



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 07:24 PM EDT

PDB ID : 3LG1 / pdb_00003lg1
Title : Structure of the Thioalkalivibrio nitratreducens cytochrome c nitrite reductase reduced by sodium borohydride (in complex with sulfite)
Authors : Trofimov, A.A.; Polyakov, K.M.; Boyko, K.M.; Filimonenkov, A.A.; Dorovatsky, P.V.; Tikhonova, T.V.; Popov, V.O.
Deposited on : 2010-01-19
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

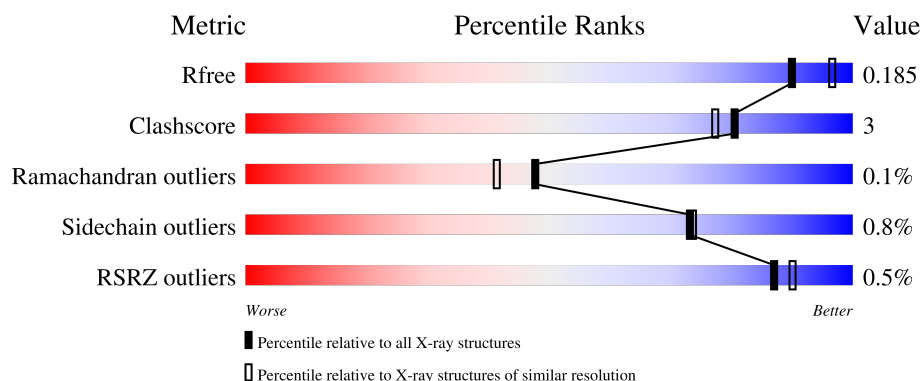
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

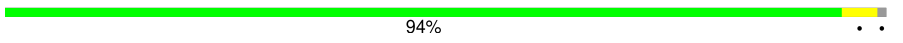
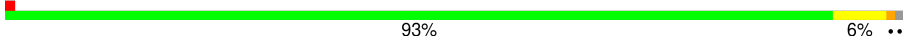
The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	525	 94%
1	B	525	 93% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	1001[A]	X	-	-	-
2	HEC	A	1002	X	-	-	-
2	HEC	A	1003[A]	X	-	-	-
2	HEC	A	1004	X	-	-	-
2	HEC	A	1005	X	-	-	-
2	HEC	A	1006	X	-	-	-
2	HEC	A	1007[A]	X	-	-	-
2	HEC	B	1001	X	-	-	-
2	HEC	B	1002	X	-	-	-
2	HEC	B	1003[A]	X	-	-	-
2	HEC	B	1004	X	-	-	-
2	HEC	B	1005	X	-	-	-
2	HEC	B	1006	X	-	-	-
2	HEC	B	1007[A]	X	-	-	-
7	PG4	A	540	-	-	-	X
7	PG4	A	545	-	-	-	X
7	PG4	A	546	-	-	-	X
7	PG4	B	537	-	-	-	X

2 Entry composition [i](#)

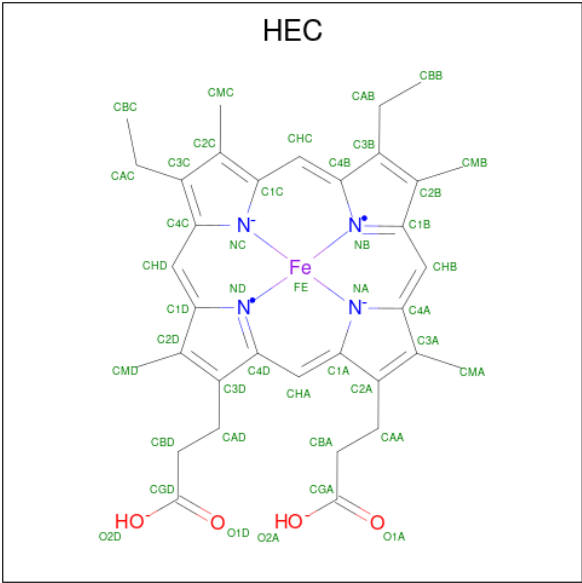
There are 8 unique types of molecules in this entry. The entry contains 10172 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	519	Total	C	N	O	S	0	10	1
			4127	2565	745	780	37			
1	B	519	Total	C	N	O	S	0	12	0
			4159	2579	758	784	38			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



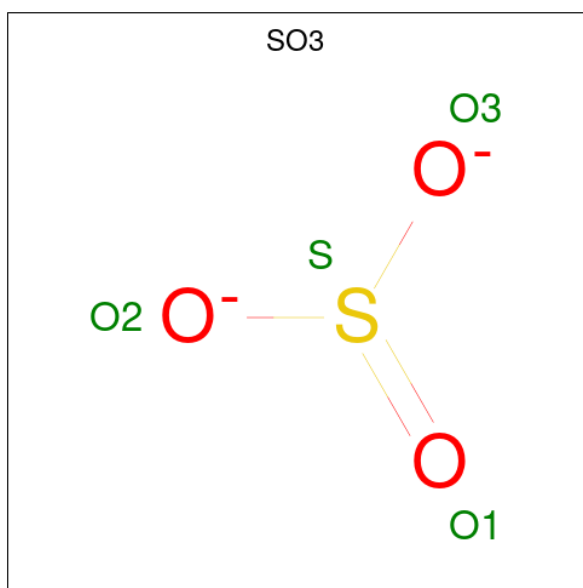
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	1
			43	34	1	4	4		

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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	1
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	1
			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
			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
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



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

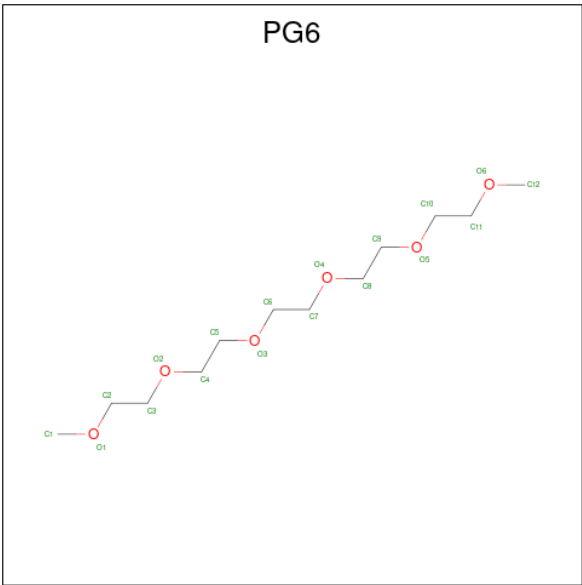
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

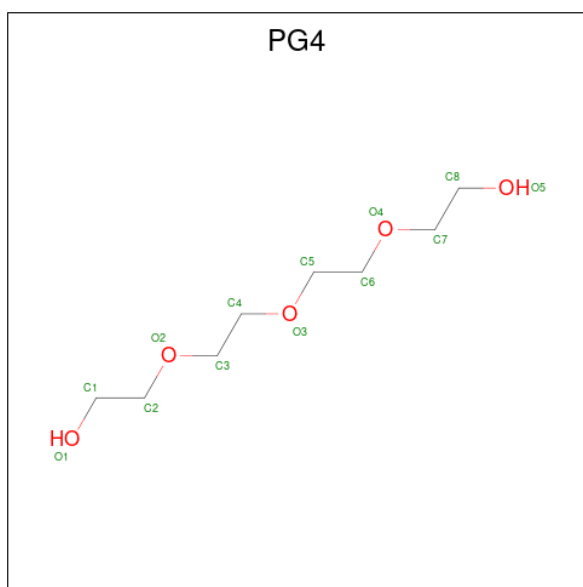
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total Na 5 5	0	0
5	B	3	Total Na 3 3	0	0

- Molecule 6 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]}-ETHANE (CCD ID: PG6) (formula: C₁₂H₂₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			17	11	6		
6	A	1	Total	C	O	0	0
			8	5	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			16	10	6		
6	A	1	Total	C	O	0	0
			10	6	4		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			17	11	6		
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	1
			10	6	4		
6	B	1	Total	C	O	0	0
			8	5	3		
6	B	1	Total	C	O	0	0
			14	9	5		
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	3	1		
7	A	1	Total	C	O	0	0
			6	4	2		
7	A	1	Total	C	O	0	0
			9	6	3		
7	A	1	Total	C	O	0	0
			5	3	2		
7	A	1	Total	C	O	0	0
			7	5	2		
7	A	1	Total	C	O	0	0
			6	4	2		
7	B	1	Total	C	O	0	0
			5	3	2		
7	B	1	Total	C	O	0	0
			6	4	2		
7	B	1	Total	C	O	0	0
			8	6	2		
7	B	1	Total	C	O	0	0
			5	3	2		

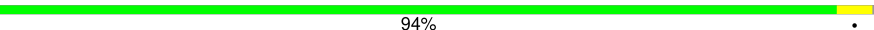
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	503	Total	O	0	0
			503	503		
8	B	471	Total	O	0	0
			471	471		

3 Residue-property plots [i](#)

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.

