG12	1:X:174:VAL:O	2.11	0.49
1:X:396:ILE:HG22	1:X:400:LYS:HE2	1.94	0.49
1:X:491:THR:H	1:X:494:GLN:HE21	1.61	0.49
4:X:709:HEC:HMC1	4:X:709:HEC:HBC2	1.92	0.49
1:X:329:HIS:HE1	4:X:715:HEC:NA	2.07	0.48
1:X:468:HIS:HD1	5:X:722:GOL:HO1	1.61	0.48
1:X:482:CYS:HG	4:X:717:HEC:HAC	1.74	0.48
1:X:456:HIS:O	1:X:461:THR:CG2	2.62	0.48
1:X:293:CYS:SG	4:X:711:HEC:HBC3	2.52	0.48
1:X:360:LYS:NZ	6:X:810:HOH:O	2.21	0.48
1:X:45:LYS:C	1:X:47:ALA:H	2.22	0.47
1:X:88:CYS:HG	4:X:705:HEC:CAC	2.16	0.47
1:X:203:CYS:SG	4:X:709:HEC:C3B	2.98	0.47
1:X:509:HIS:HE1	1:X:516:PRO:HD2	1.80	0.47
4:X:712:HEC:HBC2	4:X:712:HEC:HMC1	1.97	0.46
1:X:444:GLU:HG3	1:X:445:GLU:N	2.30	0.46
1:X:143:VAL:HG11	1:X:147:GLU:HB3	1.97	0.46
1:X:143:VAL:HG22	1:X:144:LYS:H	1.81	0.46
1:X:345:ALA:O	1:X:351:CYS:HB2	2.16	0.45
1:X:247:GLN:HB3	4:X:711:HEC:CHB	2.46	0.45
4:X:717:HEC:O1A	5:X:722:GOL:C3	2.61	0.45
1:X:133:HIS:HB3	4:X:707:HEC:HBC3	1.97	0.45
1:X:221:LEU:HD21	4:X:704:HEC:HBB3	1.97	0.45
1:X:369:ILE:HG23	6:X:1015:HOH:O	2.17	0.45
1:X:122:LYS:NZ	4:X:710:HEC:O1A	2.38	0.45
1:X:185:PRO:HA	1:X:186:VAL:HB	1.98	0.45
1:X:203:CYS:HB2	4:X:710:HEC:HBC2	1.99	0.45
1:X:133:HIS:HB3	4:X:707:HEC:CBC	2.47	0.44
1:X:346:ASN:ND2	1:X:356:ALA:HA	2.33	0.44
4:X:706:HEC:HMC3	4:X:706:HEC:HBC3	2.01	0.43
1:X:349:LYS:HE3	1:X:513:GLN:CD	2.43	0.43
1:X:203:CYS:SG	4:X:709:HEC:CBB	2.96	0.43
1:X:283:HIS:HB3	4:X:711:HEC:HBC2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:713:HEC:HBC3	4:X:713:HEC:HMC1	2.01	0.43
1:X:512:MET:O	1:X:513:GLN:HB2	2.18	0.43
4:X:713:HEC:CBC	4:X:713:HEC:HMC1	2.48	0.43
1:X:53:CYS:CB	4:X:704:HEC:C3C	2.97	0.43
1:X:85:CYS:SG	4:X:705:HEC:CBB	3.02	0.43
1:X:268:TRP:HB3	1:X:377:PRO:O	2.19	0.43
1:X:199:SER:O	1:X:203:CYS:SG	2.76	0.43
1:X:43:LEU:CD1	4:X:704:HEC:HMC1	2.48	0.42
1:X:19:ASP:O	1:X:20:THR:C	2.62	0.42
1:X:468:HIS:HD1	5:X:722:GOL:C1	2.32	0.42
1:X:488:GLN:H	1:X:488:GLN:CD	2.28	0.42
1:X:17:VAL:HG22	1:X:33:VAL:HG22	2.02	0.41
1:X:261:ASN:HD22	2:A:1:NAG:C7	2.34	0.41
1:X:491:THR:H	1:X:494:GLN:NE2	2.17	0.41
1:X:108:CYS:HG	4:X:706:HEC:CAC	2.30	0.41
1:X:50:CYS:HB2	1:X:61:LEU:HD21	2.01	0.41
1:X:140:ARG:C	1:X:142:GLN:H	2.29	0.41
4:X:716:HEC:HHB	4:X:716:HEC:HMB3	1.84	0.41
1:X:40:THR:CG2	4:X:704:HEC:HBB2	2.50	0.41
1:X:299:THR:HG23	6:X:1137:HOH:O	2.21	0.41
1:X:37:GLU:HG2	6:X:806:HOH:O	2.21	0.41
1:X:320:ASN:HD22	1:X:320:ASN:HA	1.64	0.41
4:X:711:HEC:HBC3	4:X:711:HEC:HMC1	2.01	0.41
1:X:33:VAL:O	1:X:33:VAL:HG12	2.21	0.41
1:X:337:CYS:SG	4:X:713:HEC:HBB3	2.58	0.41
1:X:368:CYS:HA	4:X:715:HEC:CHC	2.51	0.40
1:X:225:CYS:HG	4:X:710:HEC:HAC	1.83	0.40
1:X:310:CYS:SG	4:X:712:HEC:C3C	3.09	0.40
1:X:88:CYS:SG	4:X:705:HEC:CBC	3.01	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)
6:X:815:HOH:O	6:X:912:HOH:O[3_546]	2.14	0.06
1:X:437:LYS:NZ	4:X:718:HEC:O2D[2_565]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	X	510/560 (91%)	484 (95%)	21 (4%)	5 (1%)	12 9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	102	ALA
1	X	160	GLN
1	X	150	LYS
1	X	161	LYS
1	X	185	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	X	410/450 (91%)	382 (93%)	28 (7%)	14 12

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

Mol	Chain	Res	Type
1	X	18	ILE
1	X	26	LYS
1	X	43	LEU
1	X	48	LYS
1	X	72	THR
1	X	93	VAL

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Mol	Chain	Res	Type
1	X	106	LYS
1	X	119	VAL
1	X	120	THR
1	X	146	ASP
1	X	190	ARG
1	X	202	SER
1	X	217	SER
1	X	245	ARG
1	X	254	VAL
1	X	291	VAL
1	X	299	THR
1	X	320	ASN
1	X	359	GLN
1	X	405	LYS
1	X	415	LYS
1	X	421	MET
1	X	458	ASP
1	X	461	THR
1	X	472	PRO
1	X	488	GLN
1	X	489	GLU
1	X	522	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	80	GLN
1	X	231	GLN
1	X	320	ASN
1	X	330	GLN
1	X	346	ASN
1	X	359	GLN
1	X	366	ASN
1	X	382	GLN
1	X	494	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	A	1	1,2	14,14,15	0.79	1 (7%)	17,19,21	2.82	6 (35%)
2	NAA	A	2	2	14,14,15	0.88	1 (7%)	17,19,21	1.15	1 (5%)

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	NAG	A	1	1,2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAA	A	2	2	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	NAA	C8-C7	2.72	1.56	1.50
2	A	1	NAG	C3-C2	2.33	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	O3-C3-C2	6.75	123.43	109.40
2	A	1	NAG	C1-O5-C5	5.58	119.66	112.19
2	A	1	NAG	C3-C4-C5	-4.61	101.87	110.23
2	A	1	NAG	O4-C4-C5	2.95	116.59	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NAG	C1-C2-N2	-2.89	105.88	110.43
2	A	2	NAA	C3-C4-C5	2.74	115.21	110.23
2	A	1	NAG	O4-C4-C3	2.27	115.74	110.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1	NAG	C1

All (6) torsion outliers are listed below:

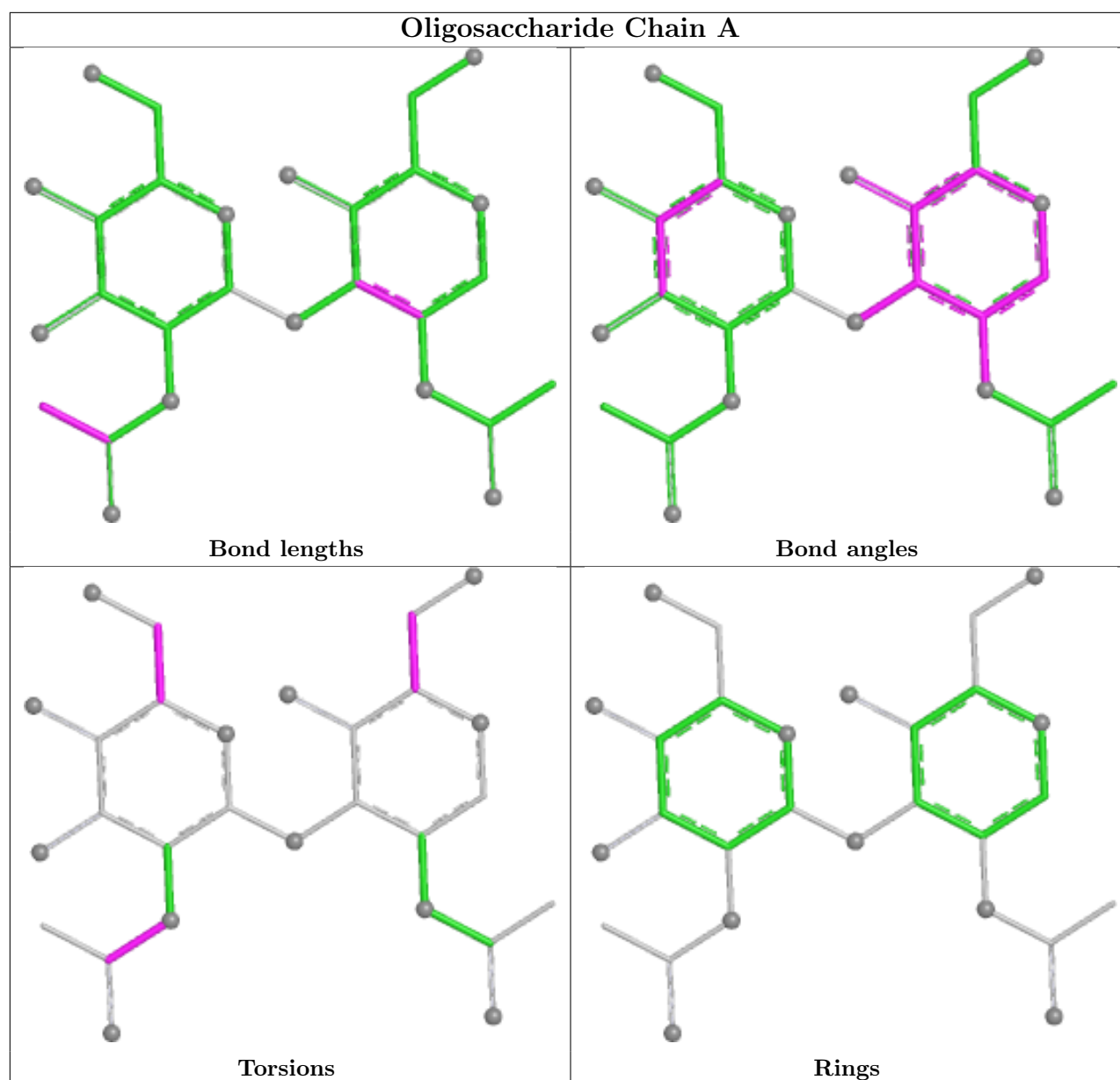
Mol	Chain	Res	Type	Atoms
2	A	1	NAG	O5-C5-C6-O6
2	A	1	NAG	C4-C5-C6-O6
2	A	2	NAA	C8-C7-N2-C2
2	A	2	NAA	O7-C7-N2-C2
2	A	2	NAA	O5-C5-C6-O6
2	A	2	NAA	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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
4	HEC	X	719	1,3	46,50,50	2.08	10 (21%)	58,82,82	2.00	14 (24%)
4	HEC	X	706	1	46,50,50	1.93	6 (13%)	58,82,82	1.95	6 (10%)
4	HEC	X	704	1	46,50,50	1.90	6 (13%)	58,82,82	2.22	15 (25%)
4	HEC	X	713	1	46,50,50	2.21	9 (19%)	58,82,82	2.30	24 (41%)
4	HEC	X	716	1	46,50,50	2.05	9 (19%)	58,82,82	2.27	15 (25%)
4	HEC	X	718	1	46,50,50	2.39	14 (30%)	58,82,82	2.56	18 (31%)
5	GOL	X	720	-	5,5,5	0.49	0	5,5,5	0.26	0
5	GOL	X	722	4	5,5,5	0.63	0	5,5,5	0.50	0
4	HEC	X	712	1	46,50,50	1.98	5 (10%)	58,82,82	1.83	11 (18%)
4	HEC	X	715	1	46,50,50	2.11	11 (23%)	58,82,82	2.64	23 (39%)
4	HEC	X	709	1	46,50,50	2.06	7 (15%)	58,82,82	1.77	7 (12%)
4	HEC	X	707	1	46,50,50	2.03	9 (19%)	58,82,82	1.88	11 (18%)
4	HEC	X	710	1	46,50,50	1.88	6 (13%)	58,82,82	1.88	11 (18%)
5	GOL	X	723	-	5,5,5	0.45	0	5,5,5	0.52	0
5	GOL	X	721	-	5,5,5	0.36	0	5,5,5	0.34	0
4	HEC	X	708	1	46,50,50	1.89	7 (15%)	58,82,82	1.87	13 (22%)
4	HEC	X	717	1,5	46,50,50	2.57	17 (36%)	58,82,82	2.30	21 (36%)
4	HEC	X	714	1	46,50,50	2.13	10 (21%)	58,82,82	2.67	21 (36%)
4	HEC	X	705	1	46,50,50	2.10	12 (26%)	58,82,82	1.88	9 (15%)
4	HEC	X	711	1	46,50,50	2.21	7 (15%)	58,82,82	2.49	17 (29%)
5	GOL	X	724	-	5,5,5	0.55	0	5,5,5	2.14	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEC	X	719	1,3	-	6/14/54/54	-
4	HEC	X	706	1	-	6/14/54/54	-
4	HEC	X	704	1	-	5/14/54/54	-
4	HEC	X	713	1	-	8/14/54/54	-
4	HEC	X	716	1	-	6/14/54/54	-
4	HEC	X	718	1	-	7/14/54/54	-
5	GOL	X	720	-	-	2/4/4/4	-
5	GOL	X	722	4	-	4/4/4/4	-
4	HEC	X	712	1	-	9/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEC	X	715	1	-	8/14/54/54	-
4	HEC	X	709	1	-	4/14/54/54	-
4	HEC	X	707	1	-	4/14/54/54	-
4	HEC	X	710	1	-	6/14/54/54	-
5	GOL	X	723	-	-	2/4/4/4	-
5	GOL	X	721	-	-	3/4/4/4	-
4	HEC	X	708	1	-	8/14/54/54	-
4	HEC	X	717	1,5	-	8/14/54/54	-
4	HEC	X	714	1	-	6/14/54/54	-
4	HEC	X	705	1	-	5/14/54/54	-
4	HEC	X	711	1	-	6/14/54/54	-
5	GOL	X	724	-	-	2/4/4/4	-