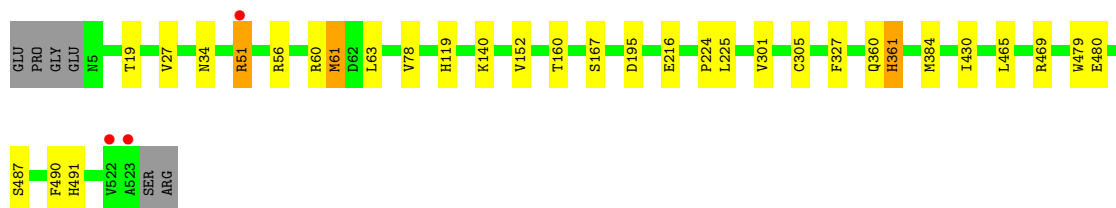
- Molecule 1: Eight-heme nitrite reductase

Chain A:  94% . .



- Molecule 1: Eight-heme nitrite reductase

Chain B:  93% 6% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	192.62Å 192.62Å 192.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 1.95 19.90 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.90-1.95) 99.7 (19.90-1.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.161 , 0.183 0.164 , 0.185	Depositor DCC
R_{free} test set	9268 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.043 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10172	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, SO3, HEC, CA, PG6, NA

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	0.86	0/4294	0.84	0/5825
1	B	0.87	0/4340	0.87	1/5883 (0.0%)
All	All	0.87	0/8634	0.85	1/11708 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	MET	CB-CA-C	-5.35	104.03	111.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4127	0	3834	17	0
1	B	4159	0	3875	21	0
2	A	344	0	160	3	0
2	B	344	0	188	5	0
3	A	8	0	0	0	0
3	B	12	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	5	0	0	0	0
5	B	3	0	0	0	0
6	A	62	0	73	1	0
6	B	69	0	71	3	0
7	A	37	0	38	1	0
7	B	24	0	24	0	0
8	A	503	0	0	4	0
8	B	471	0	0	2	0
All	All	10172	0	8263	44	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 3.

All (44) 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:51[A]:ARG:HH11	1:B:51[A]:ARG:HG3	1.38	0.85
2:B:1002:HEC:HMC1	2:B:1002:HEC:HBC3	1.73	0.70
1:B:51[A]:ARG:HG3	1:B:51[A]:ARG:NH1	2.05	0.66
1:B:167:SER:HB2	1:B:216:GLU:HG2	1.83	0.59
1:B:60:ARG:HH22	6:B:539:PG6:H31	1.68	0.57
2:B:1008:HEC:HBC3	2:B:1008:HEC:HMC1	1.86	0.57
2:A:1002:HEC:HMC1	2:A:1002:HEC:HBC3	1.85	0.57
1:A:108:GLY:HA3	6:A:544:PG6:H31	1.86	0.57
6:B:531:PG6:H111	8:B:896:HOH:O	2.05	0.56
1:A:167:SER:HB2	1:A:216:GLU:HG2	1.88	0.55
1:A:68:THR:HG23	8:A:816:HOH:O	2.07	0.55
1:A:394[B]:VAL:HG12	8:A:1036:HOH:O	2.10	0.51
1:B:51[A]:ARG:NH1	1:B:51[A]:ARG:CG	2.73	0.51
1:B:56[A]:ARG:NH2	1:B:195:ASP:OD1	2.36	0.51
1:A:61[A]:MET:SD	1:A:191:ASP:O	2.70	0.50
1:A:360:GLN:HB3	1:A:361:HIS:CE1	2.47	0.49
1:A:12:MET:HE3	8:A:952:HOH:O	2.14	0.47
1:A:487:SER:HB3	1:A:491:HIS:CE1	2.50	0.47
2:A:1004:HEC:C4D	2:A:1006:HEC:HMD2	2.44	0.47
1:B:61[C]:MET:SD	8:B:748:HOH:O	2.61	0.47
1:A:216:GLU:HG3	8:A:968:HOH:O	2.15	0.46
1:A:174:SER:HA	7:A:538:PG4:H11	1.98	0.46
1:B:487:SER:HB3	1:B:491:HIS:CE1	2.52	0.44
1:B:360:GLN:HB3	1:B:361:HIS:CE1	2.53	0.43
1:B:140:LYS:HG2	1:B:160:THR:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ILE:HG21	1:B:490:PHE:HA	1.99	0.43
1:B:360:GLN:O	1:B:361:HIS:C	2.62	0.43
1:B:34:ASN:HA	6:B:534:PG6:H21	2.01	0.42
1:A:119:HIS:CD2	2:A:1006:HEC:ND	2.88	0.42
1:B:301:VAL:HG21	1:B:327:PHE:CE2	2.55	0.42
1:A:63:LEU:HD12	1:A:63:LEU:N	2.35	0.42
1:B:78:VAL:HG12	1:B:152:VAL:HG21	2.02	0.42
1:A:360:GLN:O	1:A:361:HIS:C	2.63	0.41
1:B:479:TRP:CZ3	1:B:480:GLU:HG3	2.55	0.41
1:A:304:ASN:HB2	1:A:326:HIS:HB3	2.01	0.41
2:B:1002:HEC:HHA	2:B:1002:HEC:HBD2	2.03	0.41
1:B:119:HIS:CD2	2:B:1006:HEC:ND	2.89	0.41
1:B:224:PRO:O	1:B:225:LEU:C	2.63	0.41
1:A:61[A]:MET:HG2	1:A:228:PHE:CZ	2.56	0.41
1:B:63:LEU:HD12	1:B:63:LEU:N	2.36	0.41
1:A:140:LYS:HG2	1:A:160:THR:HG23	2.02	0.40
1:B:305:CYS:CB	2:B:1004:HEC:HMC2	2.52	0.40
1:B:465:LEU:O	1:B:469:ARG:HG3	2.21	0.40
1:A:374:ARG:HA	1:A:374:ARG:NE	2.37	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	528/525 (101%)	503 (95%)	25 (5%)	0	100	100
1	B	530/525 (101%)	503 (95%)	26 (5%)	1 (0%)	43	36
All	All	1058/1050 (101%)	1006 (95%)	51 (5%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	361	HIS

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	A	442/443 (100%)	439 (99%)	3 (1%)	76	76
1	B	449/443 (101%)	441 (98%)	8 (2%)	51	47
All	All	891/886 (101%)	880 (99%)	11 (1%)	73	61

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	THR
1	A	220	ASP
1	A	488	VAL
1	B	19[A]	THR
1	B	19[B]	THR
1	B	27	VAL
1	B	51[A]	ARG
1	B	51[B]	ARG
1	B	61[A]	MET
1	B	61[B]	MET
1	B	61[C]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	388	GLN
1	B	175	GLN
1	B	223	HIS
1	B	275	GLN
1	B	413	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 55 ligands modelled in this entry, 12 are monoatomic - leaving 43 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$
7	PG4	A	533	6	3,3,12	0.65	0	2,2,11	0.41	0
6	PG6	A	543	1	9,9,17	0.51	0	8,8,16	0.30	0
2	HEC	A	1008	1	50,50,50	1.83	7 (14%)	68,82,82	1.45	10 (14%)
2	HEC	B	1005	1	50,50,50	1.54	8 (16%)	68,82,82	1.18	5 (7%)
2	HEC	A	1006	1,4	50,50,50	1.69	9 (18%)	68,82,82	1.36	8 (11%)
6	PG6	B	541	-	13,13,17	0.62	0	12,12,16	0.39	0
3	SO3	B	533	-	1,3,3	0.63	0	0,3,3	-	-
3	SO3	A	537	-	1,3,3	0.30	0	0,3,3	-	-
3	SO3	B	526	2	1,3,3	0.30	0	0,3,3	-	-
2	HEC	B	1001	1	50,50,50	1.92	10 (20%)	68,82,82	1.49	9 (13%)
2	HEC	B	1006	1,4	50,50,50	1.74	9 (18%)	68,82,82	1.17	5 (7%)
2	HEC	A	1004	1,3,8	50,50,50	1.58	7 (14%)	68,82,82	1.24	5 (7%)
7	PG4	B	543	-	4,4,12	0.47	0	3,3,11	0.34	0
2	HEC	B	1008	1	50,50,50	1.71	8 (16%)	68,82,82	1.45	10 (14%)
6	PG6	B	531	5,7	16,16,17	0.91	0	15,15,16	1.08	1 (6%)
2	HEC	A	1002	1	50,50,50	1.85	11 (22%)	68,82,82	1.27	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	B	1004	1,3,8	50,50,50	1.67	9 (18%)	68,82,82	1.24	6 (8%)
6	PG6	A	542	-	15,15,17	0.53	0	14,14,16	0.27	0
2	HEC	B	1002	1	50,50,50	1.81	11 (22%)	68,82,82	1.37	6 (8%)
6	PG6	B	542	1	9,9,17	0.45	0	8,8,16	0.35	0
7	PG4	A	538	-	5,5,12	0.50	0	4,4,11	0.27	0
6	PG6	B	534	-	9,9,17	0.44	0	8,8,16	0.42	0
7	PG4	A	546	-	5,5,12	0.48	0	4,4,11	0.12	0
6	PG6	A	544	-	3,3,17	0.32	0	2,2,16	0.22	0
6	PG6	A	532	5,7	16,16,17	0.83	0	15,15,16	1.13	2 (13%)
3	SO3	B	536	-	1,3,3	0.50	0	0,3,3	-	-
7	PG4	A	545	-	6,6,12	0.49	0	5,5,11	0.40	0
6	PG6	B	539	-	7,7,17	0.58	0	6,6,16	0.42	0
2	HEC	A	1005	1	50,50,50	1.56	8 (16%)	68,82,82	1.16	6 (8%)
7	PG4	B	537	-	5,5,12	0.46	0	4,4,11	0.36	0
7	PG4	B	540	-	7,7,12	0.65	0	6,6,11	0.34	0
3	SO3	A	526	2	1,3,3	0.30	0	0,3,3	-	-
7	PG4	A	541	-	4,4,12	0.38	0	3,3,11	0.53	0
7	PG4	A	540	-	8,8,12	0.49	0	7,7,11	0.12	0
7	PG4	B	532	6	4,4,12	0.46	0	3,3,11	0.28	0
6	PG6	A	539	-	6,6,17	0.27	0	5,5,16	0.62	0
6	PG6	A	534	-	7,7,17	0.60	0	6,6,16	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG4	A	533	6	-	0/0/1/10	-
6	PG6	A	543	1	-	1/7/7/15	-
2	HEC	A	1008	1	-	6/14/54/54	-
2	HEC	A	1003[A]	-	1/1/3/7	-	-
2	HEC	B	1005	1	1/1/3/7	8/14/54/54	-
2	HEC	A	1006	1,4	1/1/3/7	4/14/54/54	-
6	PG6	B	541	-	-	3/11/11/15	-
2	HEC	B	1001	1	1/1/3/7	8/14/54/54	-
2	HEC	B	1006	1,4	1/1/3/7	4/14/54/54	-
2	HEC	B	1003[A]	-	1/1/3/7	-	-
2	HEC	A	1004	1,3,8	1/1/3/7	7/14/54/54	-
7	PG4	B	543	-	-	1/2/2/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	B	1008	1	-	8/14/54/54	-
6	PG6	B	531	5,7	-	7/14/14/15	-
2	HEC	A	1002	1	1/1/3/7	6/14/54/54	-
2	HEC	A	1007[A]	-	1/1/3/7	-	-
2	HEC	B	1004	1,3,8	1/1/3/7	7/14/54/54	-
6	PG6	A	542	-	-	5/13/13/15	-
2	HEC	A	1001[A]	-	1/1/3/7	-	-
2	HEC	B	1002	1	1/1/3/7	6/14/54/54	-
6	PG6	B	542	1	-	1/7/7/15	-
7	PG4	A	538	-	-	3/3/3/10	-
6	PG6	B	534	-	-	2/7/7/15	-
2	HEC	B	1007[A]	-	1/1/3/7	-	-
7	PG4	A	546	-	-	3/3/3/10	-
6	PG6	A	544	-	-	0/1/1/15	-
6	PG6	A	532	5,7	-	7/14/14/15	-
7	PG4	A	545	-	-	4/4/4/10	-
6	PG6	B	539	-	-	4/5/5/15	-
2	HEC	A	1005	1	1/1/3/7	8/14/54/54	-
7	PG4	B	537	-	-	3/3/3/10	-
7	PG4	B	540	-	-	1/5/5/10	-
7	PG4	A	541	-	-	1/2/2/10	-
7	PG4	A	540	-	-	3/6/6/10	-
7	PG4	B	532	6	-	0/2/2/10	-
6	PG6	A	539	-	-	1/4/4/15	-
6	PG6	A	534	-	-	1/5/5/15	-