All (145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	718	HEC	CAB-C3B	7.94	1.60	1.35
4	X	714	HEC	CAC-C3C	7.77	1.60	1.35
4	X	718	HEC	CAC-C3C	7.59	1.59	1.35
4	X	715	HEC	CAC-C3C	7.43	1.59	1.35
4	X	704	HEC	CAC-C3C	7.35	1.58	1.35
4	X	707	HEC	CAC-C3C	7.35	1.58	1.35
4	X	716	HEC	CAB-C3B	7.34	1.58	1.35
4	X	713	HEC	CAC-C3C	7.33	1.58	1.35
4	X	714	HEC	CAB-C3B	7.22	1.58	1.35
4	X	711	HEC	CAC-C3C	7.19	1.58	1.35
4	X	712	HEC	CAC-C3C	7.05	1.57	1.35
4	X	709	HEC	CAC-C3C	7.00	1.57	1.35
4	X	706	HEC	CAC-C3C	6.81	1.57	1.35
4	X	711	HEC	CAB-C3B	6.71	1.56	1.35
4	X	705	HEC	CAB-C3B	6.67	1.56	1.35
4	X	710	HEC	CAC-C3C	6.63	1.56	1.35
4	X	713	HEC	CAB-C3B	6.53	1.56	1.35
4	X	708	HEC	CAC-C3C	6.47	1.56	1.35
4	X	709	HEC	CAB-C3B	6.39	1.55	1.35
4	X	707	HEC	CAB-C3B	6.31	1.55	1.35
4	X	706	HEC	CAB-C3B	6.23	1.55	1.35
4	X	708	HEC	CAB-C3B	6.21	1.55	1.35
4	X	719	HEC	CAB-C3B	6.21	1.55	1.35
4	X	715	HEC	CAB-C3B	6.20	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	712	HEC	CAB-C3B	6.19	1.55	1.35
4	X	709	HEC	C3D-C2D	6.09	1.54	1.38
4	X	719	HEC	C3D-C2D	6.02	1.54	1.38
4	X	717	HEC	CAC-C3C	5.98	1.54	1.35
4	X	710	HEC	CAB-C3B	5.86	1.54	1.35
4	X	706	HEC	C3D-C2D	5.83	1.54	1.38
4	X	712	HEC	C3D-C2D	5.81	1.54	1.38
4	X	704	HEC	CAB-C3B	5.79	1.53	1.35
4	X	705	HEC	CAC-C3C	5.78	1.53	1.35
4	X	717	HEC	CAB-C3B	5.78	1.53	1.35
4	X	716	HEC	CAC-C3C	5.74	1.53	1.35
4	X	717	HEC	CBD-CAD	5.66	1.71	1.51
4	X	705	HEC	C3D-C2D	5.62	1.53	1.38
4	X	719	HEC	CAC-C3C	5.55	1.53	1.35
4	X	708	HEC	C3D-C2D	5.53	1.53	1.38
4	X	717	HEC	C3D-C2D	5.46	1.53	1.38
4	X	717	HEC	O1D-CGD	5.33	1.39	1.22
4	X	710	HEC	C3D-C2D	5.26	1.52	1.38
4	X	711	HEC	C3D-C2D	5.20	1.52	1.38
4	X	704	HEC	C3D-C2D	5.14	1.52	1.38
4	X	707	HEC	C3D-C2D	4.99	1.51	1.38
4	X	715	HEC	C3D-C2D	4.86	1.51	1.38
4	X	717	HEC	CBD-CGD	4.60	1.61	1.50
4	X	717	HEC	CAD-C3D	4.44	1.62	1.51
4	X	718	HEC	C3D-C2D	4.38	1.50	1.38
4	X	716	HEC	CMC-C2C	4.35	1.59	1.50
4	X	714	HEC	C3D-C2D	4.35	1.50	1.38
4	X	711	HEC	CMA-C3A	4.10	1.59	1.50
4	X	713	HEC	C4D-ND	-4.02	1.32	1.39
4	X	713	HEC	C1B-NB	-3.99	1.32	1.39
4	X	718	HEC	O1A-CGA	3.95	1.35	1.22
4	X	711	HEC	C4C-NC	-3.70	1.32	1.39
4	X	718	HEC	CMB-C2B	3.47	1.57	1.50
4	X	713	HEC	C3D-C2D	3.47	1.47	1.38
4	X	711	HEC	O2D-CGD	-3.44	1.19	1.30
4	X	716	HEC	CMA-C3A	3.38	1.57	1.50
4	X	717	HEC	CMD-C2D	3.14	1.57	1.50
4	X	718	HEC	C1A-C2A	3.12	1.50	1.45
4	X	718	HEC	C1B-C2B	3.07	1.50	1.43
4	X	718	HEC	C4A-C3A	3.01	1.51	1.45
4	X	717	HEC	CBB-CAB	3.00	1.60	1.49
4	X	714	HEC	C3B-C4B	2.95	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	718	HEC	CBB-CAB	2.92	1.60	1.49
4	X	717	HEC	CMB-C2B	2.90	1.56	1.50
4	X	715	HEC	C4A-NA	-2.88	1.34	1.39
4	X	719	HEC	CMD-C2D	2.87	1.56	1.50
4	X	719	HEC	CMB-C2B	2.86	1.56	1.50
4	X	718	HEC	C3B-C4B	2.85	1.51	1.46
4	X	713	HEC	CMC-C2C	2.81	1.56	1.50
4	X	717	HEC	C1B-NB	-2.80	1.34	1.39
4	X	716	HEC	C3D-C2D	2.77	1.46	1.38
4	X	705	HEC	C4B-NB	-2.74	1.34	1.39
4	X	715	HEC	C1B-C2B	2.73	1.49	1.43
4	X	706	HEC	CMB-C2B	2.71	1.56	1.50
4	X	707	HEC	O2A-CGA	-2.69	1.21	1.30
4	X	716	HEC	CAD-C3D	2.69	1.58	1.51
4	X	719	HEC	C1A-C2A	2.69	1.49	1.45
4	X	709	HEC	CMD-C2D	2.66	1.56	1.50
4	X	714	HEC	CHD-C1D	-2.64	1.33	1.39
4	X	709	HEC	CMC-C2C	2.59	1.56	1.50
4	X	705	HEC	CMD-C2D	2.54	1.56	1.50
4	X	708	HEC	CAA-C2A	2.54	1.57	1.51
4	X	717	HEC	C4B-NB	-2.52	1.34	1.39
4	X	717	HEC	CMA-C3A	2.50	1.55	1.50
4	X	715	HEC	CMB-C2B	2.49	1.55	1.50
4	X	707	HEC	CMD-C2D	2.49	1.55	1.50
4	X	717	HEC	C1D-ND	-2.47	1.35	1.39
4	X	719	HEC	C4C-NC	-2.46	1.35	1.39
4	X	715	HEC	C1C-C2C	2.45	1.48	1.43
4	X	719	HEC	CBD-CAD	2.43	1.60	1.51
4	X	707	HEC	CMC-C2C	2.41	1.55	1.50
4	X	714	HEC	CBB-CAB	2.41	1.58	1.49
4	X	714	HEC	C1C-NC	-2.39	1.35	1.39
4	X	705	HEC	C4C-NC	-2.39	1.35	1.39
4	X	712	HEC	CBB-CAB	2.38	1.58	1.49
4	X	714	HEC	C1D-C2D	2.36	1.48	1.43
4	X	705	HEC	CHB-C1B	-2.36	1.34	1.39
4	X	715	HEC	O1D-CGD	2.36	1.29	1.22
4	X	708	HEC	CBA-CGA	2.36	1.56	1.50
4	X	706	HEC	CMD-C2D	2.35	1.55	1.50
4	X	709	HEC	C2A-C3A	-2.35	1.31	1.36
4	X	704	HEC	CMA-C3A	2.33	1.55	1.50
4	X	705	HEC	CHC-C1C	-2.33	1.34	1.39
4	X	717	HEC	CAA-C2A	2.33	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	715	HEC	CMC-C2C	2.33	1.55	1.50
4	X	718	HEC	C1C-C2C	2.30	1.48	1.43
4	X	712	HEC	CMD-C2D	2.29	1.55	1.50
4	X	710	HEC	C3B-C2B	-2.26	1.33	1.41
4	X	719	HEC	C4A-C3A	2.25	1.49	1.45
4	X	718	HEC	C1D-C2D	2.24	1.48	1.43
4	X	715	HEC	CMA-C3A	2.23	1.55	1.50
4	X	704	HEC	CMD-C2D	2.23	1.55	1.50
4	X	714	HEC	C1A-C2A	2.23	1.49	1.45
4	X	719	HEC	C1C-NC	-2.23	1.35	1.39
4	X	713	HEC	C4B-NB	-2.23	1.35	1.39
4	X	716	HEC	O2D-CGD	-2.20	1.23	1.30
4	X	708	HEC	CMA-C3A	2.20	1.55	1.50
4	X	707	HEC	CMA-C3A	2.19	1.55	1.50
4	X	705	HEC	C3B-C2B	-2.18	1.33	1.41
4	X	715	HEC	CBB-CAB	2.15	1.57	1.49
4	X	705	HEC	CBB-CAB	2.15	1.57	1.49
4	X	717	HEC	C1D-C2D	2.14	1.48	1.43
4	X	710	HEC	CMA-C3A	2.12	1.55	1.50
4	X	705	HEC	C1C-NC	-2.11	1.35	1.39
4	X	707	HEC	CBB-CAB	2.11	1.57	1.49
4	X	711	HEC	C3B-C2B	-2.09	1.34	1.41
4	X	716	HEC	CMD-C2D	2.09	1.55	1.50
4	X	707	HEC	C4B-NB	-2.07	1.35	1.39
4	X	706	HEC	CMC-C2C	2.07	1.55	1.50
4	X	717	HEC	C3C-C2C	-2.06	1.34	1.41
4	X	718	HEC	CAD-C3D	2.05	1.56	1.51
4	X	710	HEC	O1D-CGD	2.04	1.28	1.22
4	X	705	HEC	CAA-C2A	2.04	1.56	1.51
4	X	716	HEC	C1C-NC	2.03	1.43	1.39
4	X	713	HEC	C1D-ND	-2.03	1.35	1.39
4	X	713	HEC	CAD-C3D	2.03	1.56	1.51
4	X	708	HEC	O1A-CGA	2.03	1.28	1.22
4	X	704	HEC	O1D-CGD	2.02	1.28	1.22
4	X	709	HEC	CBB-CAB	2.02	1.57	1.49
4	X	714	HEC	C4B-NB	-2.01	1.35	1.39
4	X	718	HEC	CBC-CAC	2.00	1.56	1.49

All (238) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	704	HEC	CBB-CAB-C3B	-10.22	107.00	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	714	HEC	CBC-CAC-C3C	-9.19	109.07	127.43
4	X	711	HEC	CBC-CAC-C3C	-9.07	109.30	127.43
4	X	715	HEC	CBB-CAB-C3B	-9.01	109.42	127.43
4	X	718	HEC	CBB-CAB-C3B	-8.98	109.49	127.43
4	X	706	HEC	CBB-CAB-C3B	-8.88	109.69	127.43
4	X	716	HEC	CBB-CAB-C3B	-8.80	109.84	127.43
4	X	710	HEC	CBB-CAB-C3B	-8.75	109.95	127.43
4	X	718	HEC	CBC-CAC-C3C	-8.56	110.33	127.43
4	X	707	HEC	CBB-CAB-C3B	-8.11	111.22	127.43
4	X	705	HEC	CBB-CAB-C3B	-7.69	112.06	127.43
4	X	714	HEC	CMC-C2C-C1C	-7.40	114.15	125.42
4	X	714	HEC	CBB-CAB-C3B	-7.28	112.89	127.43
4	X	717	HEC	CAD-CBD-CGD	7.15	132.64	113.67
4	X	711	HEC	CMC-C2C-C1C	-7.12	114.58	125.42
4	X	716	HEC	CBC-CAC-C3C	-6.90	113.64	127.43
4	X	708	HEC	CBB-CAB-C3B	-6.82	113.80	127.43
4	X	709	HEC	CBC-CAC-C3C	-6.64	114.16	127.43
4	X	719	HEC	CMC-C2C-C1C	-6.49	115.54	125.42
4	X	704	HEC	CBC-CAC-C3C	-6.47	114.49	127.43
4	X	713	HEC	CHB-C4A-NA	6.47	131.50	124.45
4	X	709	HEC	CBB-CAB-C3B	-6.20	115.05	127.43
4	X	712	HEC	CBB-CAB-C3B	-6.16	115.12	127.43
4	X	717	HEC	CBB-CAB-C3B	-6.11	115.22	127.43
4	X	715	HEC	CAD-CBD-CGD	-6.11	97.45	113.67
4	X	711	HEC	CBB-CAB-C3B	-6.02	115.40	127.43
4	X	714	HEC	C2A-C1A-NA	-5.62	104.90	110.32
4	X	718	HEC	CMC-C2C-C1C	-5.58	116.92	125.42
4	X	705	HEC	CBC-CAC-C3C	-5.30	116.83	127.43
4	X	707	HEC	CBC-CAC-C3C	-5.27	116.90	127.43
4	X	712	HEC	CBC-CAC-C3C	-5.25	116.94	127.43
4	X	706	HEC	CBC-CAC-C3C	-5.21	117.03	127.43
4	X	711	HEC	CAD-CBD-CGD	-5.19	99.91	113.67
4	X	716	HEC	CMB-C2B-C1B	-5.18	117.53	125.42
4	X	719	HEC	CBB-CAB-C3B	-5.13	117.17	127.43
4	X	715	HEC	CMD-C2D-C1D	5.06	133.13	125.42
4	X	719	HEC	CBD-CAD-C3D	-4.90	98.98	112.53
4	X	716	HEC	CHB-C4A-NA	-4.87	119.15	124.45
4	X	705	HEC	CHA-C1A-NA	4.83	129.71	124.45
4	X	714	HEC	C4A-NA-C1A	4.78	113.61	105.82
4	X	712	HEC	CMC-C2C-C1C	-4.67	118.30	125.42
4	X	713	HEC	CMD-C2D-C3D	4.66	135.50	125.62
4	X	704	HEC	CMC-C2C-C1C	-4.60	118.41	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	708	HEC	CBC-CAC-C3C	-4.57	118.30	127.43
4	X	711	HEC	C2A-C1A-NA	-4.54	105.94	110.32
4	X	717	HEC	CBC-CAC-C3C	-4.46	118.51	127.43
4	X	718	HEC	CBD-CAD-C3D	-4.45	100.22	112.53
4	X	718	HEC	C4D-ND-C1D	4.45	113.08	105.82
4	X	715	HEC	C4D-ND-C1D	4.44	113.05	105.82
4	X	715	HEC	C4A-NA-C1A	4.41	113.01	105.82
4	X	715	HEC	CMC-C2C-C1C	-4.40	118.72	125.42
4	X	708	HEC	C4D-ND-C1D	4.40	112.99	105.82
4	X	713	HEC	CHC-C4B-NB	4.39	129.24	124.45
4	X	717	HEC	O1D-CGD-CBD	4.36	136.93	123.09
4	X	717	HEC	CHA-C1A-NA	4.25	129.08	124.45
4	X	712	HEC	C4D-ND-C1D	4.20	112.66	105.82
4	X	713	HEC	CMB-C2B-C1B	-4.17	119.06	125.42
4	X	717	HEC	C4D-C3D-C2D	-4.09	100.54	106.87
4	X	715	HEC	CAA-CBA-CGA	-4.05	102.94	113.67
4	X	713	HEC	CHB-C4A-C3A	-4.02	117.14	125.49
4	X	719	HEC	CAD-CBD-CGD	4.01	124.31	113.67
4	X	715	HEC	C2A-C1A-NA	-3.98	106.48	110.32
4	X	706	HEC	C4D-ND-C1D	3.96	112.27	105.82
4	X	713	HEC	CBB-CAB-C3B	-3.94	119.55	127.43
4	X	707	HEC	CBA-CAA-C2A	-3.94	101.63	112.53
4	X	710	HEC	CBC-CAC-C3C	-3.89	119.66	127.43
4	X	710	HEC	CHA-C1A-NA	3.88	128.68	124.45
4	X	713	HEC	CAD-CBD-CGD	-3.87	103.40	113.67
4	X	715	HEC	CBC-CAC-C3C	-3.86	119.73	127.43
4	X	706	HEC	CBD-CAD-C3D	-3.83	101.94	112.53
4	X	710	HEC	C4D-ND-C1D	3.77	111.97	105.82
4	X	716	HEC	CBD-CAD-C3D	-3.75	102.17	112.53
4	X	718	HEC	CMB-C2B-C1B	-3.73	119.74	125.42
4	X	713	HEC	C4B-NB-C1B	3.73	111.90	105.82
4	X	715	HEC	CHB-C4A-NA	3.72	128.51	124.45
4	X	711	HEC	C4D-ND-C1D	3.64	111.76	105.82
4	X	709	HEC	C4D-ND-C1D	3.64	111.75	105.82
5	X	724	GOL	C3-C2-C1	-3.59	98.64	111.80
4	X	718	HEC	CMC-C2C-C3C	3.55	134.90	126.55
4	X	714	HEC	C2C-C1C-NC	-3.51	104.51	110.14
4	X	719	HEC	CHB-C4A-NA	3.47	128.23	124.45
4	X	717	HEC	CHD-C4C-NC	3.46	128.22	124.45
4	X	708	HEC	CBA-CAA-C2A	3.46	122.09	112.53
4	X	717	HEC	CHC-C4B-NB	3.43	128.19	124.45
4	X	705	HEC	C4D-ND-C1D	3.42	111.40	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	718	HEC	CAD-CBD-CGD	-3.41	104.63	113.67
4	X	717	HEC	C4D-ND-C1D	3.40	111.37	105.82
4	X	713	HEC	CMD-C2D-C1D	-3.40	120.24	125.42
4	X	711	HEC	C4C-NC-C1C	3.37	111.32	105.82
4	X	714	HEC	C4C-NC-C1C	3.33	111.24	105.82
4	X	707	HEC	CMD-C2D-C1D	3.27	130.40	125.42
4	X	719	HEC	O1D-CGD-CBD	-3.27	112.72	123.09
4	X	714	HEC	CBA-CAA-C2A	-3.26	103.52	112.53
4	X	715	HEC	CBD-CAD-C3D	-3.23	103.60	112.53
4	X	706	HEC	C2A-C1A-NA	-3.23	107.21	110.32
4	X	716	HEC	CHB-C1B-NB	3.23	129.71	123.86
4	X	713	HEC	CHD-C4C-NC	-3.21	120.95	124.45
4	X	704	HEC	CAA-CBA-CGA	-3.20	105.17	113.67
4	X	708	HEC	C4B-NB-C1B	3.19	111.03	105.82
4	X	715	HEC	CMC-C2C-C3C	3.18	134.03	126.55
4	X	714	HEC	CHC-C1C-NC	3.16	129.60	123.86
4	X	707	HEC	C2A-C1A-NA	-3.16	107.27	110.32
4	X	717	HEC	CHB-C4A-NA	3.15	127.89	124.45
4	X	716	HEC	CMB-C2B-C3B	3.15	133.95	126.55
4	X	719	HEC	CBC-CAC-C3C	-3.14	121.17	127.43
4	X	715	HEC	CMA-C3A-C4A	-3.13	119.22	124.73
4	X	713	HEC	CHA-C1A-NA	3.09	127.81	124.45
4	X	715	HEC	CAA-C2A-C3A	3.08	133.63	127.87
4	X	712	HEC	C4B-NB-C1B	3.07	110.82	105.82
4	X	713	HEC	CAA-C2A-C1A	3.06	131.08	124.85
4	X	709	HEC	CAA-CBA-CGA	-3.03	105.63	113.67
4	X	706	HEC	CBA-CAA-C2A	-3.03	104.15	112.53
4	X	714	HEC	C4D-ND-C1D	3.02	110.75	105.82
4	X	704	HEC	C2A-C1A-NA	-2.99	107.44	110.32
4	X	711	HEC	CHD-C4C-NC	2.92	127.63	124.45
5	X	724	GOL	O1-C1-C2	-2.90	97.33	110.38
4	X	711	HEC	CMC-C2C-C3C	2.90	133.36	126.55
4	X	716	HEC	O2A-CGA-CBA	2.89	123.13	114.00
4	X	705	HEC	CHA-C1A-C2A	-2.88	120.32	124.86
4	X	718	HEC	C4A-NA-C1A	2.85	110.47	105.82
4	X	711	HEC	CAD-C3D-C4D	2.85	130.50	124.94
4	X	718	HEC	O2A-CGA-O1A	2.84	130.64	123.33
4	X	715	HEC	C3A-C4A-NA	-2.82	104.43	109.64
4	X	704	HEC	CAD-C3D-C4D	2.81	130.44	124.94
4	X	713	HEC	CHD-C1D-ND	2.81	128.95	123.86
4	X	711	HEC	CBD-CAD-C3D	2.80	120.28	112.53
4	X	704	HEC	CBD-CAD-C3D	-2.79	104.81	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	708	HEC	O1D-CGD-CBD	-2.78	114.27	123.09
4	X	719	HEC	CMD-C2D-C1D	2.78	129.65	125.42
4	X	711	HEC	C4A-NA-C1A	2.78	110.35	105.82
4	X	713	HEC	C4D-ND-C1D	2.77	110.34	105.82
4	X	714	HEC	CMD-C2D-C1D	2.77	129.63	125.42
4	X	714	HEC	CHC-C4B-C3B	2.77	129.88	125.21
4	X	719	HEC	O2D-CGD-CBD	2.76	122.71	114.00
4	X	711	HEC	CAA-CBA-CGA	-2.74	106.39	113.67
4	X	707	HEC	CMC-C2C-C1C	-2.74	121.25	125.42
4	X	710	HEC	CAD-CBD-CGD	-2.74	106.40	113.67
4	X	713	HEC	CAA-CBA-CGA	-2.74	106.40	113.67
4	X	718	HEC	O2D-CGD-CBD	2.72	122.59	114.00
4	X	717	HEC	CAD-C3D-C2D	2.71	133.14	127.07
4	X	707	HEC	CAA-CBA-CGA	-2.71	106.49	113.67
4	X	705	HEC	CAD-C3D-C4D	2.68	130.18	124.94
4	X	717	HEC	O2D-CGD-CBD	-2.68	105.53	114.00
4	X	713	HEC	CAA-C2A-C3A	-2.66	122.88	127.87
4	X	715	HEC	C4C-NC-C1C	2.66	110.15	105.82
4	X	715	HEC	CHA-C4D-ND	2.65	128.67	123.86
4	X	710	HEC	CBD-CAD-C3D	-2.65	105.20	112.53
4	X	719	HEC	CMC-C2C-C3C	2.65	132.78	126.55
4	X	711	HEC	CMD-C2D-C1D	2.64	129.44	125.42
4	X	709	HEC	CHC-C4B-NB	2.62	127.31	124.45
4	X	708	HEC	CMB-C2B-C1B	-2.62	121.43	125.42
4	X	715	HEC	CAA-C2A-C1A	-2.62	119.53	124.85
4	X	705	HEC	CMB-C2B-C3B	2.61	132.69	126.55
4	X	718	HEC	C2A-C1A-NA	-2.59	107.82	110.32
4	X	717	HEC	C4B-NB-C1B	2.58	110.03	105.82
4	X	714	HEC	O2A-CGA-CBA	2.56	122.08	114.00
4	X	705	HEC	CMD-C2D-C1D	2.54	129.29	125.42
4	X	713	HEC	CMB-C2B-C3B	2.53	132.50	126.55
4	X	715	HEC	C1D-CHD-C4C	2.52	132.43	124.66
4	X	719	HEC	C4A-NA-C1A	2.51	109.91	105.82
4	X	712	HEC	CMD-C2D-C3D	2.50	130.92	125.62
4	X	704	HEC	CMD-C2D-C1D	2.50	129.22	125.42
4	X	708	HEC	C2B-C1B-NB	-2.49	106.15	110.14
4	X	708	HEC	CMC-C2C-C1C	-2.47	121.65	125.42
4	X	718	HEC	CAA-CBA-CGA	-2.47	107.12	113.67
4	X	712	HEC	C2B-C1B-NB	-2.46	106.20	110.14
4	X	714	HEC	C4B-NB-C1B	2.44	109.81	105.82
4	X	713	HEC	CHA-C1A-C2A	-2.44	121.00	124.86
4	X	704	HEC	C4D-ND-C1D	2.43	109.78	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	718	HEC	CBA-CAA-C2A	-2.42	105.85	112.53
4	X	716	HEC	CHB-C1B-C2B	-2.42	120.41	127.43
4	X	708	HEC	C3D-C4D-ND	-2.41	107.48	110.15
4	X	715	HEC	C4B-NB-C1B	2.40	109.74	105.82
4	X	719	HEC	C4C-NC-C1C	2.40	109.73	105.82
4	X	709	HEC	CHA-C4D-ND	2.40	128.21	123.86
4	X	710	HEC	C4B-NB-C1B	2.38	109.70	105.82
4	X	704	HEC	C2B-C1B-NB	-2.37	106.34	110.14
4	X	714	HEC	CHA-C1A-C2A	2.37	128.60	124.86
4	X	716	HEC	O2D-CGD-CBD	2.37	121.48	114.00
4	X	704	HEC	O2A-CGA-CBA	2.35	121.43	114.00
4	X	707	HEC	C4B-NB-C1B	2.33	109.62	105.82
4	X	716	HEC	CMD-C2D-C3D	2.33	130.56	125.62
4	X	707	HEC	C4D-ND-C1D	2.32	109.61	105.82
4	X	714	HEC	O1A-CGA-CBA	-2.32	115.75	123.09
4	X	718	HEC	CMB-C2B-C3B	2.31	131.98	126.55
4	X	710	HEC	CHD-C4C-NC	2.30	126.95	124.45
4	X	712	HEC	CAD-CBD-CGD	-2.29	107.58	113.67
4	X	716	HEC	C1D-C2D-C3D	-2.29	104.20	106.82
4	X	716	HEC	C4D-CHA-C1A	2.29	131.72	124.66
4	X	717	HEC	CMB-C2B-C1B	-2.28	121.95	125.42
4	X	714	HEC	CAA-CBA-CGA	-2.27	107.63	113.67
4	X	715	HEC	C1B-CHB-C4A	2.27	131.68	124.66
4	X	718	HEC	C4B-NB-C1B	2.27	109.53	105.82
4	X	707	HEC	C1D-C2D-C3D	-2.27	104.22	106.82
4	X	713	HEC	C1D-C2D-C3D	-2.26	104.23	106.82
4	X	717	HEC	O2D-CGD-O1D	-2.25	117.54	123.33
4	X	715	HEC	O1D-CGD-CBD	-2.25	115.95	123.09
4	X	718	HEC	C4D-CHA-C1A	2.25	131.60	124.66
4	X	704	HEC	C4B-NB-C1B	2.24	109.47	105.82
4	X	714	HEC	CBD-CAD-C3D	-2.22	106.38	112.53
4	X	717	HEC	C3D-C4D-ND	2.22	112.62	110.15
4	X	709	HEC	CBA-CAA-C2A	2.22	118.67	112.53
4	X	711	HEC	CBA-CAA-C2A	2.22	118.66	112.53
4	X	708	HEC	CHC-C1C-NC	2.21	127.87	123.86
4	X	713	HEC	CBC-CAC-C3C	-2.20	123.03	127.43
4	X	713	HEC	O2A-CGA-CBA	2.20	120.96	114.00
4	X	716	HEC	O2D-CGD-O1D	-2.19	117.70	123.33
4	X	713	HEC	CAD-C3D-C2D	2.18	131.97	127.07
4	X	717	HEC	C2D-C1D-ND	-2.17	106.66	110.14
4	X	718	HEC	CHA-C4D-ND	2.17	127.79	123.86
4	X	712	HEC	CHD-C1D-ND	2.17	127.79	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	713	HEC	CBA-CAA-C2A	-2.16	106.57	112.53
4	X	713	HEC	CHD-C1D-C2D	-2.16	121.16	127.43
4	X	719	HEC	CHC-C1C-NC	2.16	127.77	123.86
4	X	715	HEC	C3D-C4D-ND	-2.15	107.76	110.15
4	X	716	HEC	CAA-C2A-C3A	-2.15	123.84	127.87
4	X	714	HEC	C1D-C2D-C3D	-2.14	104.37	106.82
4	X	717	HEC	O2A-CGA-CBA	2.13	120.75	114.00
4	X	708	HEC	O2D-CGD-CBD	2.13	120.74	114.00
4	X	717	HEC	C2A-C1A-NA	-2.13	108.27	110.32
4	X	705	HEC	C1C-CHC-C4B	2.12	131.20	124.66
4	X	714	HEC	CHC-C4B-NB	-2.10	122.17	124.45
4	X	712	HEC	C2A-C1A-NA	-2.09	108.30	110.32
4	X	708	HEC	CAD-CBD-CGD	-2.09	108.13	113.67
4	X	710	HEC	CMD-C2D-C3D	2.08	130.03	125.62
4	X	714	HEC	CMC-C2C-C3C	2.08	131.44	126.55
4	X	717	HEC	CMC-C2C-C1C	-2.08	122.25	125.42
4	X	704	HEC	C2C-C1C-NC	-2.07	106.82	110.14
4	X	704	HEC	CHA-C1A-NA	2.07	126.71	124.45
4	X	711	HEC	CHA-C1A-NA	2.06	126.70	124.45
4	X	710	HEC	O2A-CGA-CBA	2.05	120.47	114.00
4	X	717	HEC	CBD-CAD-C3D	2.04	118.19	112.53
4	X	707	HEC	C4A-NA-C1A	2.03	109.13	105.82
4	X	719	HEC	CMA-C3A-C4A	-2.03	121.16	124.73
4	X	711	HEC	CHC-C1C-NC	2.01	127.50	123.86
4	X	712	HEC	CAA-CBA-CGA	2.01	118.99	113.67
4	X	704	HEC	C4C-NC-C1C	2.01	109.09	105.82
4	X	710	HEC	CHB-C4A-NA	2.00	126.64	124.45