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1008	HEC	C3D-C2D	7.61	1.53	1.36
2	B	1002	HEC	C3D-C2D	7.39	1.52	1.36
2	A	1002	HEC	C3D-C2D	7.37	1.52	1.36
2	B	1001	HEC	C3D-C2D	7.34	1.52	1.36
2	B	1008	HEC	C3D-C2D	7.30	1.52	1.36
2	B	1006	HEC	C3D-C2D	6.87	1.51	1.36
2	B	1004	HEC	C3D-C2D	6.65	1.51	1.36
2	A	1005	HEC	C3D-C2D	6.63	1.51	1.36
2	A	1006	HEC	C3D-C2D	6.40	1.50	1.36
2	B	1005	HEC	C3D-C2D	6.21	1.50	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1004	HEC	C3D-C2D	6.21	1.50	1.36
2	B	1001	HEC	FE-NA	5.02	2.11	1.95
2	A	1006	HEC	FE-NC	4.85	2.11	1.95
2	A	1002	HEC	FE-ND	4.73	2.09	1.94
2	B	1001	HEC	FE-NC	4.52	2.10	1.95
2	B	1006	HEC	FE-NC	4.52	2.10	1.95
2	A	1008	HEC	FE-NA	4.34	2.09	1.95
2	A	1008	HEC	FE-ND	4.16	2.07	1.94
2	B	1001	HEC	FE-NB	4.15	2.07	1.94
2	B	1002	HEC	FE-NA	4.03	2.08	1.95
2	B	1002	HEC	FE-NC	3.78	2.07	1.95
2	B	1005	HEC	CMA-C3A	3.35	1.57	1.50
2	B	1002	HEC	FE-ND	3.32	2.05	1.94
2	B	1008	HEC	FE-NC	3.28	2.06	1.95
2	B	1001	HEC	FE-ND	3.26	2.04	1.94
2	B	1004	HEC	FE-ND	3.26	2.04	1.94
2	B	1008	HEC	FE-ND	3.24	2.04	1.94
2	B	1008	HEC	CMC-C2C	3.20	1.57	1.50
2	A	1005	HEC	CMA-C3A	3.19	1.57	1.50
2	A	1004	HEC	FE-ND	3.16	2.04	1.94
2	B	1004	HEC	FE-NB	3.12	2.04	1.94
2	A	1002	HEC	FE-NC	3.09	2.05	1.95
2	B	1004	HEC	CMC-C2C	3.04	1.57	1.50
2	B	1002	HEC	FE-NB	3.03	2.04	1.94
2	A	1008	HEC	CMC-C2C	3.02	1.57	1.50
2	A	1004	HEC	CAB-C3B	3.01	1.58	1.51
2	A	1002	HEC	CMB-C2B	2.96	1.56	1.50
2	B	1006	HEC	CMC-C2C	2.95	1.56	1.50
2	B	1004	HEC	CAB-C3B	2.91	1.58	1.51
2	B	1006	HEC	FE-NA	2.91	2.04	1.95
2	A	1008	HEC	CAC-C3C	2.86	1.58	1.51
2	A	1002	HEC	FE-NA	2.84	2.04	1.95
2	B	1008	HEC	FE-NA	2.82	2.04	1.95
2	A	1004	HEC	FE-NC	2.80	2.04	1.95
2	B	1008	HEC	CMD-C2D	2.80	1.56	1.50
2	A	1006	HEC	CMB-C2B	2.77	1.56	1.50
2	B	1006	HEC	CMB-C2B	2.75	1.56	1.50
2	B	1005	HEC	CMB-C2B	2.75	1.56	1.50
2	A	1005	HEC	CAC-C3C	2.73	1.58	1.51
2	A	1004	HEC	CMD-C2D	2.70	1.56	1.50
2	B	1006	HEC	CAB-C3B	2.68	1.57	1.51
2	A	1002	HEC	FE-NB	2.66	2.03	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	HEC	CMA-C3A	2.64	1.56	1.50
2	A	1006	HEC	CMC-C2C	2.58	1.56	1.50
2	A	1006	HEC	CMA-C3A	2.55	1.56	1.50
2	B	1005	HEC	CAC-C3C	2.54	1.57	1.51
2	A	1002	HEC	CAB-C3B	2.53	1.57	1.51
2	A	1005	HEC	CMB-C2B	2.53	1.56	1.50
2	B	1001	HEC	CMB-C2B	2.53	1.55	1.50
2	B	1001	HEC	CMA-C3A	2.49	1.55	1.50
2	B	1005	HEC	CMD-C2D	2.47	1.55	1.50
2	A	1006	HEC	FE-NA	2.45	2.03	1.95
2	B	1004	HEC	FE-NC	2.45	2.03	1.95
2	A	1008	HEC	CMA-C3A	2.42	1.55	1.50
2	A	1008	HEC	CMD-C2D	2.40	1.55	1.50
2	A	1002	HEC	CMD-C2D	2.40	1.55	1.50
2	A	1005	HEC	O2D-CGD	-2.40	1.22	1.30
2	A	1006	HEC	CAB-C3B	2.39	1.57	1.51
2	A	1005	HEC	FE-ND	2.39	2.02	1.94
2	B	1005	HEC	CMC-C2C	2.39	1.55	1.50
2	B	1005	HEC	FE-ND	2.34	2.02	1.94
2	B	1004	HEC	FE-NA	2.34	2.02	1.95
2	A	1002	HEC	CMC-C2C	2.33	1.55	1.50
2	A	1002	HEC	CAC-C3C	2.33	1.57	1.51
2	B	1001	HEC	CAC-C3C	2.32	1.57	1.51
2	A	1005	HEC	CAA-C2A	2.31	1.57	1.51
2	B	1002	HEC	CAB-C3B	2.30	1.57	1.51
2	B	1002	HEC	CMB-C2B	2.29	1.55	1.50
2	A	1006	HEC	CMD-C2D	2.28	1.55	1.50
2	B	1002	HEC	CMC-C2C	2.28	1.55	1.50
2	B	1008	HEC	CMA-C3A	2.28	1.55	1.50
2	B	1006	HEC	CMA-C3A	2.28	1.55	1.50
2	B	1002	HEC	CMD-C2D	2.25	1.55	1.50
2	B	1008	HEC	CAC-C3C	2.23	1.56	1.51
2	B	1002	HEC	CAC-C3C	2.23	1.56	1.51
2	A	1004	HEC	CMC-C2C	2.23	1.55	1.50
2	A	1005	HEC	CMC-C2C	2.22	1.55	1.50
2	B	1005	HEC	FE-NB	2.20	2.01	1.94
2	B	1004	HEC	CMB-C2B	2.20	1.55	1.50
2	B	1002	HEC	CMA-C3A	2.18	1.55	1.50
2	B	1001	HEC	CAB-C3B	2.12	1.56	1.51
2	B	1006	HEC	CAC-C3C	2.09	1.56	1.51
2	B	1006	HEC	CMD-C2D	2.06	1.55	1.50
2	A	1004	HEC	FE-NB	2.04	2.01	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1006	HEC	C4C-C3C	2.04	1.48	1.44
2	B	1001	HEC	CMC-C2C	2.01	1.54	1.50
2	B	1004	HEC	CMD-C2D	2.01	1.54	1.50

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1008	HEC	C1D-ND-C4D	5.62	111.87	105.21
2	B	1008	HEC	C1D-ND-C4D	5.34	111.53	105.21
2	B	1001	HEC	C1D-ND-C4D	5.29	111.47	105.21
2	B	1002	HEC	CMC-C2C-C1C	-4.23	118.98	125.42
2	B	1002	HEC	C1D-ND-C4D	3.69	109.57	105.21
2	B	1002	HEC	CAA-CBA-CGA	-3.66	103.95	113.67
2	B	1004	HEC	C1D-ND-C4D	3.54	109.40	105.21
2	A	1005	HEC	C1D-ND-C4D	3.51	109.36	105.21
2	A	1002	HEC	C1D-ND-C4D	3.44	109.28	105.21
2	A	1002	HEC	CAA-CBA-CGA	-3.37	104.73	113.67
2	B	1001	HEC	CBD-CAD-C3D	-3.20	103.69	112.53
2	B	1005	HEC	C1D-ND-C4D	3.13	108.92	105.21
2	A	1008	HEC	CBB-CAB-C3B	-3.10	104.01	112.42
2	B	1008	HEC	CHA-C4D-ND	3.05	127.71	124.42
2	A	1006	HEC	CMC-C2C-C1C	-3.05	120.77	125.42
2	B	1001	HEC	CHD-C1D-ND	3.05	128.14	124.37
2	B	1008	HEC	CBD-CAD-C3D	-3.01	104.20	112.53
2	A	1004	HEC	CMB-C2B-C1B	-3.01	120.33	125.03
2	A	1006	HEC	C2A-C1A-NA	-2.98	107.45	110.32
2	A	1004	HEC	CAD-C3D-C4D	2.98	129.88	124.70
2	A	1002	HEC	CMC-C2C-C1C	-2.93	120.96	125.42
2	A	1008	HEC	C3D-C4D-ND	-2.91	107.53	110.35
2	B	1001	HEC	C2A-C1A-NA	-2.89	107.53	110.32
2	B	1004	HEC	CAD-C3D-C4D	2.88	129.71	124.70
2	A	1004	HEC	C1D-ND-C4D	2.84	108.57	105.21
2	B	1004	HEC	CHA-C1A-NA	2.80	127.50	124.45
2	B	1001	HEC	CBA-CAA-C2A	-2.79	104.81	112.53
2	B	1004	HEC	CMC-C2C-C1C	-2.78	121.18	125.42
2	B	1006	HEC	CMC-C2C-C1C	-2.75	121.24	125.42
2	A	1006	HEC	CBB-CAB-C3B	-2.68	105.15	112.42
2	B	1002	HEC	C2A-C1A-NA	-2.65	107.77	110.32
2	A	1005	HEC	CMC-C2C-C1C	-2.63	121.41	125.42
2	A	1008	HEC	CBD-CAD-C3D	-2.63	105.25	112.53
2	A	1008	HEC	CMC-C2C-C1C	-2.63	121.42	125.42
2	A	1002	HEC	C2A-C1A-NA	-2.61	107.80	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	HEC	C1B-C2B-C3B	2.61	109.72	106.98
2	B	1008	HEC	CBB-CAB-C3B	-2.57	105.45	112.42
2	B	1005	HEC	CMC-C2C-C1C	-2.56	121.51	125.42
2	B	1001	HEC	CHB-C1B-NB	2.50	127.11	124.42
2	B	1008	HEC	C3D-C4D-ND	-2.44	107.99	110.35
2	B	1006	HEC	C1D-ND-C4D	2.42	108.08	105.21
2	A	1008	HEC	C2A-C1A-NA	-2.42	107.98	110.32
2	A	1008	HEC	CHB-C1B-NB	2.42	127.03	124.42
2	B	1005	HEC	CMD-C2D-C1D	2.40	128.79	125.03
6	A	532	PG6	C6-O3-C5	2.40	123.77	113.26
2	B	1004	HEC	CMB-C2B-C1B	-2.39	121.30	125.03
2	B	1001	HEC	C4B-NB-C1B	2.35	107.98	105.21
2	A	1004	HEC	CMC-C2C-C1C	-2.33	121.87	125.42
2	A	1005	HEC	CMD-C2D-C1D	2.32	128.67	125.03
2	B	1006	HEC	CAD-C3D-C4D	2.32	128.74	124.70
2	B	1006	HEC	CBB-CAB-C3B	-2.30	106.19	112.42
2	B	1008	HEC	C2A-C1A-NA	-2.30	108.11	110.32
2	A	1006	HEC	C4C-NC-C1C	2.29	109.55	105.82
2	B	1006	HEC	C2A-C1A-NA	-2.26	108.14	110.32
2	A	1006	HEC	CBD-CAD-C3D	-2.25	106.30	112.53
2	B	1005	HEC	CAD-C3D-C4D	2.21	128.56	124.70
2	A	1005	HEC	CBD-CAD-C3D	-2.18	106.49	112.53
2	B	1008	HEC	O2A-CGA-CBA	2.18	120.89	114.00
2	B	1001	HEC	C4A-NA-C1A	2.18	109.37	105.82
2	B	1005	HEC	CBD-CAD-C3D	-2.16	106.57	112.53
2	B	1004	HEC	C2A-C1A-NA	-2.15	108.25	110.32
2	A	1006	HEC	CMC-C2C-C3C	2.14	130.16	125.62
2	B	1001	HEC	CMC-C2C-C1C	-2.14	122.16	125.42
2	A	1006	HEC	CBA-CAA-C2A	-2.14	106.62	112.53
2	A	1008	HEC	CBC-CAC-C3C	2.13	118.21	112.42
6	B	531	PG6	C8-O4-C7	2.12	122.53	113.26
2	A	1005	HEC	CBB-CAB-C3B	-2.11	106.69	112.42
6	A	532	PG6	C8-O4-C7	2.07	122.34	113.26
2	B	1008	HEC	CMD-C2D-C1D	2.07	128.27	125.03
2	A	1004	HEC	CHD-C1D-ND	2.06	126.92	124.37
2	A	1008	HEC	C1D-C2D-C3D	-2.06	104.81	106.98
2	A	1002	HEC	CHA-C1A-NA	2.06	126.69	124.45
2	A	1002	HEC	C3C-C4C-NC	-2.05	107.88	110.15
2	A	1008	HEC	CHD-C1D-ND	2.04	126.89	124.37
2	A	1005	HEC	CAD-CBD-CGD	-2.04	108.25	113.67
2	B	1002	HEC	CHB-C1B-NB	2.04	126.62	124.42
2	B	1008	HEC	CHD-C1D-ND	2.04	126.89	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	HEC	CHB-C1B-NB	2.03	126.61	124.42
2	B	1008	HEC	O1A-CGA-CBA	-2.02	116.67	123.09
2	A	1006	HEC	C1D-ND-C4D	2.00	107.58	105.21

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1004	HEC	NA
2	A	1005	HEC	NA
2	A	1006	HEC	NA
2	A	1007[A]	HEC	NA
2	A	1002	HEC	NA
2	A	1003[A]	HEC	NA
2	A	1001[A]	HEC	NA
2	B	1004	HEC	NA
2	B	1005	HEC	NA
2	B	1006	HEC	NA
2	B	1007[A]	HEC	NA
2	B	1002	HEC	NA
2	B	1003[A]	HEC	NA
2	B	1001	HEC	NA

All (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1002	HEC	C2C-C3C-CAC-CBC
2	B	1002	HEC	C2C-C3C-CAC-CBC
2	A	1002	HEC	C4C-C3C-CAC-CBC
2	B	1002	HEC	C4C-C3C-CAC-CBC
2	B	1008	HEC	C2C-C3C-CAC-CBC
7	A	546	PG4	C1-C2-O2-C3
2	A	1004	HEC	C2B-C3B-CAB-CBB
2	B	1008	HEC	C2B-C3B-CAB-CBB
2	B	1004	HEC	C2C-C3C-CAC-CBC
7	A	545	PG4	O2-C3-C4-O3
2	A	1008	HEC	C2B-C3B-CAB-CBB
2	A	1005	HEC	C2C-C3C-CAC-CBC
2	B	1001	HEC	C2C-C3C-CAC-CBC
2	B	1008	HEC	C4C-C3C-CAC-CBC
2	B	1004	HEC	C2B-C3B-CAB-CBB
6	A	542	PG6	O1-C2-C3-O2
6	A	542	PG6	O5-C10-C11-O6

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Mol	Chain	Res	Type	Atoms
6	A	543	PG6	O3-C6-C7-O4
7	A	545	PG4	C6-C5-O3-C4
2	B	1001	HEC	C2B-C3B-CAB-CBB
2	B	1004	HEC	C4C-C3C-CAC-CBC
2	B	1001	HEC	C4C-C3C-CAC-CBC
7	A	540	PG4	O3-C5-C6-O4
2	A	1008	HEC	C2C-C3C-CAC-CBC
2	A	1004	HEC	C4B-C3B-CAB-CBB
2	B	1005	HEC	C2B-C3B-CAB-CBB
7	A	538	PG4	O1-C1-C2-O2
6	A	542	PG6	O4-C8-C9-O5
2	A	1005	HEC	C4C-C3C-CAC-CBC
6	B	531	PG6	O5-C10-C11-O6
7	A	546	PG4	O1-C1-C2-O2
2	B	1006	HEC	C2B-C3B-CAB-CBB
6	B	539	PG6	O2-C4-C5-O3
7	A	541	PG4	O1-C1-C2-O2
7	B	537	PG4	O1-C1-C2-O2
2	B	1006	HEC	C2C-C3C-CAC-CBC
7	B	537	PG4	C4-C3-O2-C2
2	A	1004	HEC	C2C-C3C-CAC-CBC
2	B	1004	HEC	C4B-C3B-CAB-CBB
2	B	1005	HEC	C2C-C3C-CAC-CBC
6	A	539	PG6	O2-C4-C5-O3
6	B	539	PG6	O1-C2-C3-O2
2	A	1008	HEC	C4C-C3C-CAC-CBC
7	A	546	PG4	C4-C3-O2-C2
2	A	1005	HEC	C2B-C3B-CAB-CBB
7	A	540	PG4	O4-C7-C8-O5
2	A	1006	HEC	C2B-C3B-CAB-CBB
2	B	1005	HEC	C4C-C3C-CAC-CBC
2	B	1001	HEC	C4B-C3B-CAB-CBB
2	A	1008	HEC	C4B-C3B-CAB-CBB
6	A	532	PG6	C4-C5-O3-C6
6	A	534	PG6	C2-C3-O2-C4
6	A	532	PG6	C5-C4-O2-C3
7	B	540	PG4	C4-C3-O2-C2
6	A	532	PG6	O4-C8-C9-O5
2	A	1004	HEC	C4C-C3C-CAC-CBC
2	B	1006	HEC	C4C-C3C-CAC-CBC
6	B	531	PG6	C8-C9-O5-C10
6	B	541	PG6	O1-C2-C3-O2