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	704	HEC	C2C-C3C-CAC-CBC
4	X	704	HEC	C4C-C3C-CAC-CBC
4	X	704	HEC	C3D-CAD-CBD-CGD
4	X	705	HEC	C2B-C3B-CAB-CBB
4	X	705	HEC	C4B-C3B-CAB-CBB
4	X	705	HEC	C2C-C3C-CAC-CBC
4	X	705	HEC	C4C-C3C-CAC-CBC
4	X	706	HEC	C2C-C3C-CAC-CBC
4	X	706	HEC	C4C-C3C-CAC-CBC
4	X	707	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
4	X	707	HEC	C4B-C3B-CAB-CBB
4	X	707	HEC	C4C-C3C-CAC-CBC
4	X	708	HEC	C2B-C3B-CAB-CBB
4	X	708	HEC	C4B-C3B-CAB-CBB
4	X	708	HEC	C2C-C3C-CAC-CBC
4	X	708	HEC	C4C-C3C-CAC-CBC
4	X	709	HEC	C2B-C3B-CAB-CBB
4	X	709	HEC	C4B-C3B-CAB-CBB
4	X	710	HEC	C2B-C3B-CAB-CBB
4	X	710	HEC	C4B-C3B-CAB-CBB
4	X	710	HEC	C2C-C3C-CAC-CBC
4	X	710	HEC	C4C-C3C-CAC-CBC
4	X	711	HEC	C2B-C3B-CAB-CBB
4	X	711	HEC	C4B-C3B-CAB-CBB
4	X	711	HEC	C2C-C3C-CAC-CBC
4	X	711	HEC	C4C-C3C-CAC-CBC
4	X	712	HEC	C2B-C3B-CAB-CBB
4	X	712	HEC	C4B-C3B-CAB-CBB
4	X	712	HEC	C2C-C3C-CAC-CBC
4	X	712	HEC	C4C-C3C-CAC-CBC
4	X	713	HEC	C2B-C3B-CAB-CBB
4	X	713	HEC	C4B-C3B-CAB-CBB
4	X	714	HEC	C2B-C3B-CAB-CBB
4	X	714	HEC	C4B-C3B-CAB-CBB
4	X	714	HEC	C2C-C3C-CAC-CBC
4	X	714	HEC	C4C-C3C-CAC-CBC
4	X	715	HEC	C2B-C3B-CAB-CBB
4	X	715	HEC	C4B-C3B-CAB-CBB
4	X	715	HEC	C2C-C3C-CAC-CBC
4	X	715	HEC	C4C-C3C-CAC-CBC
4	X	716	HEC	C2B-C3B-CAB-CBB
4	X	716	HEC	C4B-C3B-CAB-CBB
4	X	716	HEC	C2C-C3C-CAC-CBC
4	X	716	HEC	C4C-C3C-CAC-CBC
4	X	717	HEC	C2B-C3B-CAB-CBB
4	X	717	HEC	C4B-C3B-CAB-CBB
4	X	717	HEC	C2C-C3C-CAC-CBC
4	X	717	HEC	C4C-C3C-CAC-CBC
4	X	718	HEC	C2B-C3B-CAB-CBB
4	X	718	HEC	C4B-C3B-CAB-CBB
4	X	718	HEC	C2C-C3C-CAC-CBC
4	X	718	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
4	X	719	HEC	C2B-C3B-CAB-CBB
4	X	719	HEC	C4B-C3B-CAB-CBB
4	X	719	HEC	C4C-C3C-CAC-CBC
5	X	720	GOL	O1-C1-C2-C3
5	X	721	GOL	C1-C2-C3-O3
5	X	722	GOL	C1-C2-C3-O3
5	X	722	GOL	O2-C2-C3-O3
5	X	723	GOL	C1-C2-C3-O3
4	X	713	HEC	C2D-C3D-CAD-CBD
4	X	713	HEC	C4D-C3D-CAD-CBD
4	X	712	HEC	C2A-CAA-CBA-CGA
5	X	720	GOL	O1-C1-C2-O2
5	X	721	GOL	O2-C2-C3-O3
5	X	723	GOL	O2-C2-C3-O3
5	X	724	GOL	O1-C1-C2-O2
5	X	722	GOL	O1-C1-C2-C3
5	X	724	GOL	O1-C1-C2-C3
4	X	717	HEC	C3D-CAD-CBD-CGD
4	X	713	HEC	C3D-CAD-CBD-CGD
5	X	722	GOL	O1-C1-C2-O2
4	X	706	HEC	C4B-C3B-CAB-CBB
4	X	704	HEC	C2B-C3B-CAB-CBB
4	X	706	HEC	C2B-C3B-CAB-CBB
4	X	707	HEC	C2C-C3C-CAC-CBC
4	X	705	HEC	C3D-CAD-CBD-CGD
4	X	710	HEC	CAD-CBD-CGD-O2D
4	X	712	HEC	CAA-CBA-CGA-O1A
4	X	718	HEC	CAD-CBD-CGD-O2D
5	X	721	GOL	O1-C1-C2-C3
4	X	709	HEC	CAD-CBD-CGD-O2D
4	X	712	HEC	CAA-CBA-CGA-O2A
4	X	713	HEC	CAA-CBA-CGA-O1A
4	X	718	HEC	CAD-CBD-CGD-O1D
4	X	713	HEC	CAA-CBA-CGA-O2A
4	X	708	HEC	CAD-CBD-CGD-O1D
4	X	710	HEC	CAD-CBD-CGD-O1D
4	X	714	HEC	CAA-CBA-CGA-O2A
4	X	714	HEC	CAA-CBA-CGA-O1A
4	X	706	HEC	CAA-CBA-CGA-O2A
4	X	709	HEC	CAD-CBD-CGD-O1D
4	X	706	HEC	CAA-CBA-CGA-O1A
4	X	708	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
4	X	711	HEC	CAD-CBD-CGD-O2D
4	X	715	HEC	CAD-CBD-CGD-O2D
4	X	717	HEC	CAA-CBA-CGA-O1A
4	X	715	HEC	CAD-CBD-CGD-O1D
4	X	717	HEC	CAA-CBA-CGA-O2A
4	X	712	HEC	CAD-CBD-CGD-O2D
4	X	719	HEC	CAD-CBD-CGD-O1D
4	X	719	HEC	CAD-CBD-CGD-O2D
4	X	715	HEC	CAA-CBA-CGA-O1A
4	X	715	HEC	CAA-CBA-CGA-O2A
4	X	711	HEC	CAD-CBD-CGD-O1D
4	X	712	HEC	CAD-CBD-CGD-O1D
4	X	719	HEC	C3D-CAD-CBD-CGD
4	X	716	HEC	CAA-CBA-CGA-O1A
4	X	716	HEC	CAA-CBA-CGA-O2A
4	X	708	HEC	CAA-CBA-CGA-O2A
4	X	718	HEC	CAA-CBA-CGA-O1A
4	X	708	HEC	CAA-CBA-CGA-O1A
4	X	704	HEC	C4B-C3B-CAB-CBB
4	X	713	HEC	CAD-CBD-CGD-O2D
4	X	717	HEC	CAD-CBD-CGD-O2D

There are no ring outliers.

17 monomers are involved in 107 short contacts:

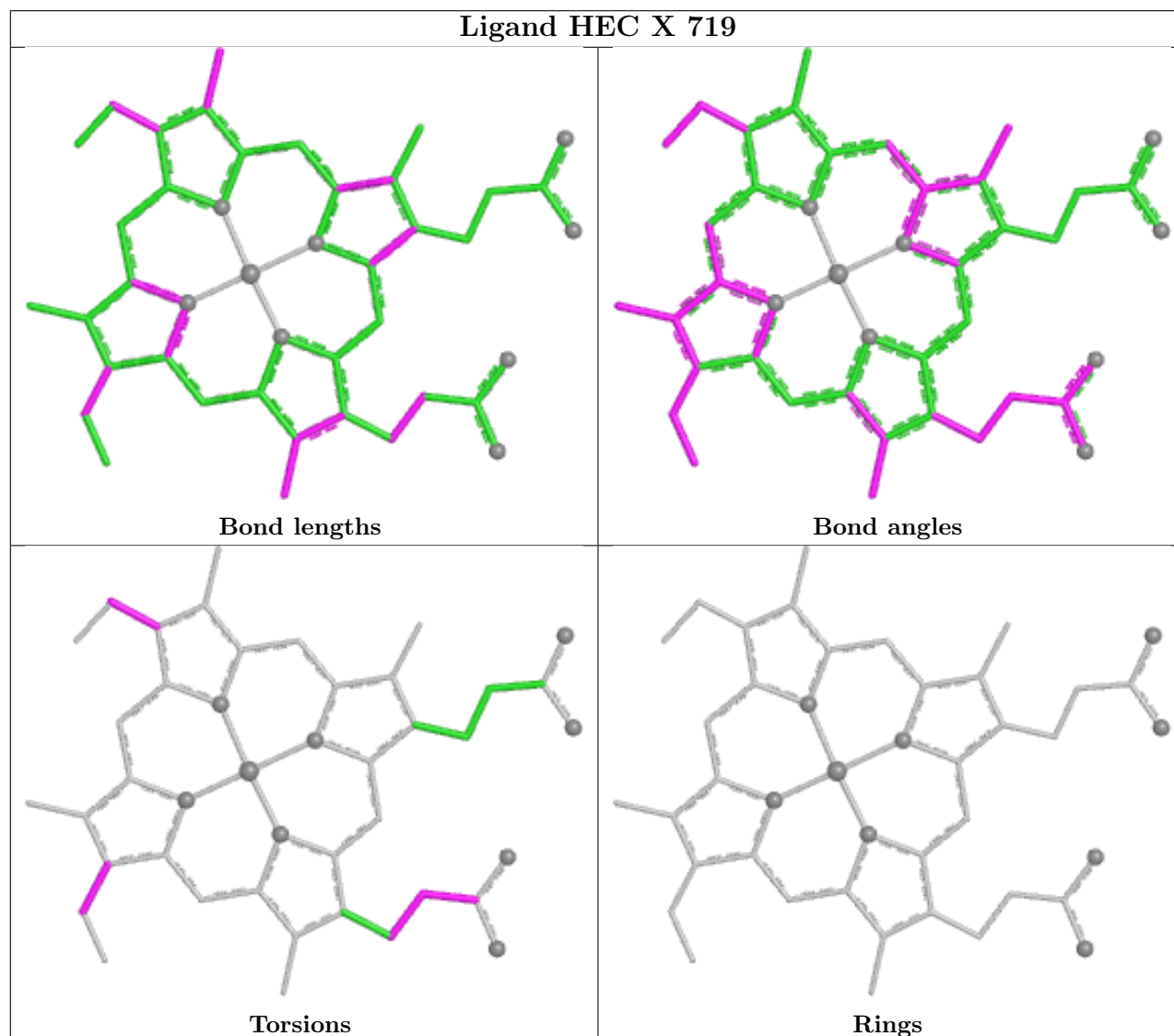
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	719	HEC	10	0
4	X	706	HEC	4	0
4	X	704	HEC	14	0
4	X	713	HEC	9	0
4	X	716	HEC	2	0
4	X	718	HEC	7	1
5	X	722	GOL	6	0
4	X	712	HEC	4	0
4	X	715	HEC	4	0
4	X	709	HEC	6	0
4	X	707	HEC	6	0
4	X	710	HEC	7	0
5	X	723	GOL	1	0
4	X	708	HEC	2	0
4	X	717	HEC	9	0
4	X	705	HEC	11	0

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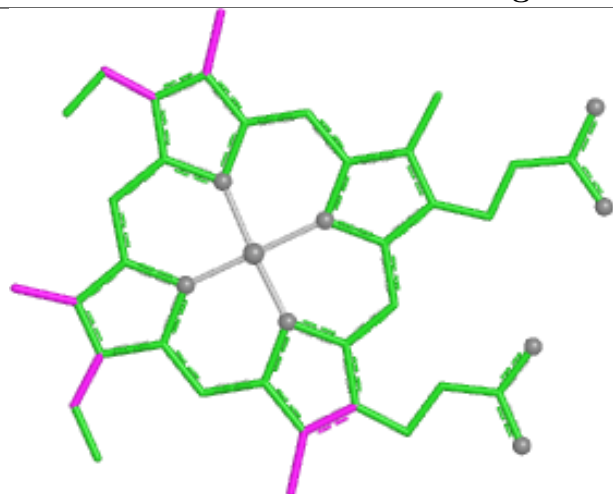
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	711	HEC	10	0

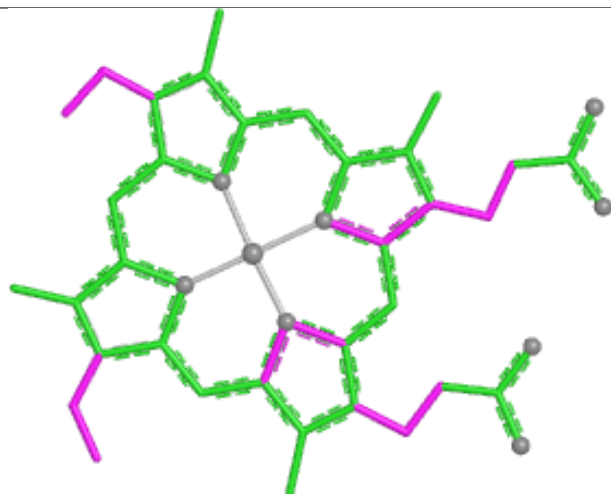
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



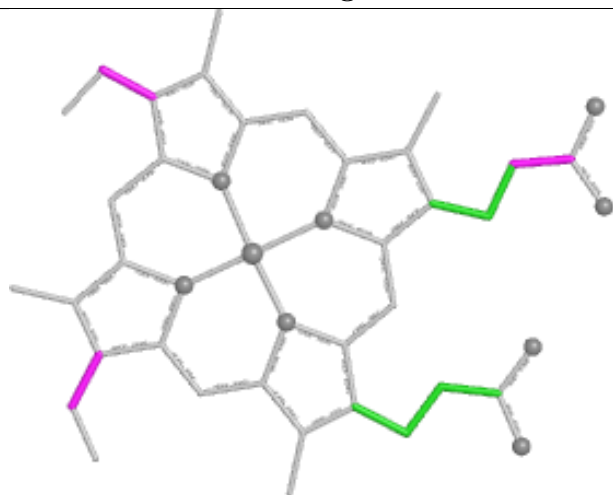
Ligand HEC X 706



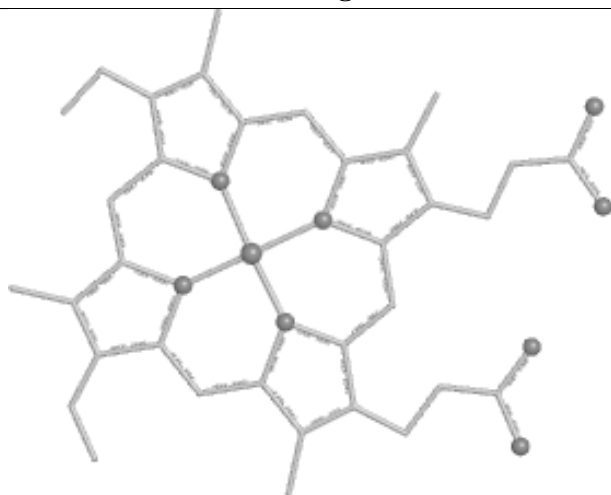
Bond lengths



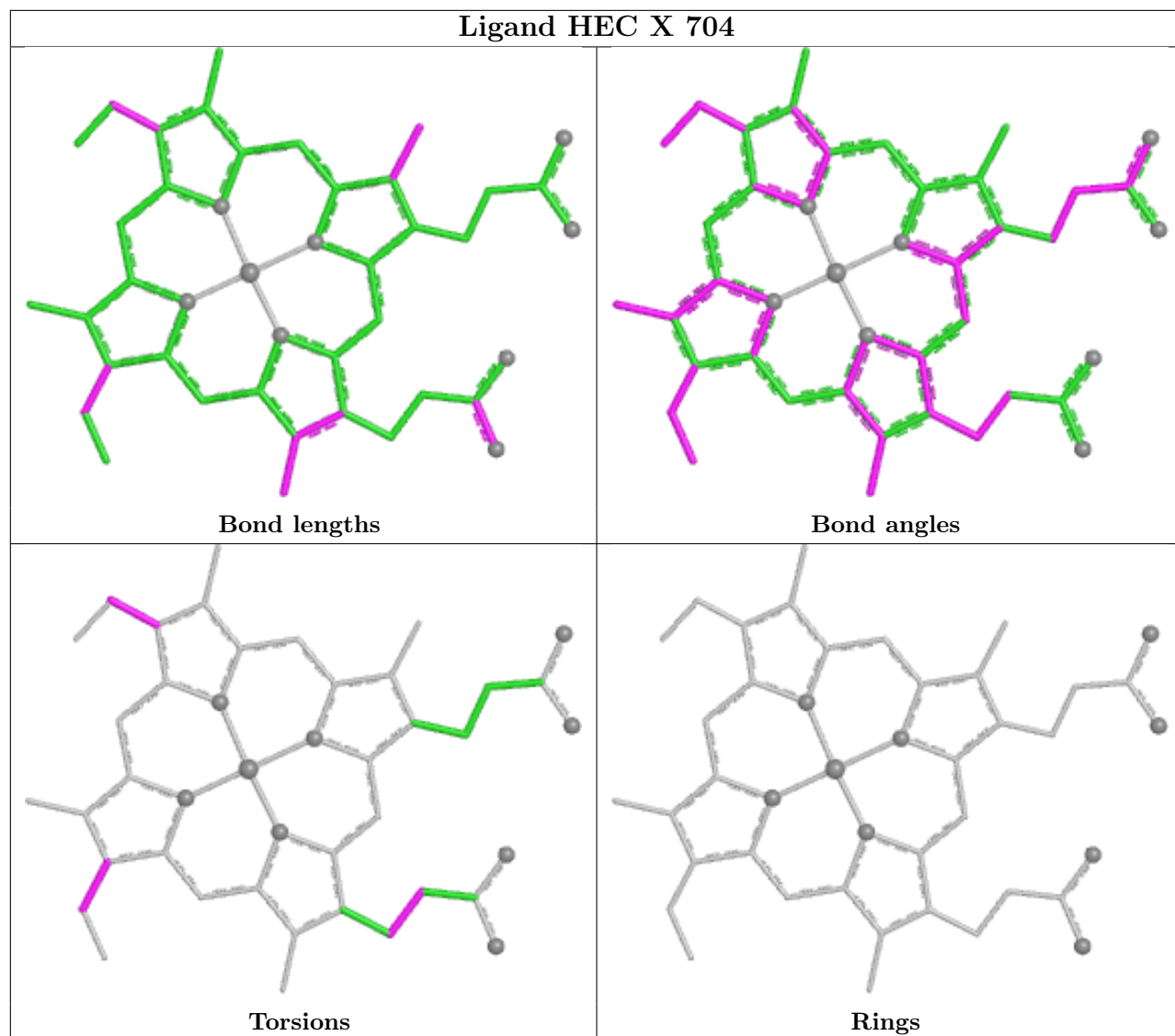
Bond angles



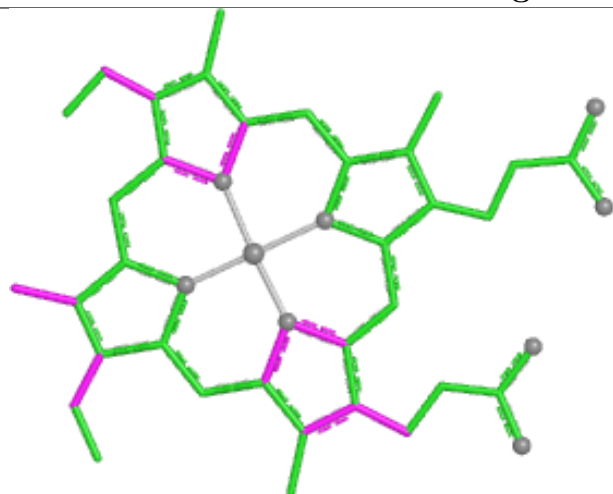
Torsions



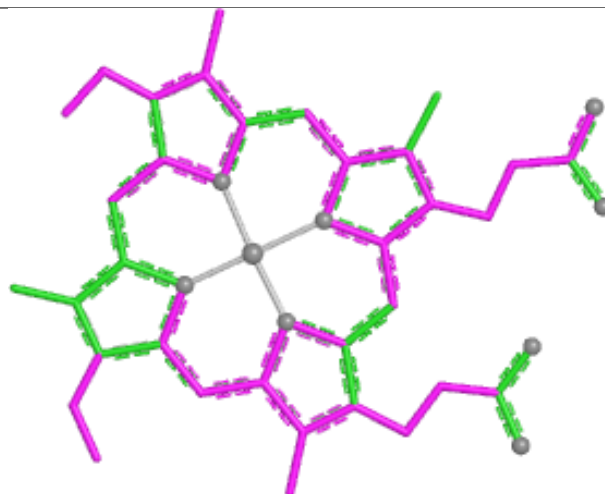
Rings



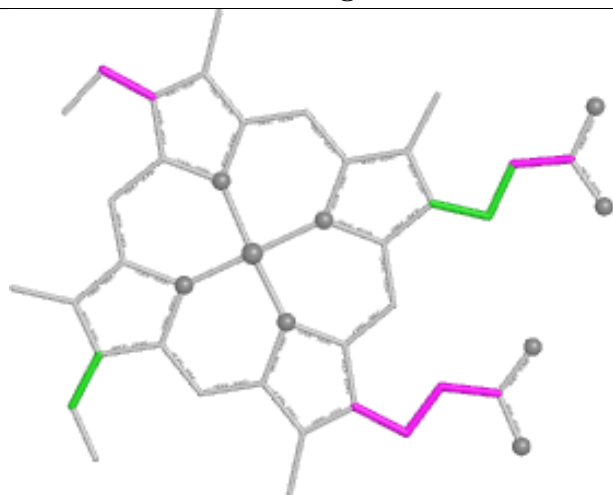
Ligand HEC X 713



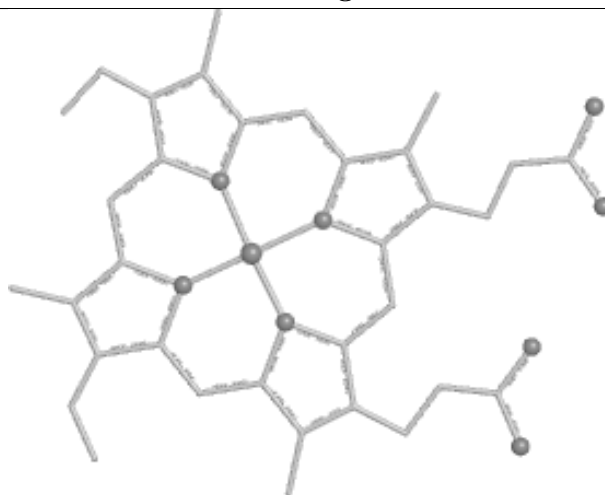
Bond lengths



Bond angles

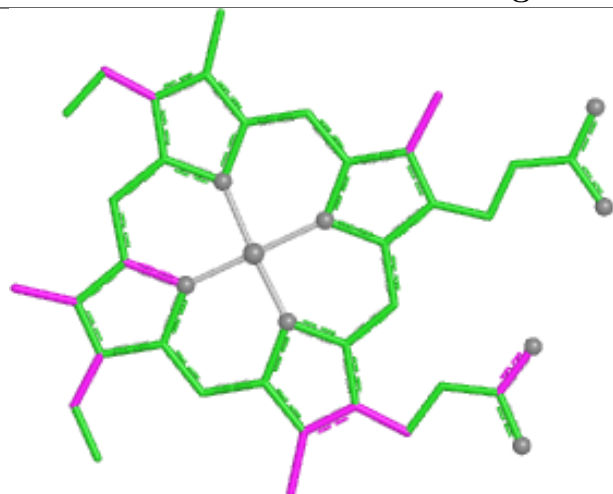


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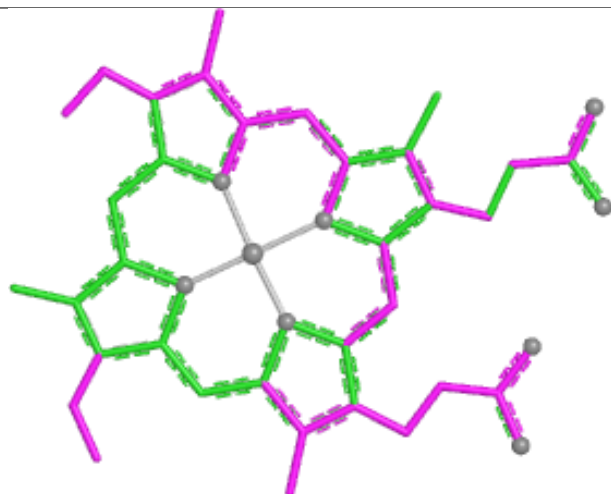