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Mol	Chain	Res	Type	Atoms
6	B	531	PG6	C5-C4-O2-C3
2	B	1008	HEC	C4B-C3B-CAB-CBB
7	A	545	PG4	C3-C4-O3-C5
6	B	542	PG6	O1-C2-C3-O2
7	B	543	PG4	C1-C2-O2-C3
6	A	532	PG6	C8-C9-O5-C10
6	B	531	PG6	C7-C6-O3-C5
7	A	545	PG4	C4-C3-O2-C2
7	A	540	PG4	C3-C4-O3-C5
6	B	531	PG6	C6-C7-O4-C8
6	A	542	PG6	C11-C10-O5-C9
2	B	1005	HEC	C4B-C3B-CAB-CBB
2	A	1005	HEC	C4B-C3B-CAB-CBB
2	B	1004	HEC	C2A-CAA-CBA-CGA
2	A	1002	HEC	C2B-C3B-CAB-CBB
2	A	1004	HEC	CAA-CBA-CGA-O1A
2	A	1005	HEC	CAA-CBA-CGA-O2A
6	A	532	PG6	C7-C6-O3-C5
2	B	1002	HEC	CAA-CBA-CGA-O1A
2	A	1005	HEC	CAA-CBA-CGA-O1A
2	A	1006	HEC	C4C-C3C-CAC-CBC
7	B	537	PG4	C1-C2-O2-C3
2	B	1004	HEC	CAA-CBA-CGA-O1A
2	B	1006	HEC	C4B-C3B-CAB-CBB
2	B	1005	HEC	CAA-CBA-CGA-O2A
6	A	532	PG6	O5-C10-C11-O6
2	A	1002	HEC	CAA-CBA-CGA-O1A
2	A	1004	HEC	CAA-CBA-CGA-O2A
2	B	1005	HEC	CAA-CBA-CGA-O1A
6	B	534	PG6	C7-C6-O3-C5
2	B	1004	HEC	CAA-CBA-CGA-O2A
6	B	531	PG6	C4-C5-O3-C6
2	A	1002	HEC	CAA-CBA-CGA-O2A
2	A	1008	HEC	CAD-CBD-CGD-O1D
2	B	1002	HEC	CAA-CBA-CGA-O2A
6	B	539	PG6	C5-C4-O2-C3
6	B	541	PG6	C2-C3-O2-C4
6	B	534	PG6	C5-C4-O2-C3
6	B	531	PG6	C2-C3-O2-C4
2	A	1008	HEC	CAD-CBD-CGD-O2D
6	A	542	PG6	C5-C4-O2-C3
7	A	538	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
2	B	1001	HEC	CAD-CBD-CGD-O2D
2	B	1002	HEC	C2B-C3B-CAB-CBB
2	B	1001	HEC	CAD-CBD-CGD-O1D
7	A	538	PG4	C4-C3-O2-C2
6	B	541	PG6	C9-C8-O4-C7
2	B	1008	HEC	CAD-CBD-CGD-O2D
2	A	1005	HEC	CAD-CBD-CGD-O2D
2	B	1008	HEC	CAA-CBA-CGA-O1A
2	B	1001	HEC	CAA-CBA-CGA-O2A
2	A	1006	HEC	C2C-C3C-CAC-CBC
2	A	1006	HEC	C4B-C3B-CAB-CBB
2	B	1008	HEC	CAA-CBA-CGA-O2A
2	B	1005	HEC	CAD-CBD-CGD-O2D
2	B	1001	HEC	CAA-CBA-CGA-O1A
2	A	1002	HEC	C4B-C3B-CAB-CBB
2	B	1002	HEC	C4D-C3D-CAD-CBD
2	B	1008	HEC	CAD-CBD-CGD-O1D
6	A	532	PG6	C2-C3-O2-C4
2	A	1004	HEC	C2A-CAA-CBA-CGA
6	B	539	PG6	C2-C3-O2-C4
2	A	1005	HEC	CAD-CBD-CGD-O1D
2	B	1005	HEC	CAD-CBD-CGD-O1D

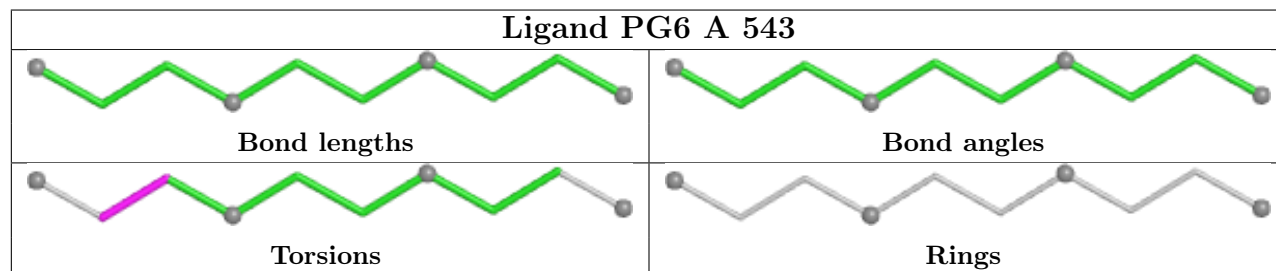
There are no ring outliers.

12 monomers are involved in 13 short contacts:

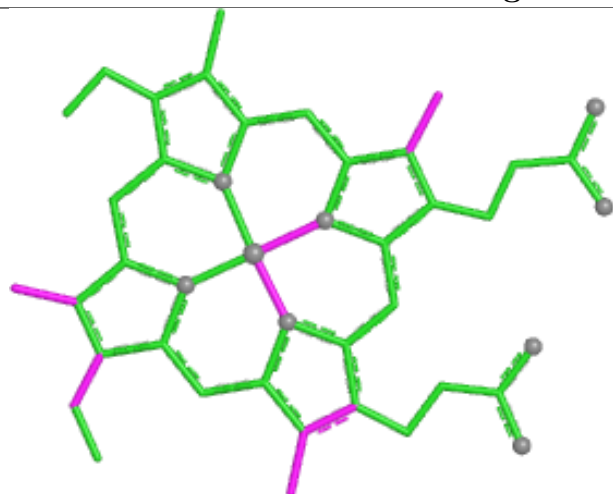
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1006	HEC	2	0
2	B	1006	HEC	1	0
2	A	1004	HEC	1	0
2	B	1008	HEC	1	0
6	B	531	PG6	1	0
2	A	1002	HEC	1	0
2	B	1004	HEC	1	0
2	B	1002	HEC	2	0
7	A	538	PG4	1	0
6	B	534	PG6	1	0
6	A	544	PG6	1	0
6	B	539	PG6	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

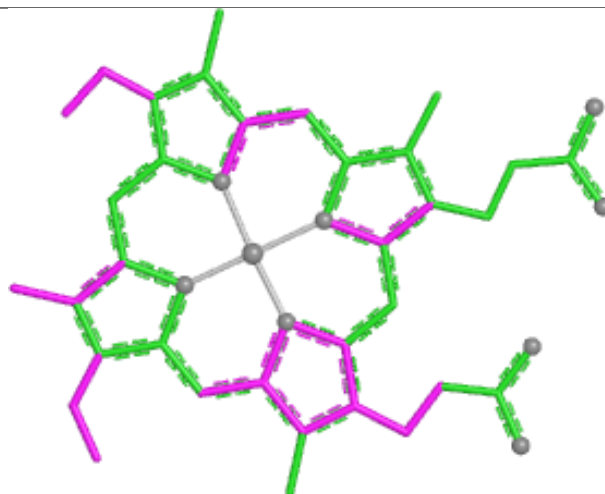
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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



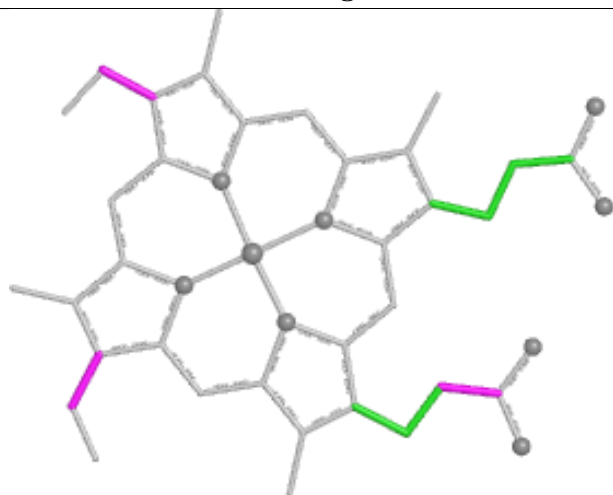
Ligand HEC A 1008



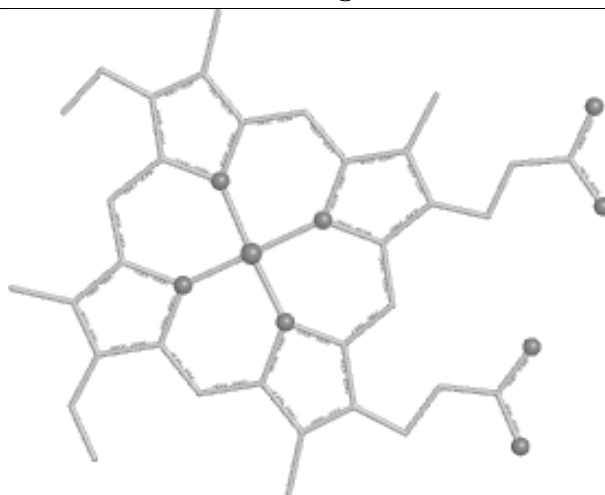
Bond lengths



Bond angles

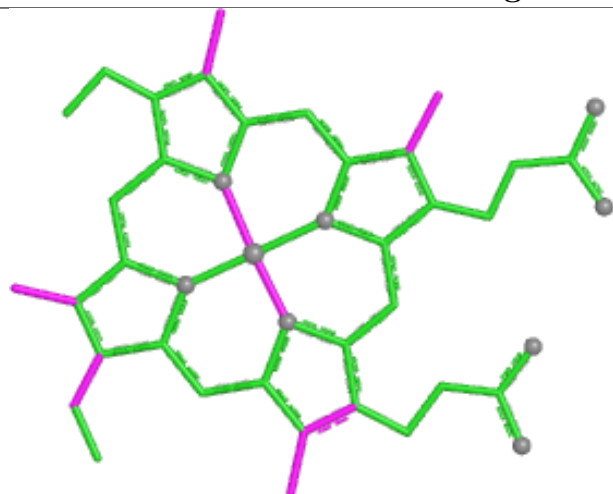


Torsions

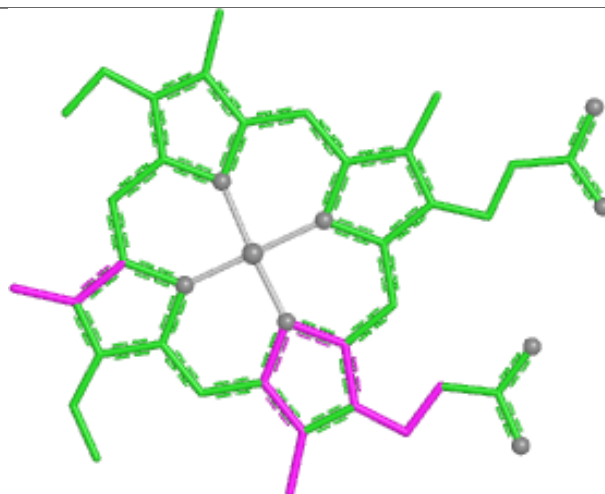


Rings

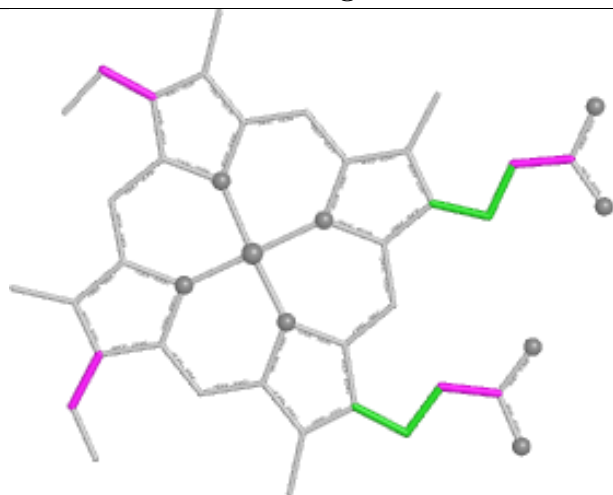
Ligand HEC B 1005



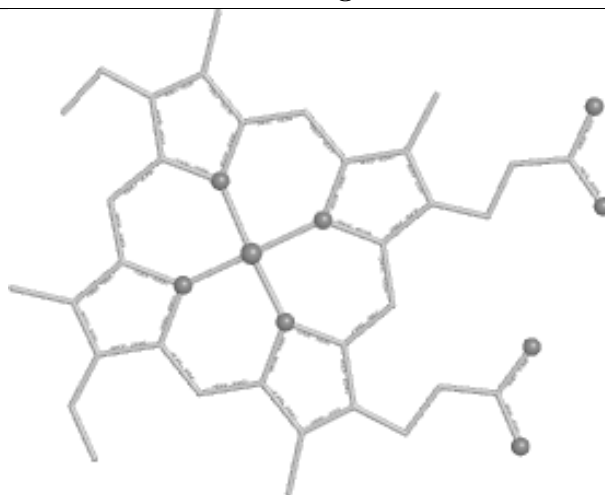
Bond lengths



Bond angles

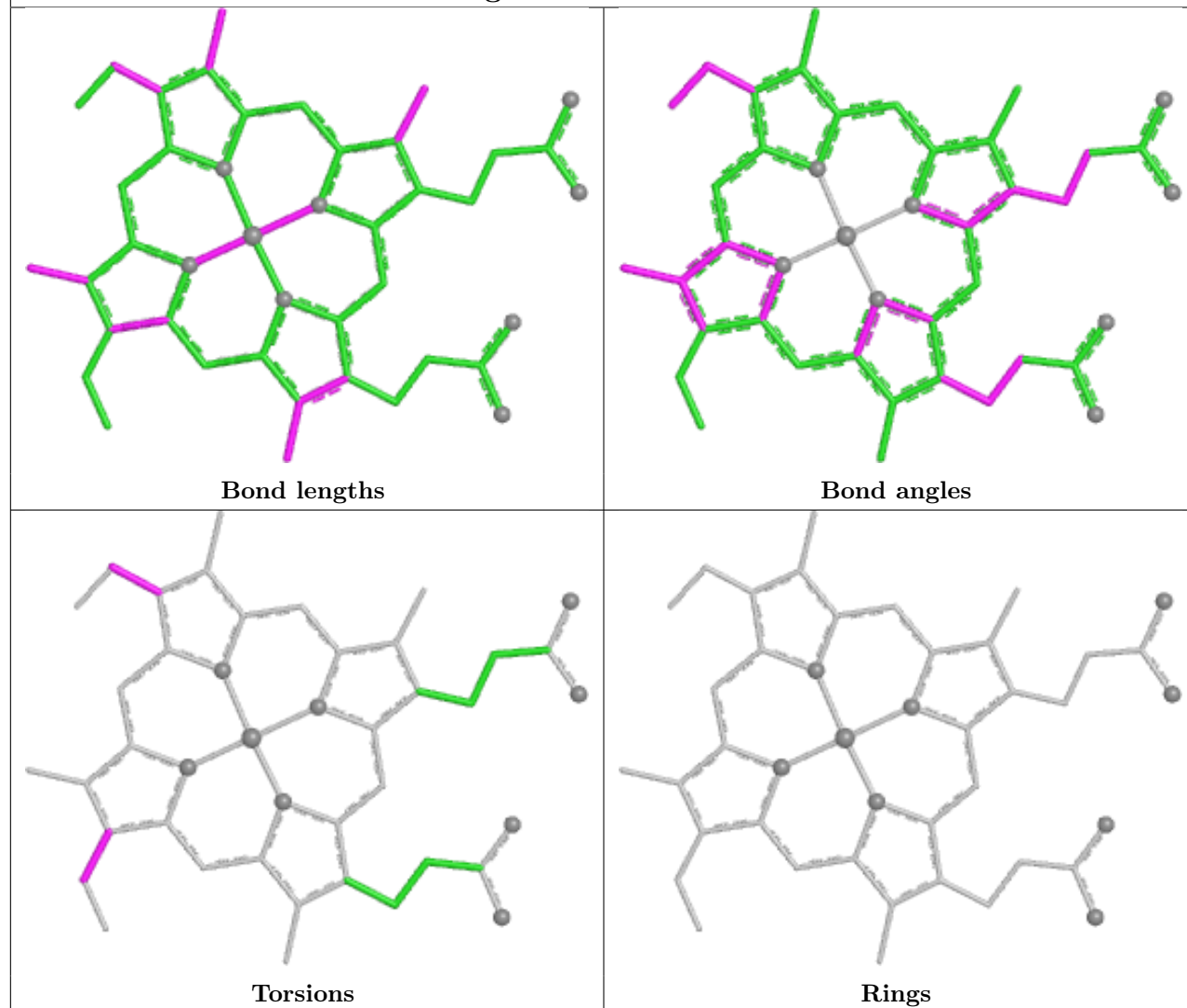