Rings

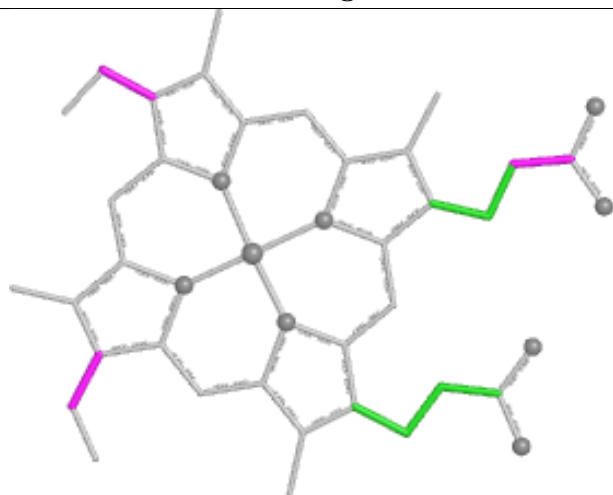
Ligand HEC X 716



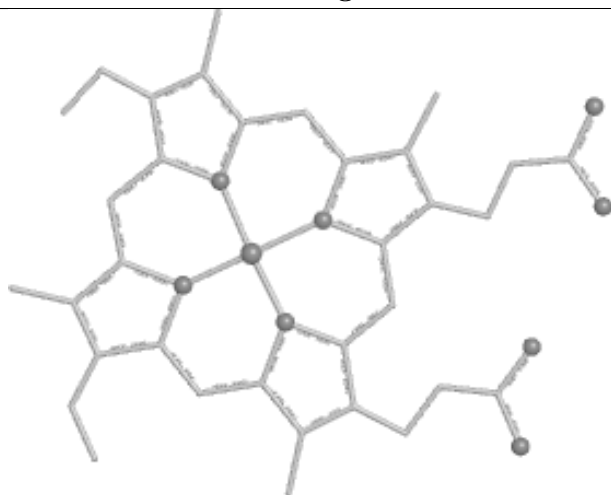
Bond lengths



Bond angles

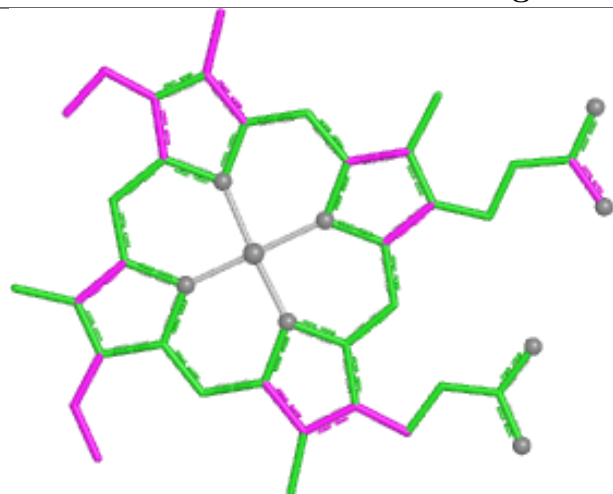


Torsions

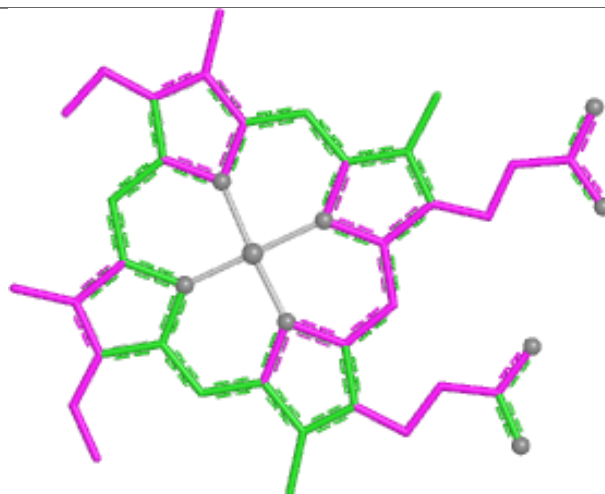


Rings

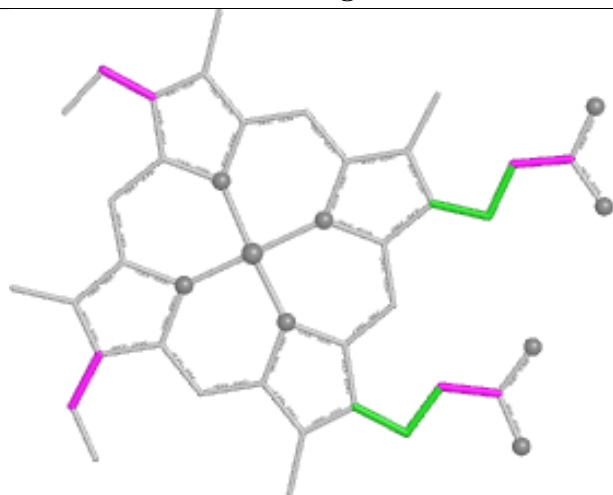
Ligand HEC X 718



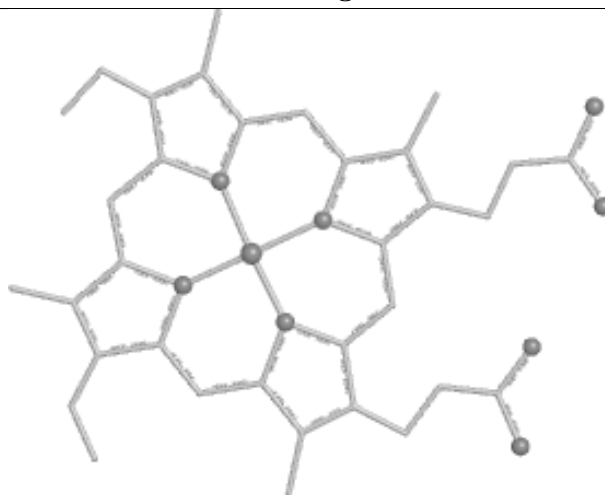
Bond lengths



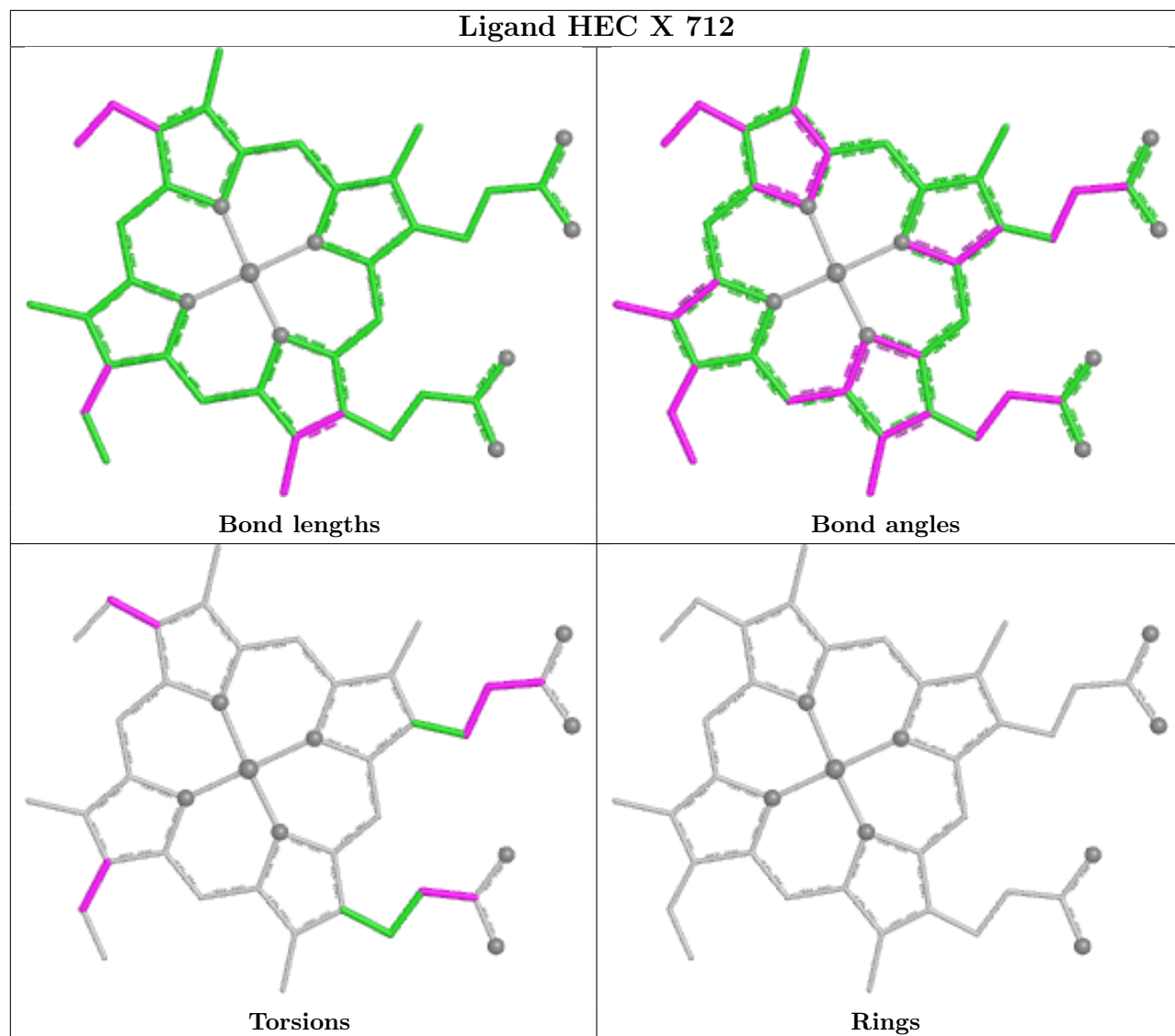
Bond angles

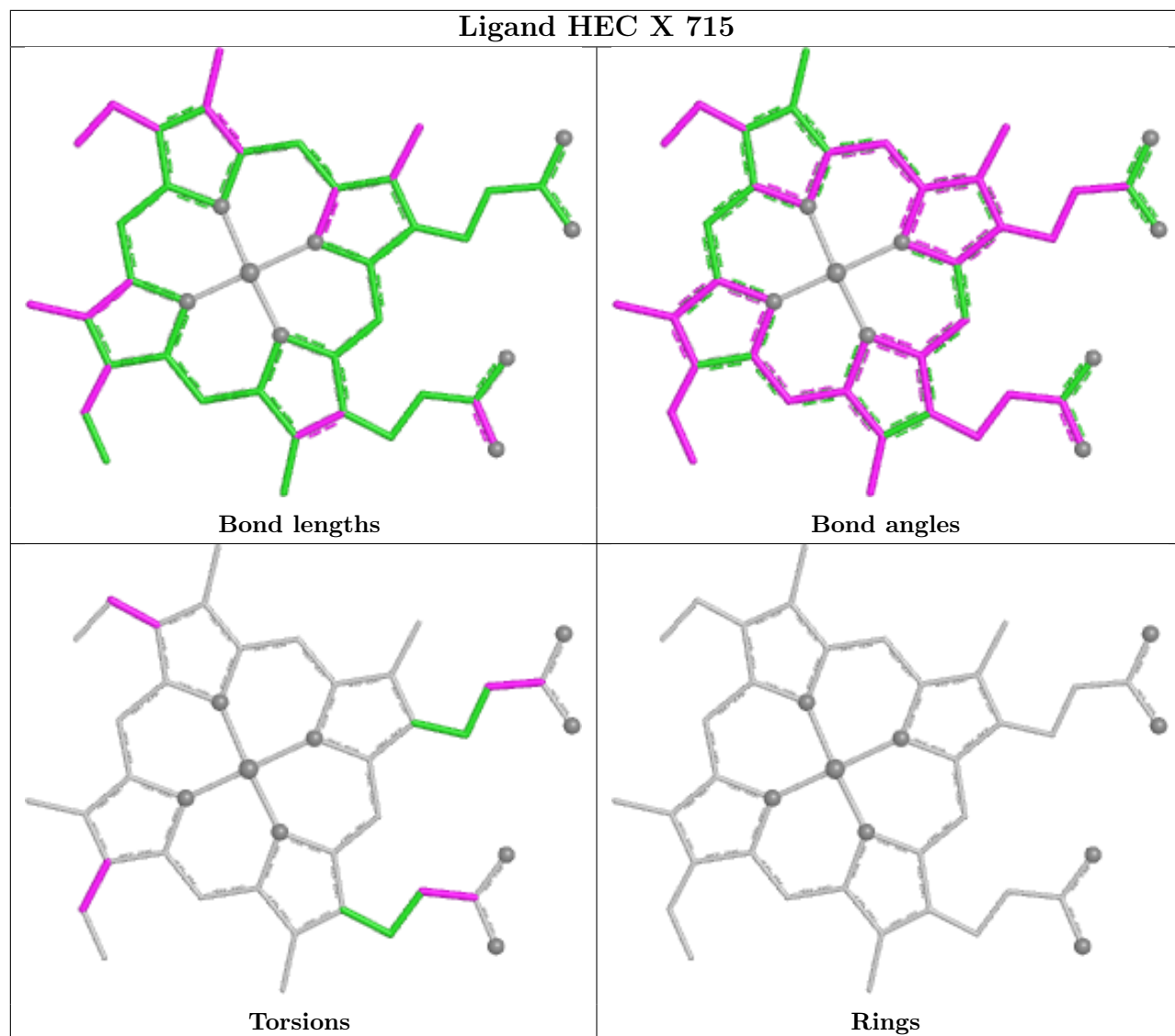


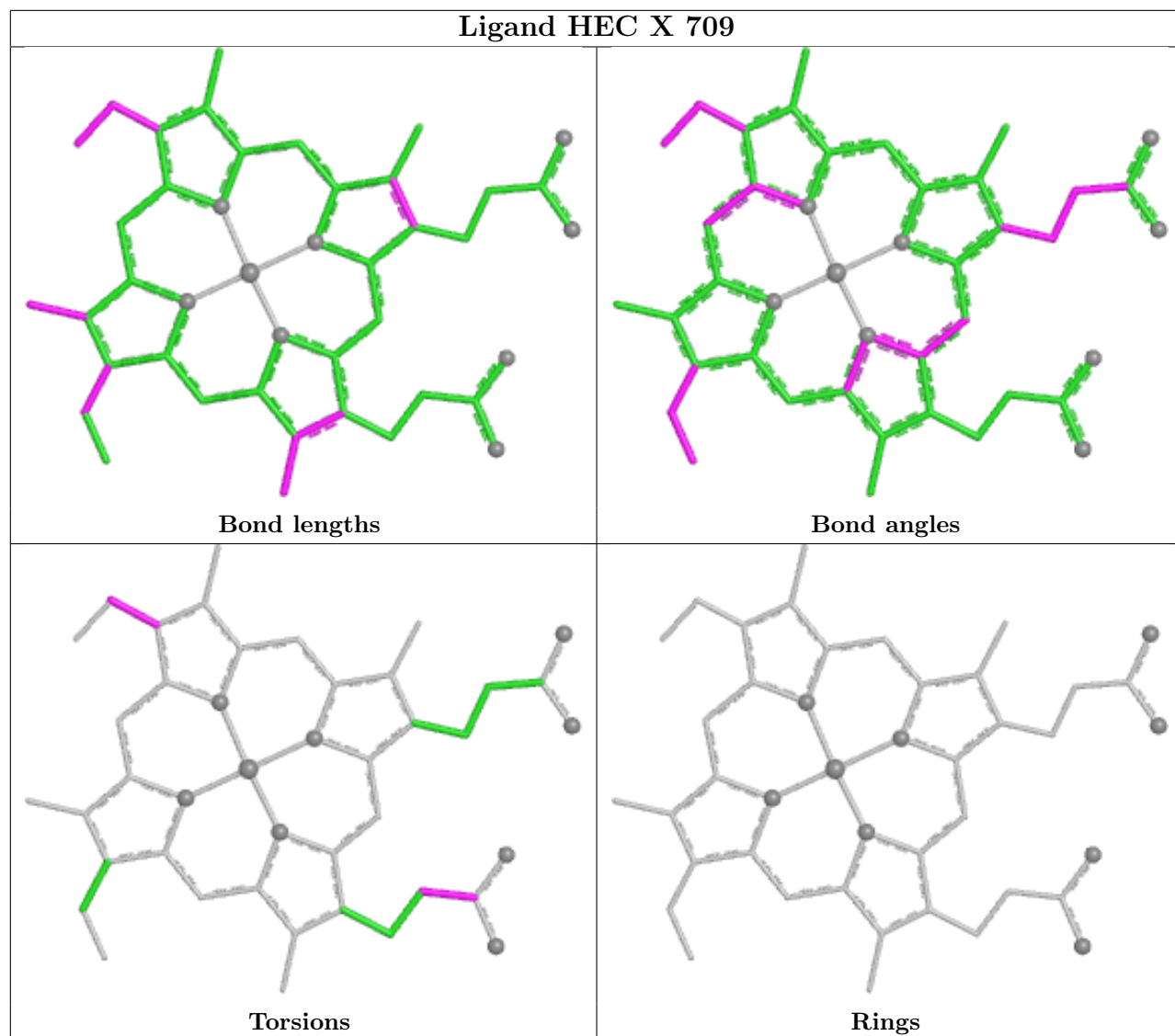
Torsions



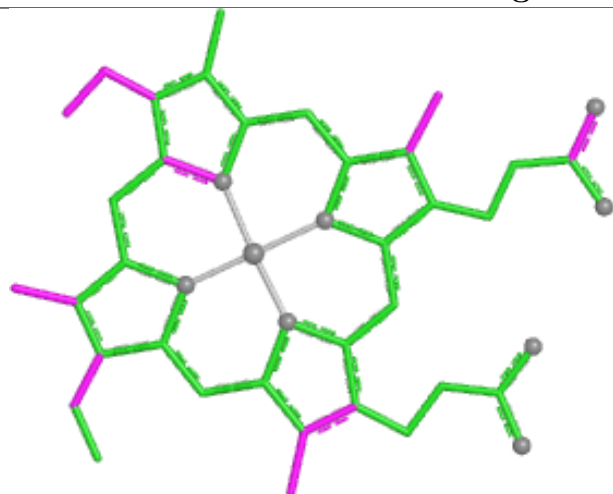
Rings



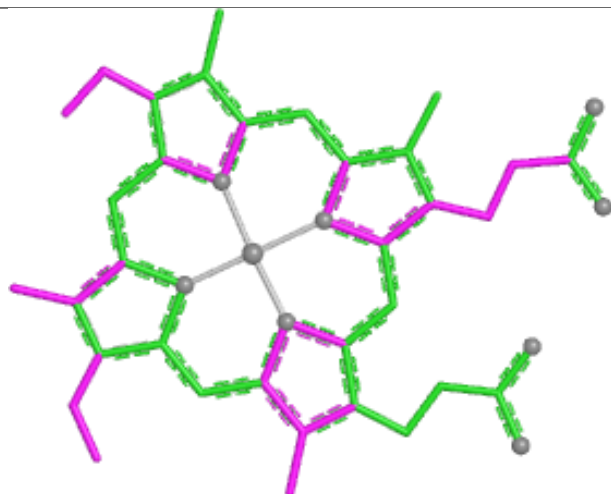




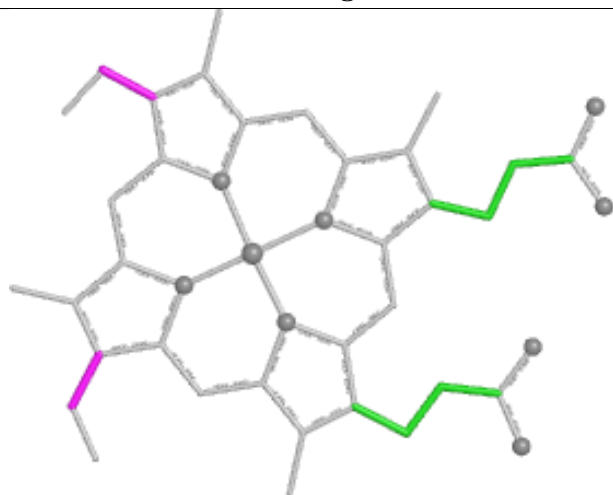
Ligand HEC X 707



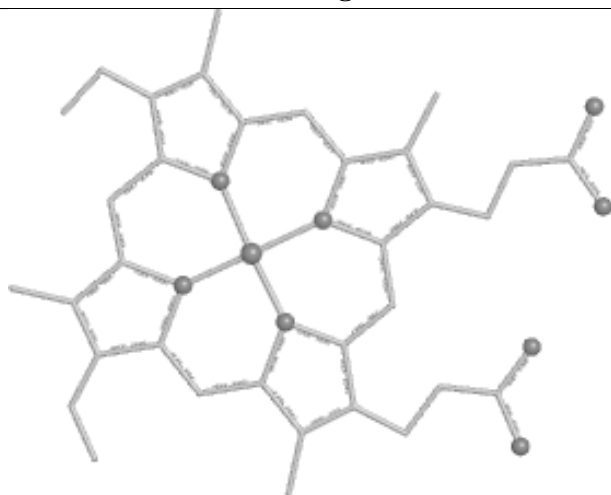
Bond lengths



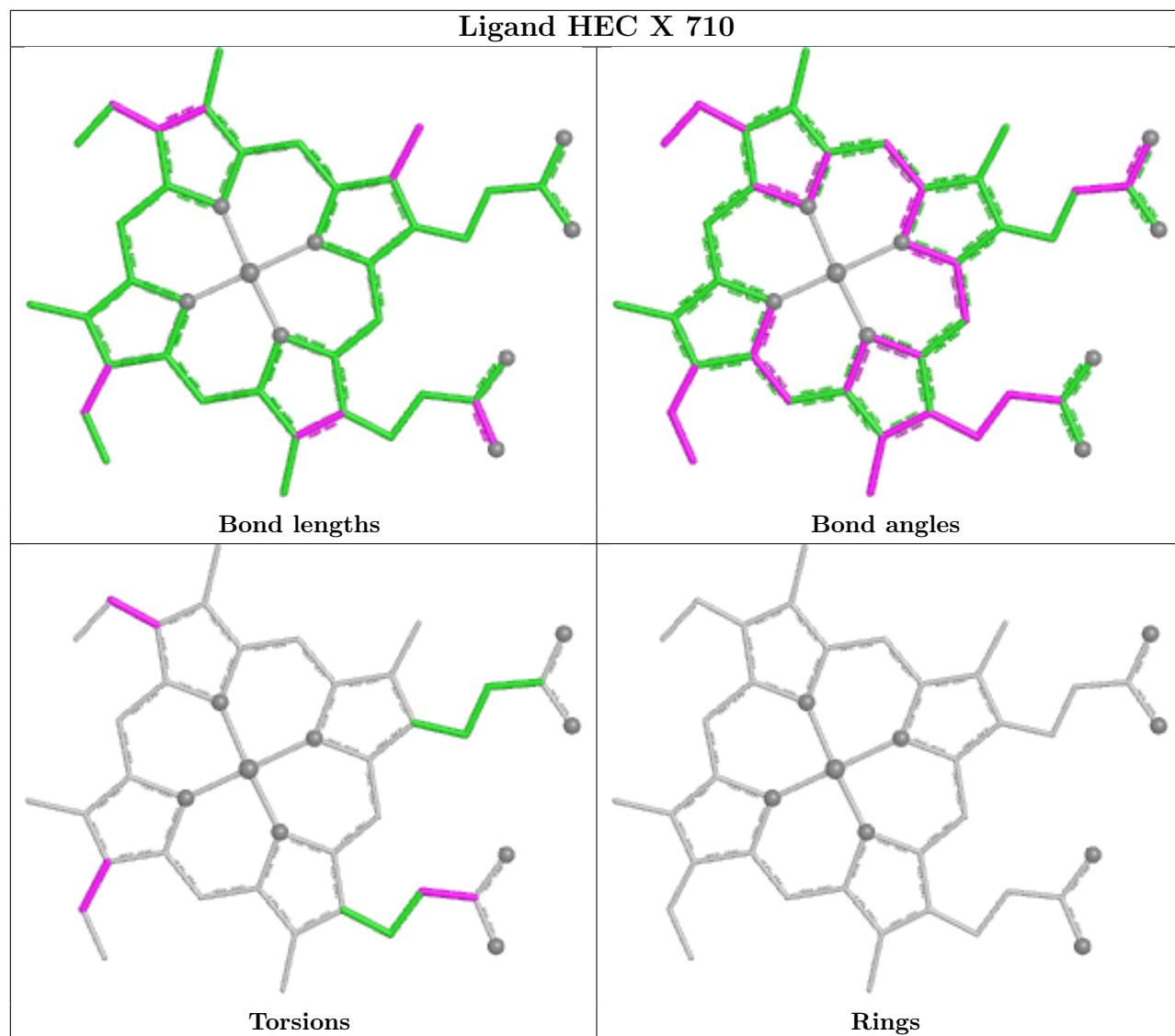
Bond angles



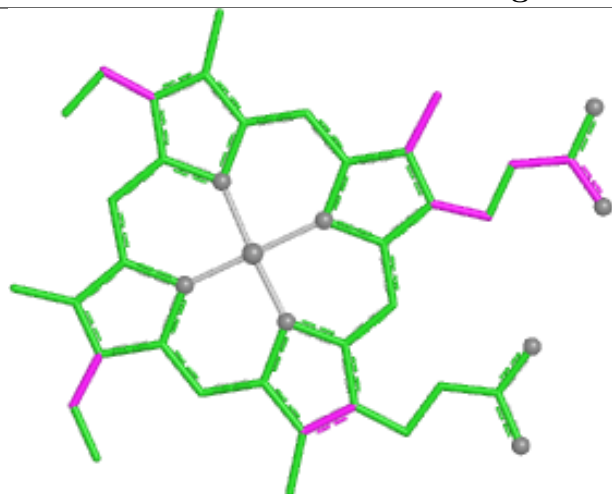
Torsions



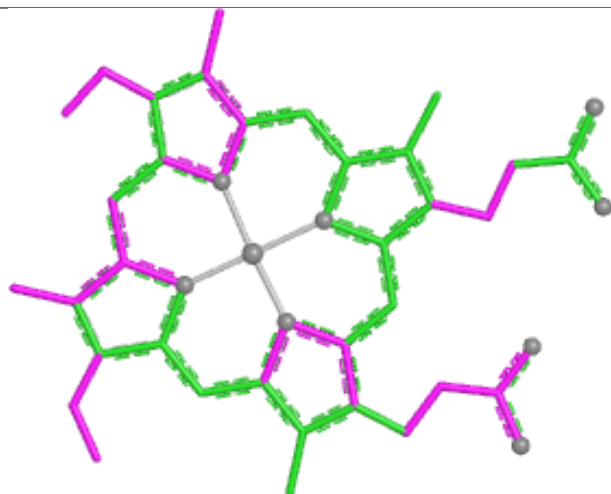
Rings



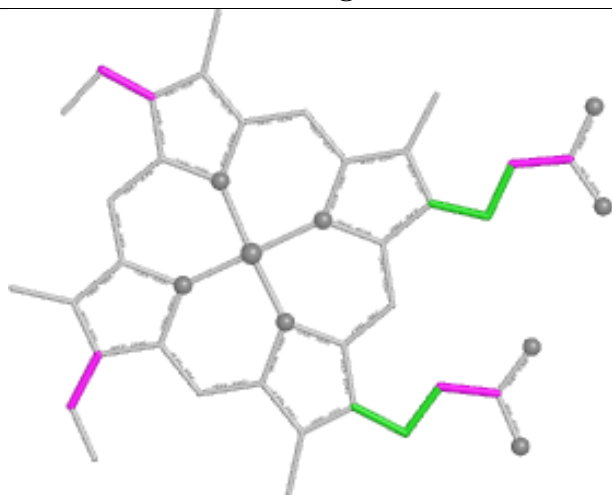
Ligand HEC X 708



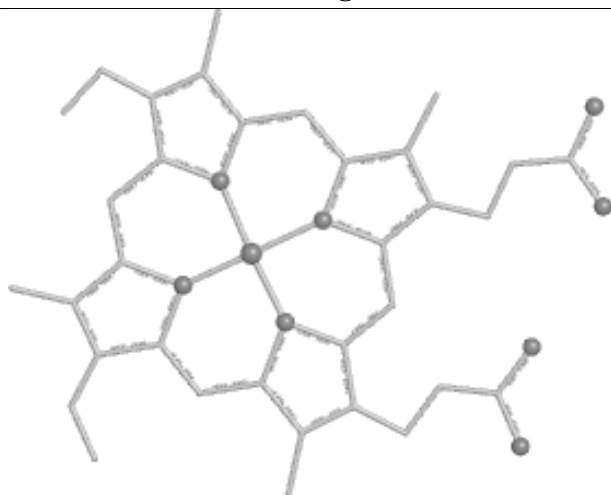
Bond lengths



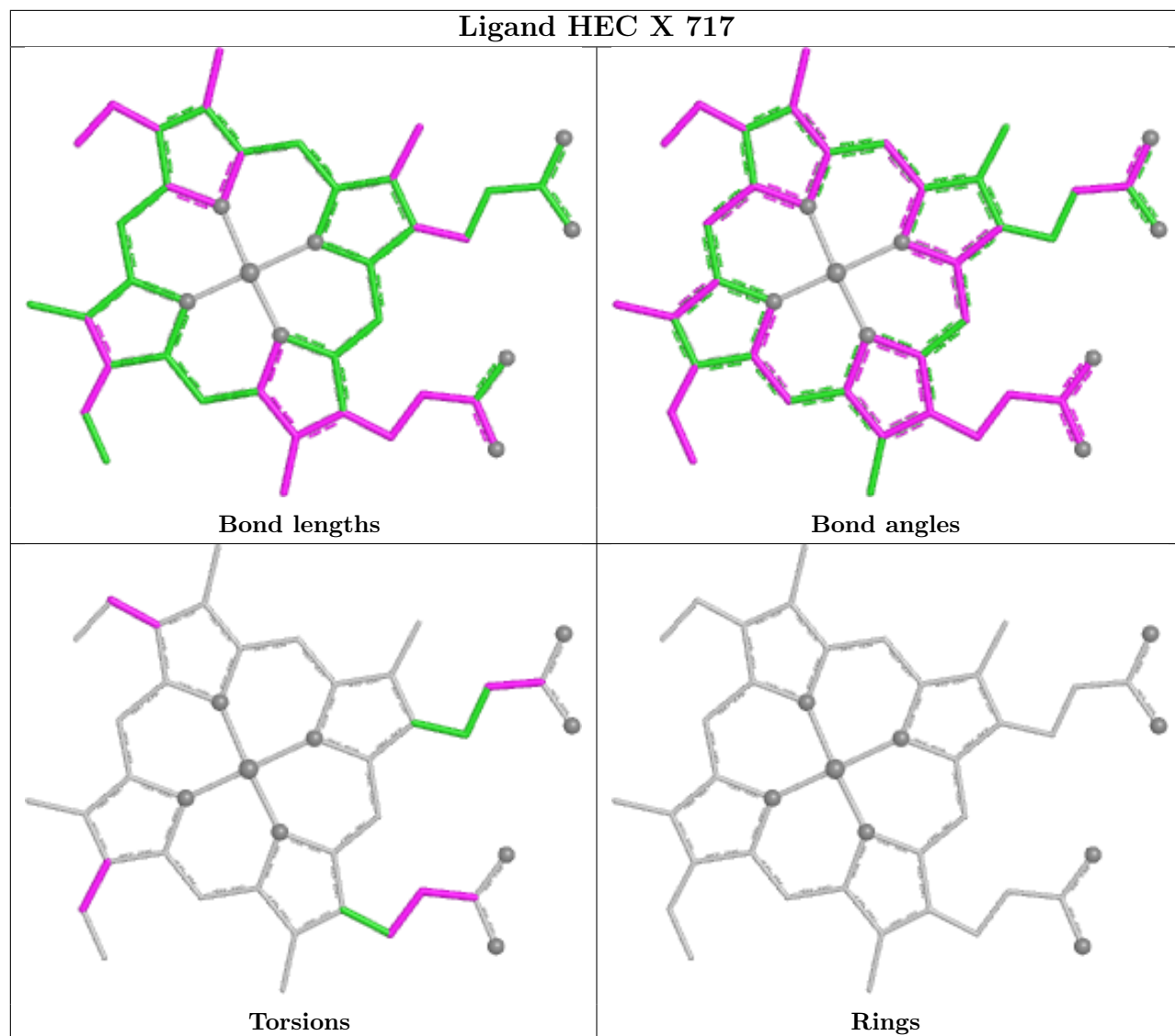
Bond angles



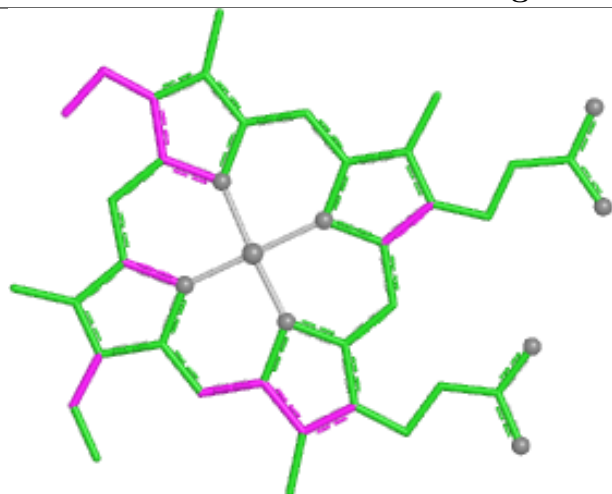
Torsions



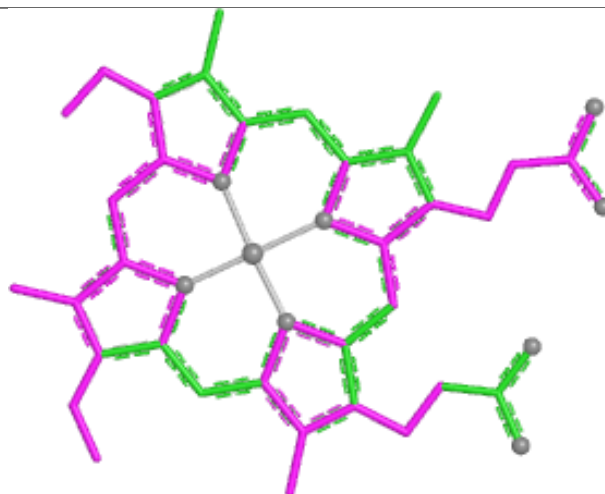
Rings



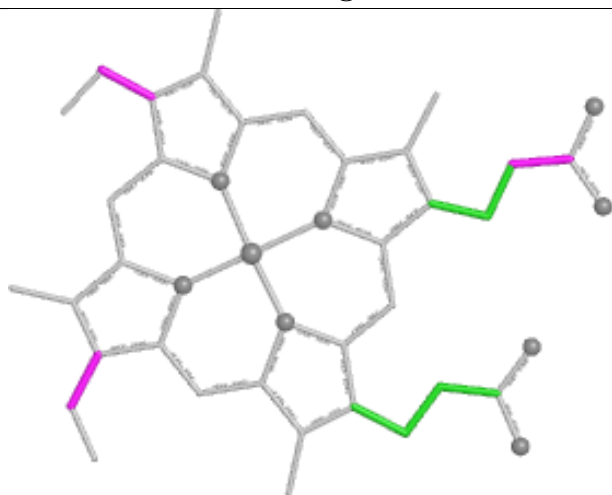
Ligand HEC X 714



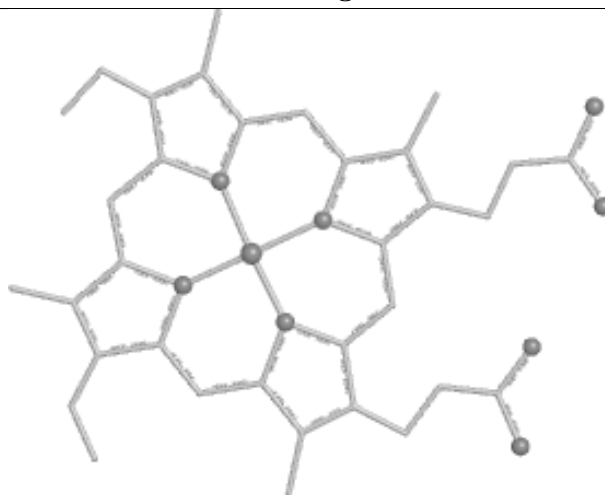
Bond lengths



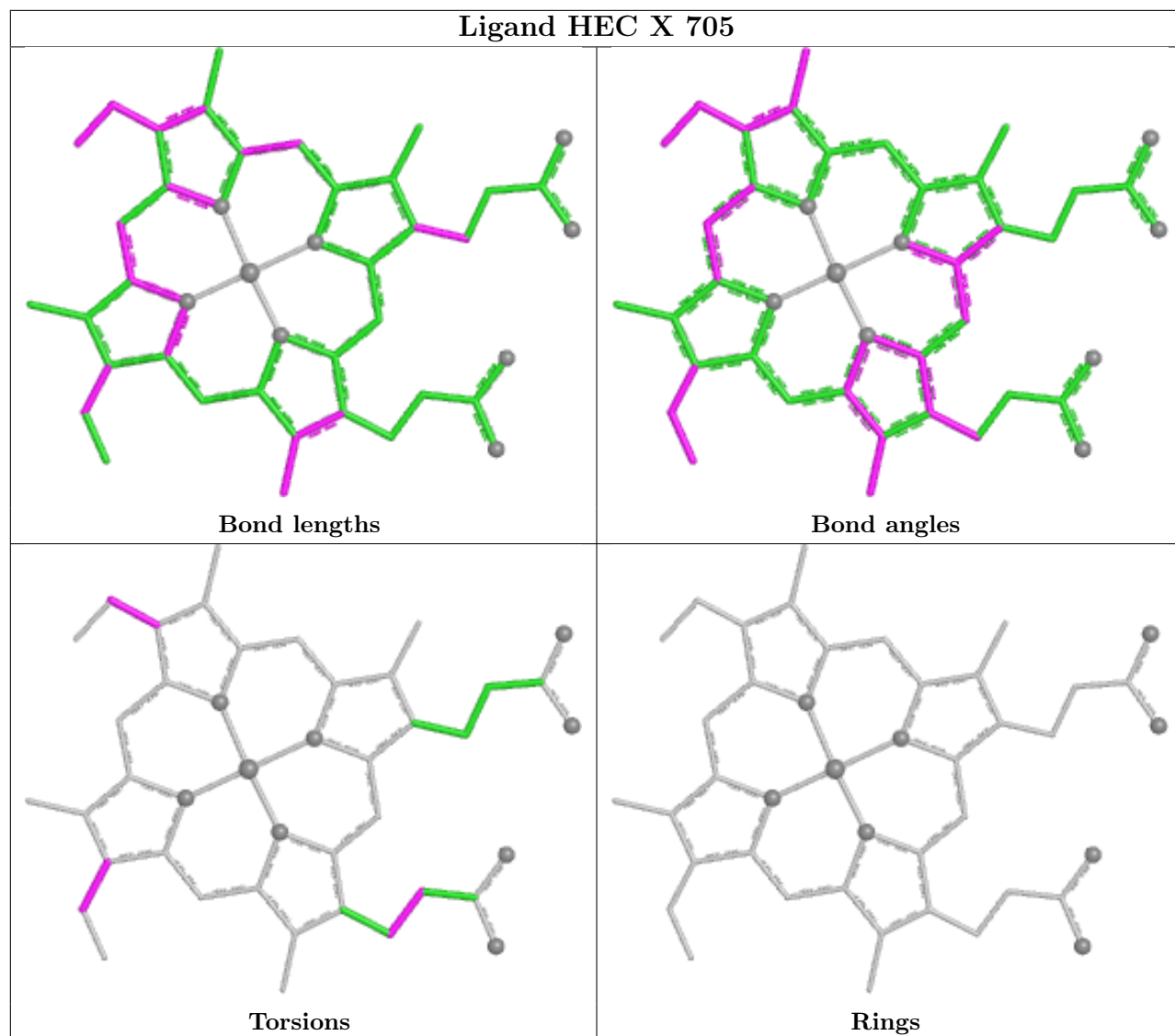
Bond angles

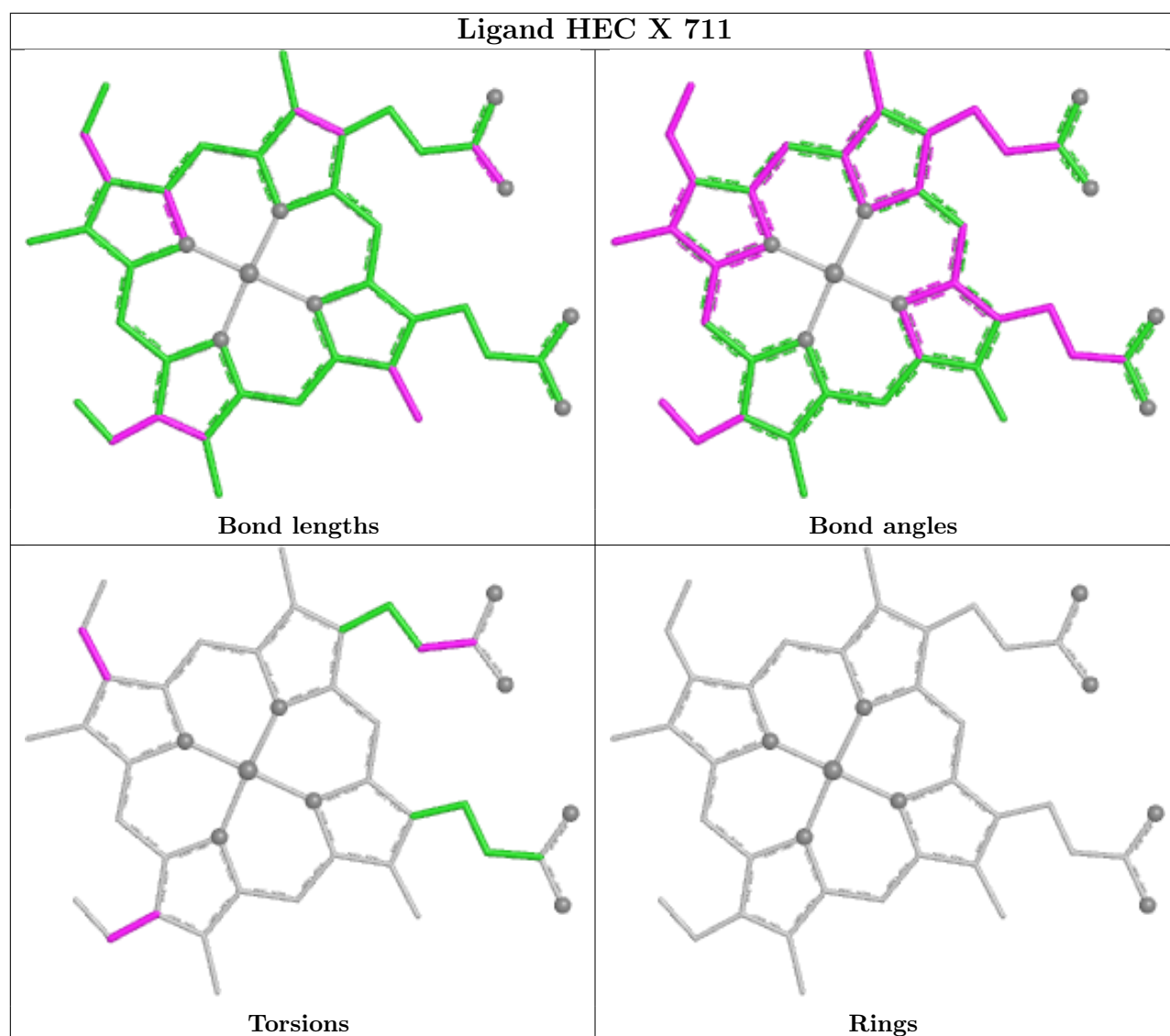


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	X	516/560 (92%)	0.22	10 (1%) 66 69	28, 55, 82, 91	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	530	SER	5.4
1	X	22	ALA	3.2
1	X	16	ILE	3.0
1	X	102	ALA	2.9
1	X	186	VAL	2.8
1	X	183	PRO	2.5
1	X	34	PHE	2.3
1	X	420	TYR	2.3
1	X	81	TYR	2.2
1	X	97	PRO	2.1

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

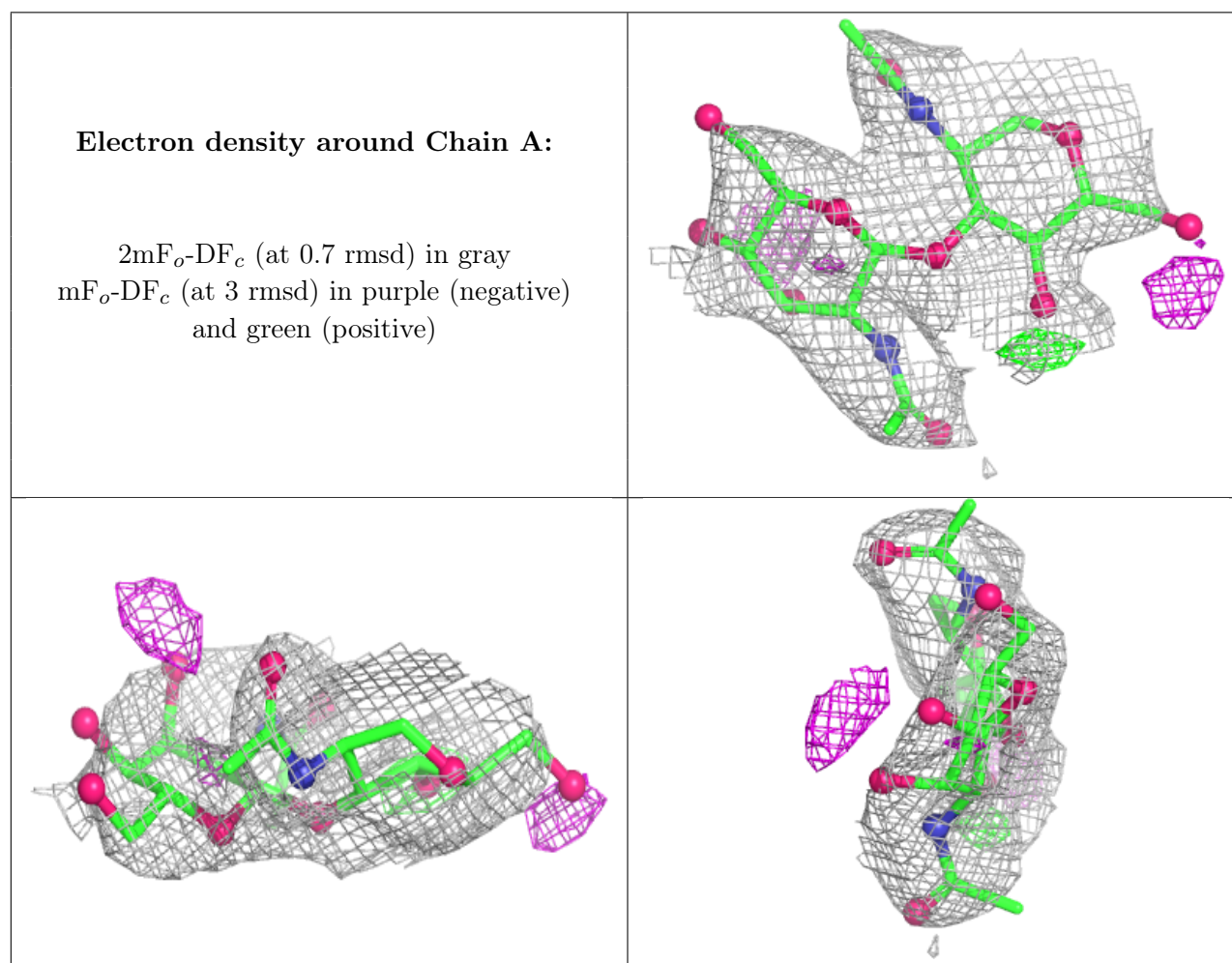
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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
2	NAG	A	1	14/15	-	-	75,79,86,86	0
2	NAA	A	2	14/15	-	-	89,91,94,94	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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($\text{\AA}^2$)	Q<0.9
5	GOL	X	724	6/6	0.73	0.17	57,62,66,73	0
5	GOL	X	720	6/6	0.79	0.10	86,88,89,90	0
5	GOL	X	723	6/6	0.82	0.13	53,61,66,70	0
5	GOL	X	721	6/6	0.85	0.11	62,69,71,73	0
3	ZN	X	702	1/1	0.88	0.07	72,72,72,72	0
5	GOL	X	722	6/6	0.92	0.13	28,54,59,60	0
4	HEC	X	717	43/43	0.93	0.10	20,31,41,50	0
3	ZN	X	703	1/1	0.93	0.11	69,69,69,69	0

Continued on next page...

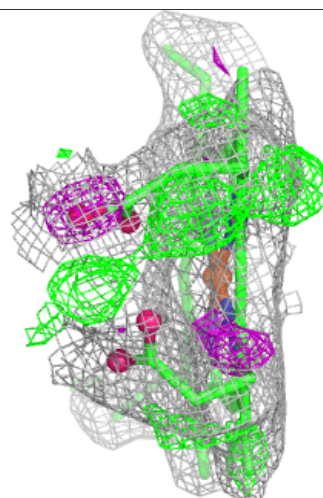
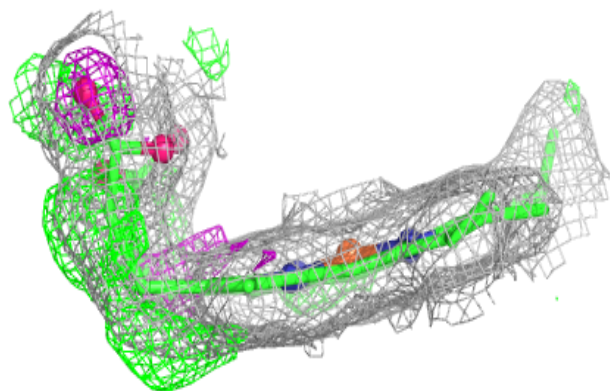
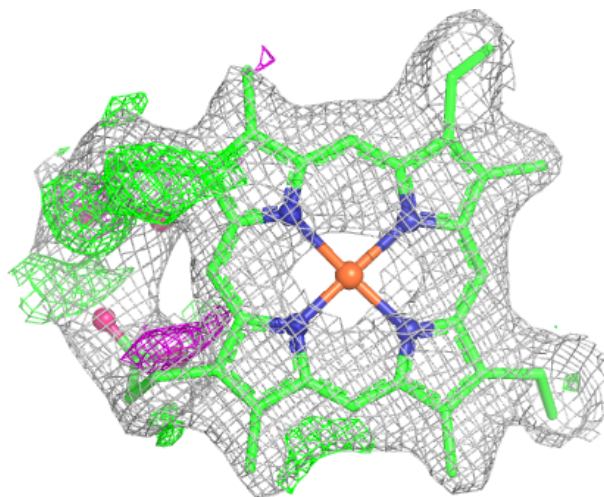
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	HEC	X	706	43/43	0.93	0.11	58,73,75,77	0
4	HEC	X	704	43/43	0.95	0.10	52,59,63,65	0
4	HEC	X	708	43/43	0.95	0.09	48,58,73,78	0
4	HEC	X	709	43/43	0.95	0.09	45,49,65,71	0
4	HEC	X	710	43/43	0.95	0.09	49,55,65,72	0
4	HEC	X	705	43/43	0.95	0.09	45,51,75,80	0
4	HEC	X	719	43/43	0.96	0.08	29,38,50,64	0
4	HEC	X	712	43/43	0.96	0.09	40,50,61,67	0
4	HEC	X	714	43/43	0.97	0.07	28,33,52,58	0
4	HEC	X	715	43/43	0.97	0.07	30,38,56,65	0
4	HEC	X	711	43/43	0.97	0.07	27,37,52,61	0
4	HEC	X	718	43/43	0.97	0.06	25,31,49,56	0
4	HEC	X	707	43/43	0.97	0.07	38,48,54,57	0
4	HEC	X	713	43/43	0.98	0.06	20,26,41,47	0
4	HEC	X	716	43/43	0.98	0.06	28,31,43,53	0
3	ZN	X	701	1/1	1.00	0.01	42,42,42,42	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.

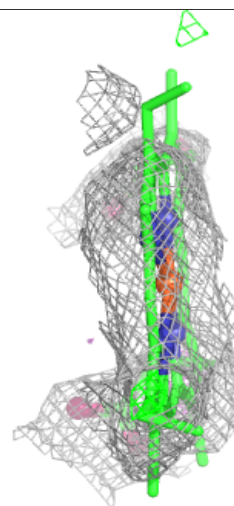
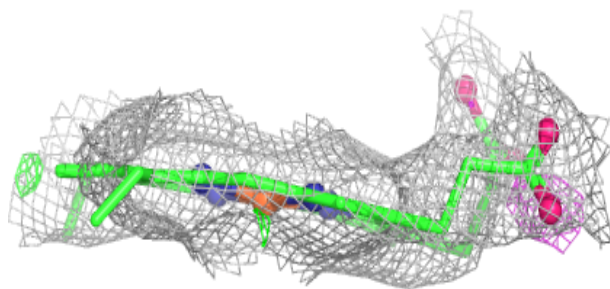
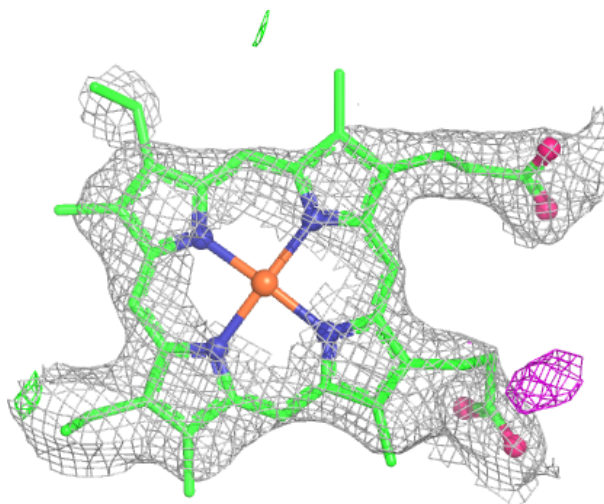
Electron density around HEC X 717:

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



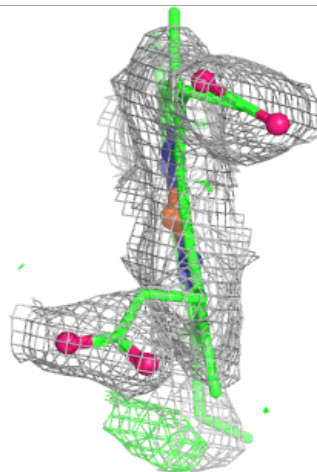
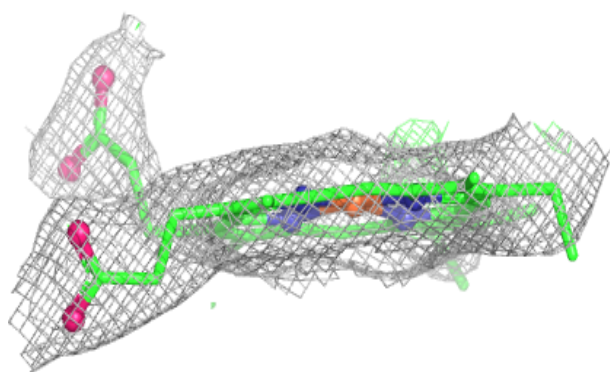
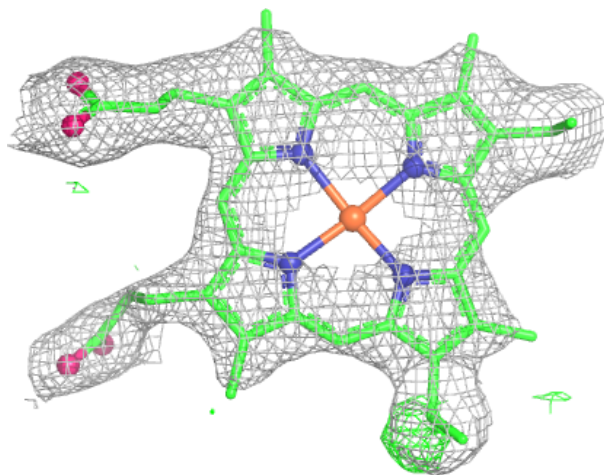
Electron density around HEC X 706:

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and green (positive)



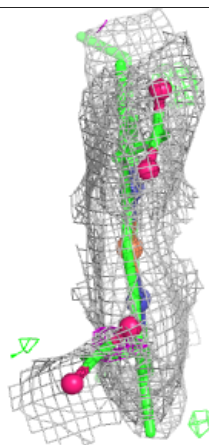
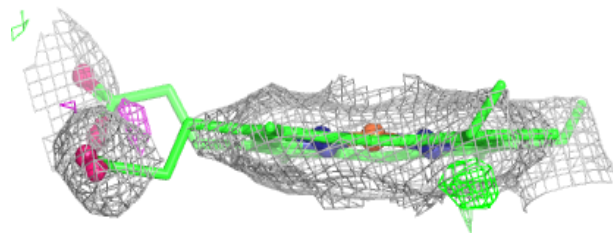
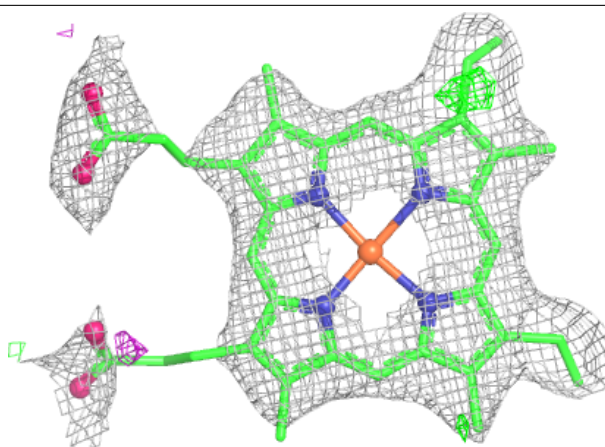
Electron density around HEC X 704:

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



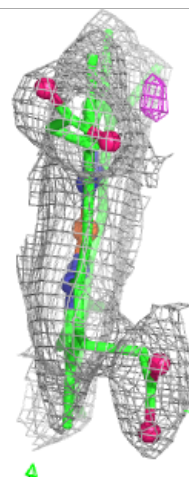
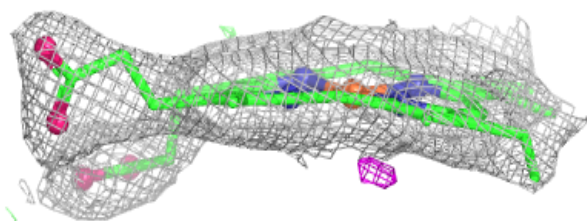
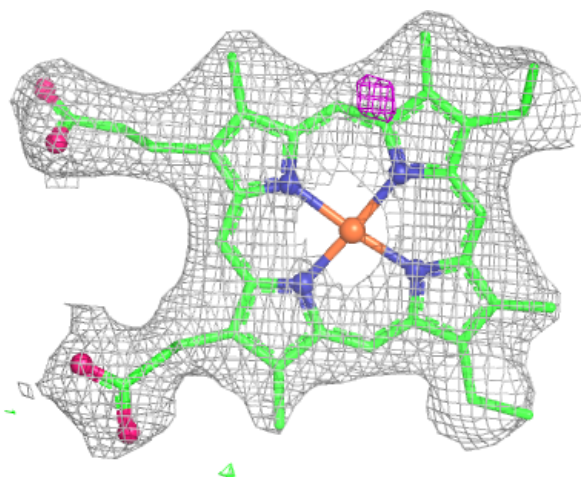
Electron density around HEC X 708:

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



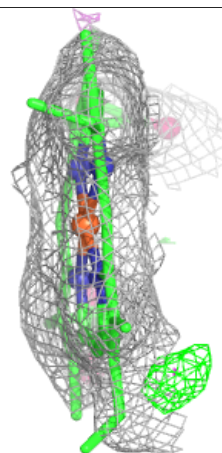
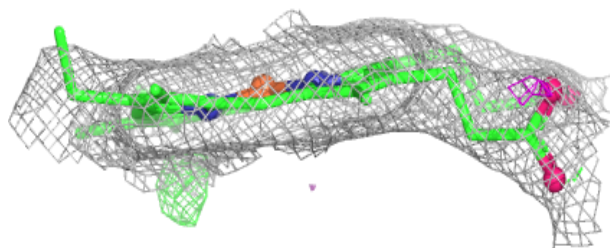
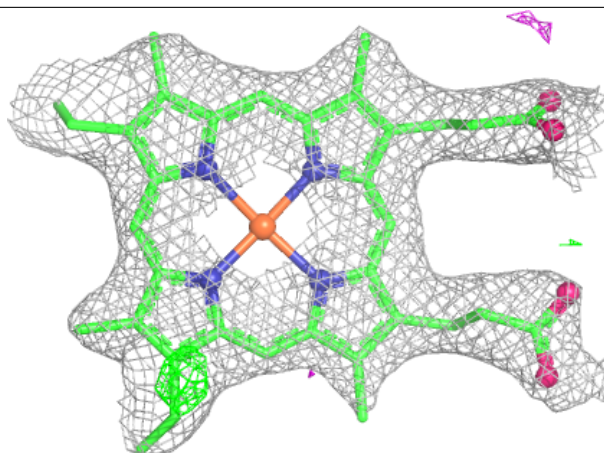
Electron density around HEC X 709:

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



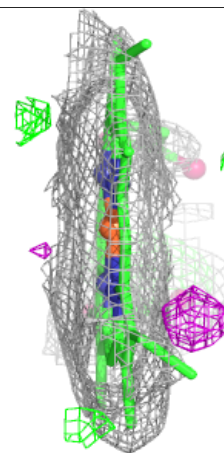
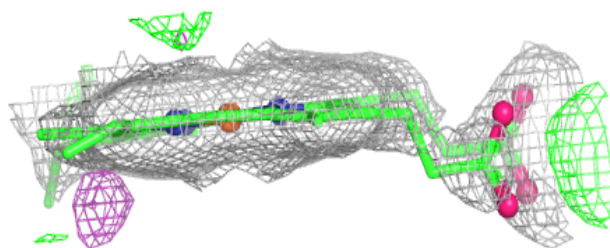
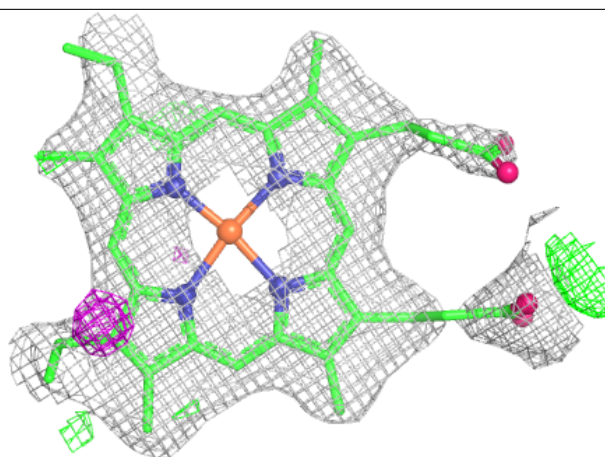
Electron density around HEC X 710:

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



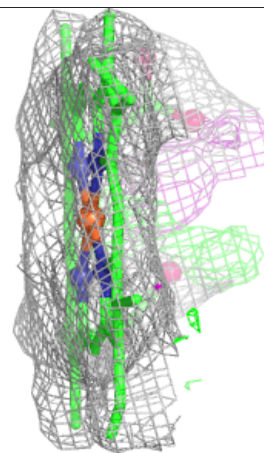
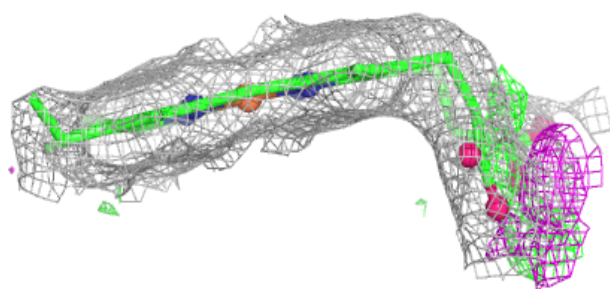
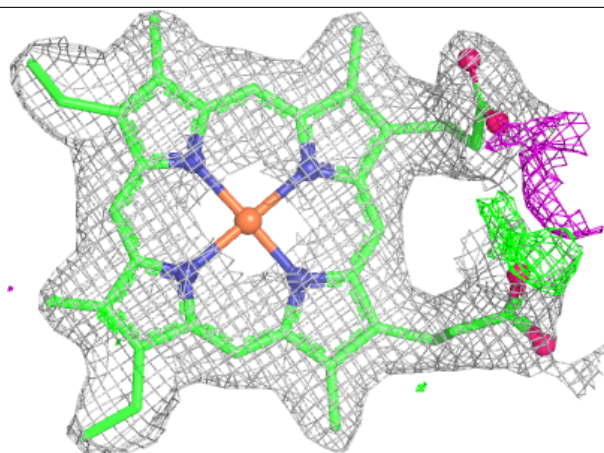
Electron density around HEC X 705:

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



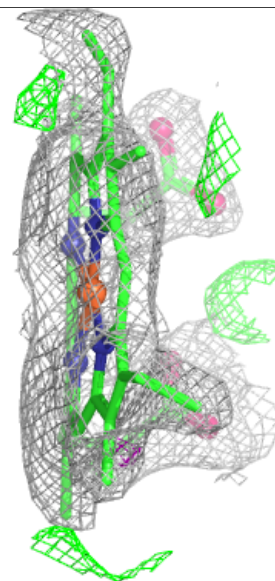
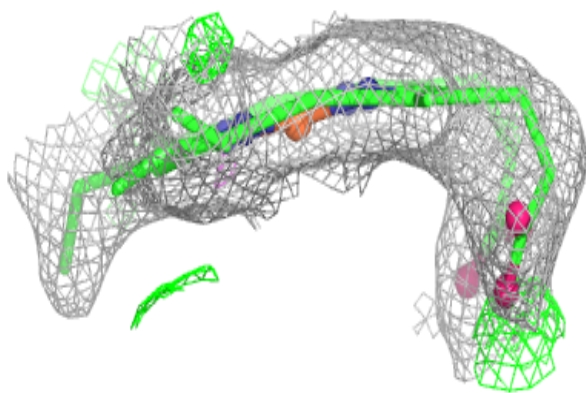
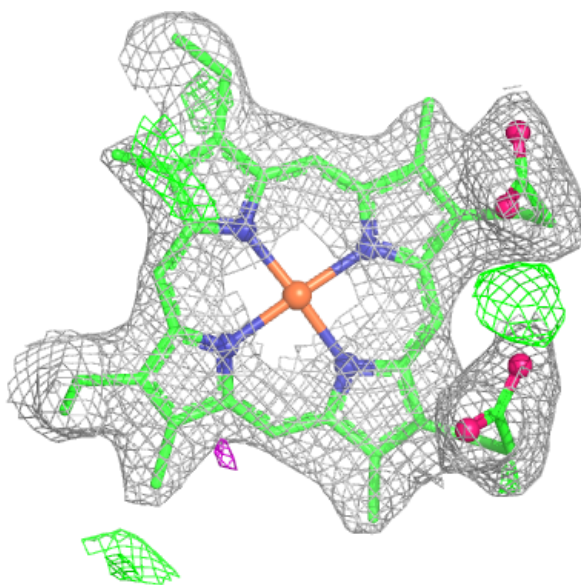
Electron density around HEC X 719:

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and green (positive)



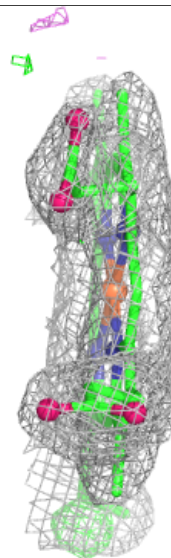
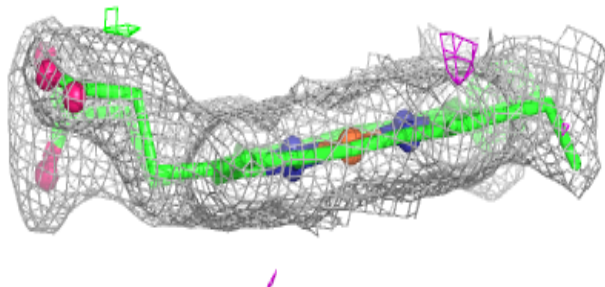
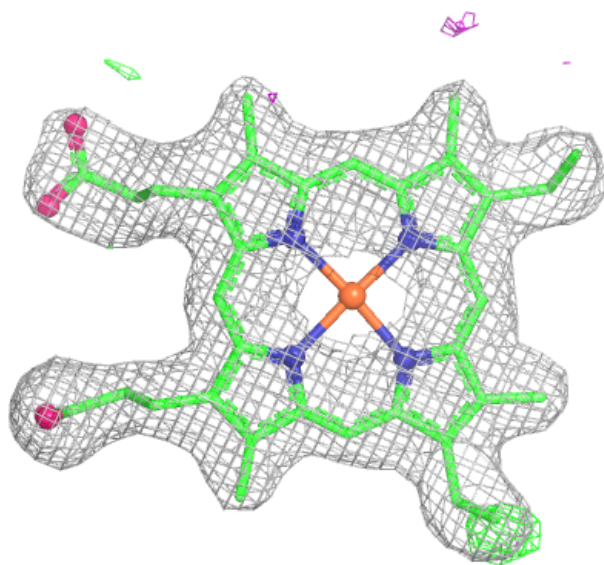
Electron density around HEC X 712:

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



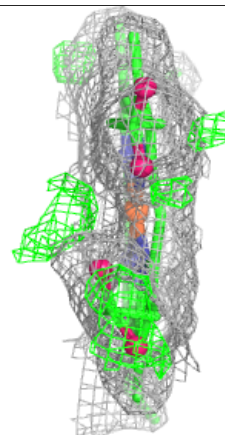
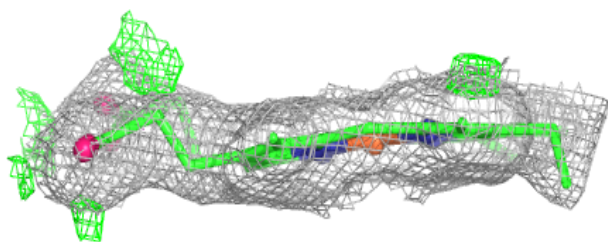
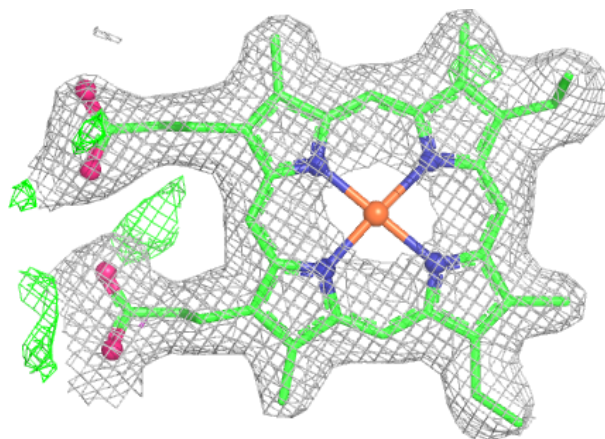
Electron density around HEC X 714:

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



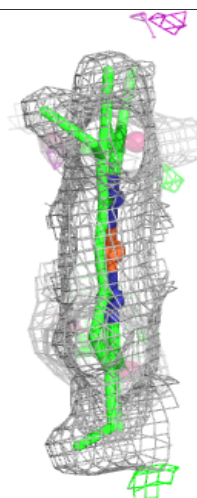
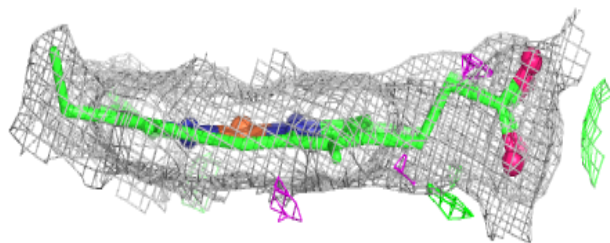
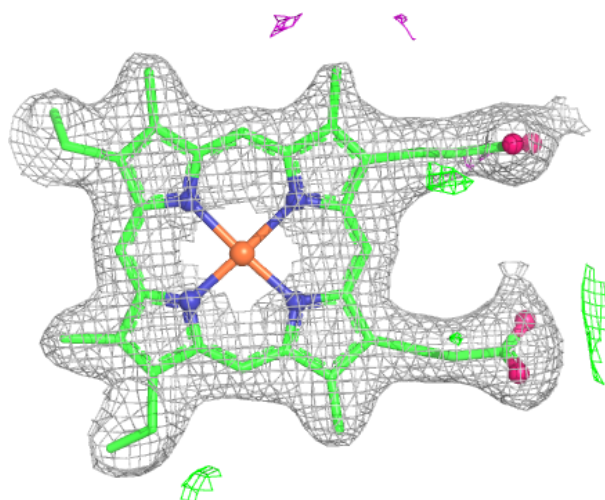
Electron density around HEC X 715:

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



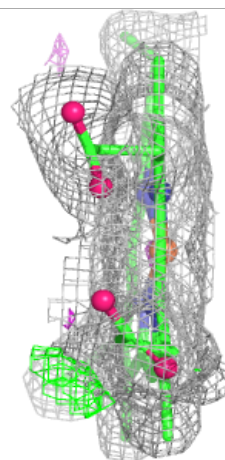
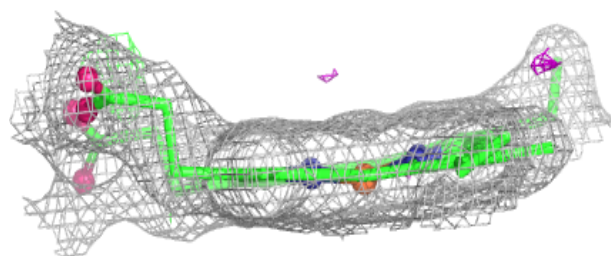
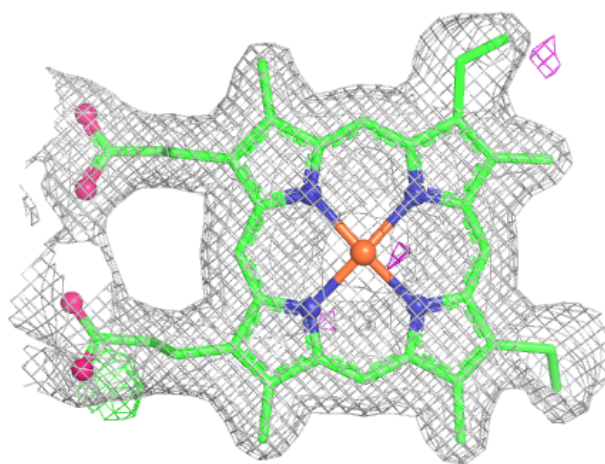
Electron density around HEC X 711:

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and green (positive)



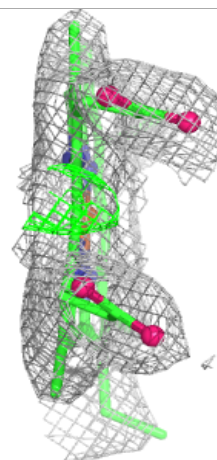
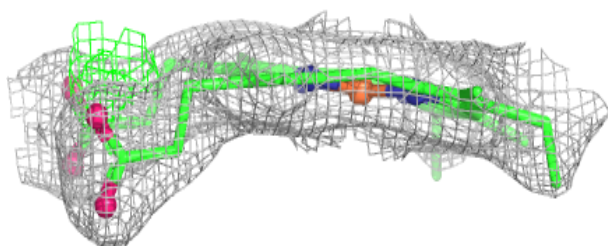
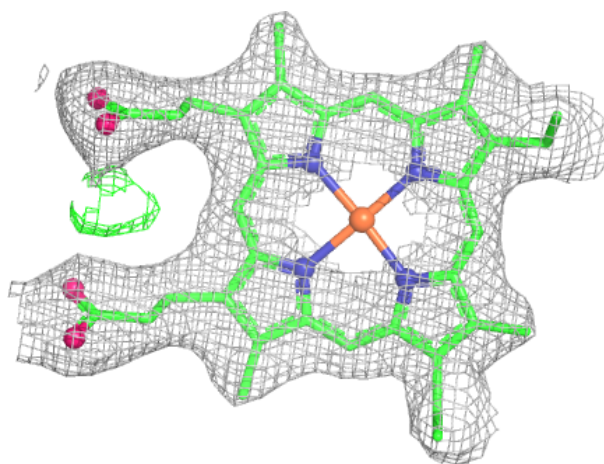
Electron density around HEC X 718:

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



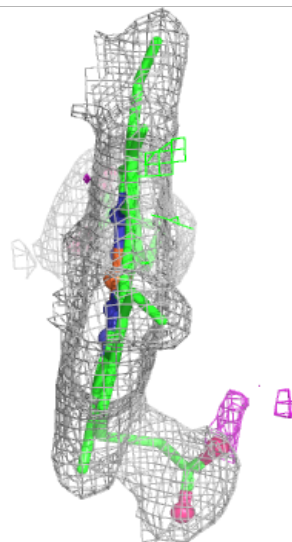
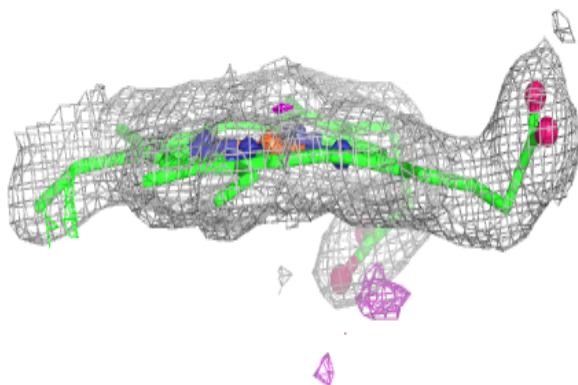
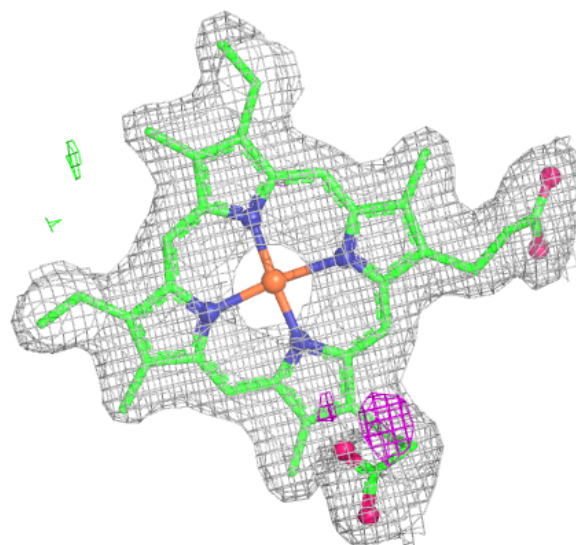
Electron density around HEC X 707:

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and green (positive)



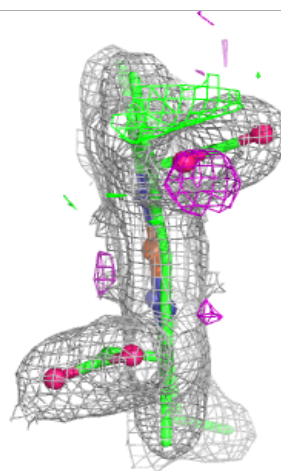
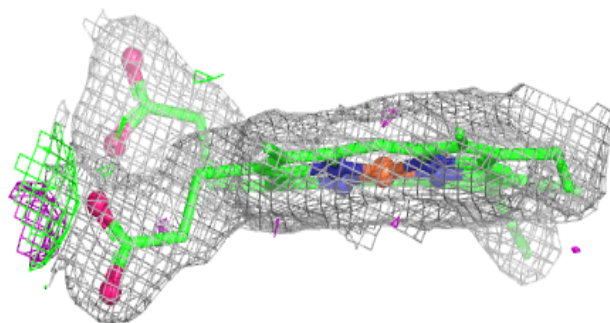
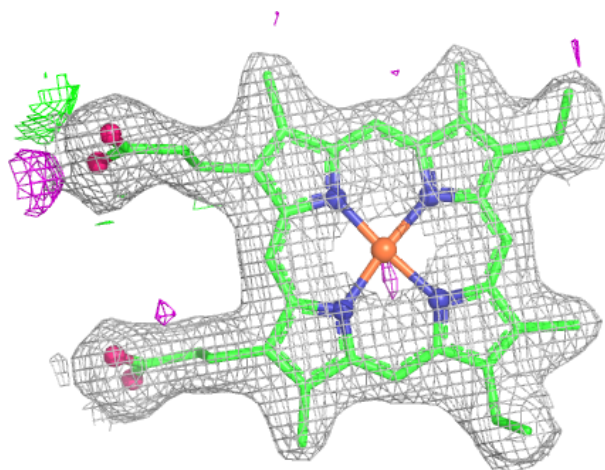
Electron density around HEC X 713:

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



Electron density around HEC X 716:

$2mF_o-DF_c$ (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.