Torsions

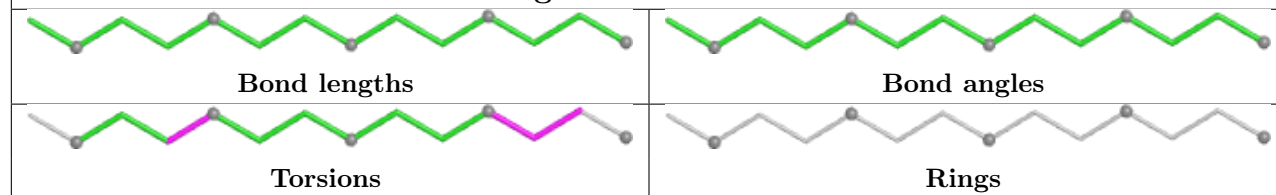


Rings

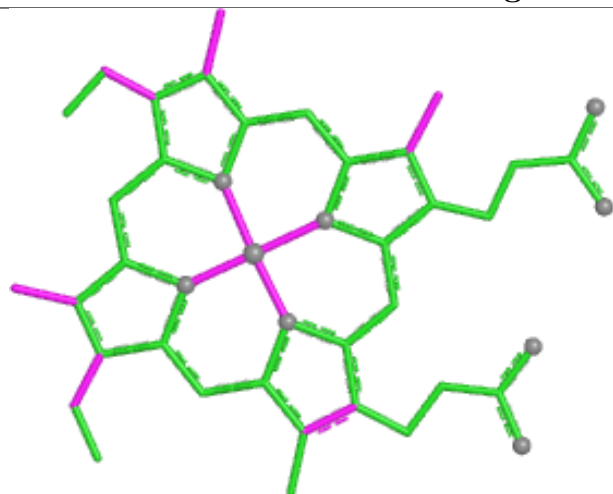
Ligand HEC A 1006



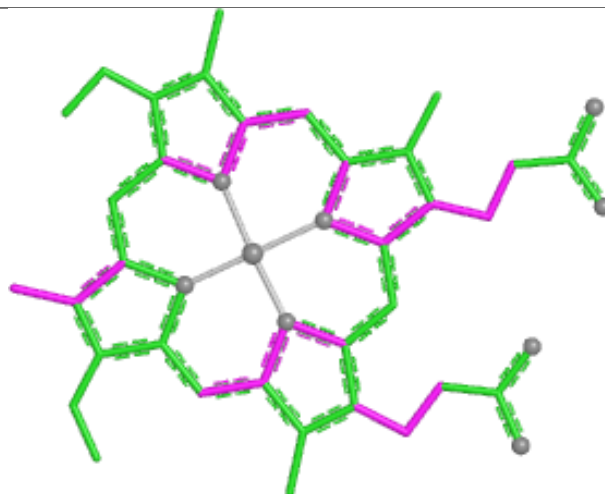
Ligand PG6 B 541



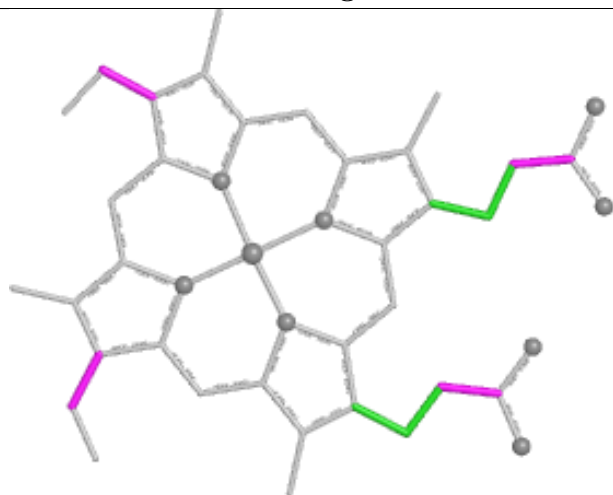
Ligand HEC B 1001



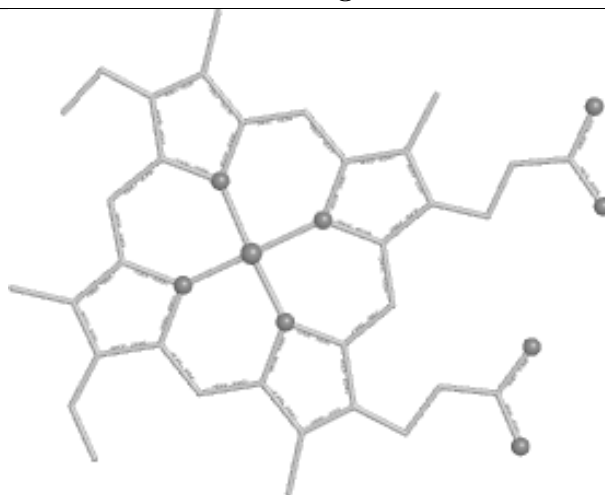
Bond lengths



Bond angles

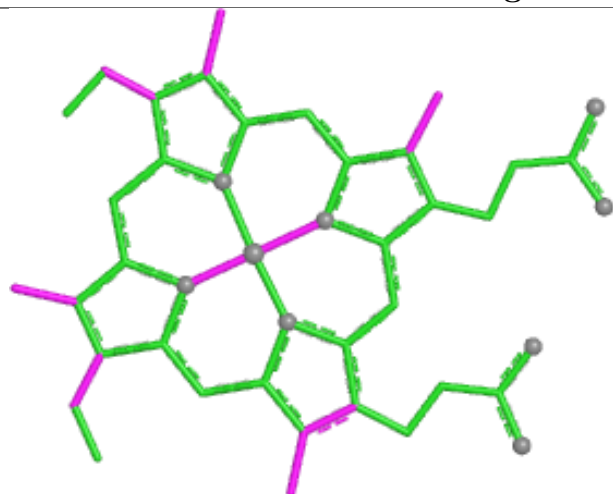


Torsions

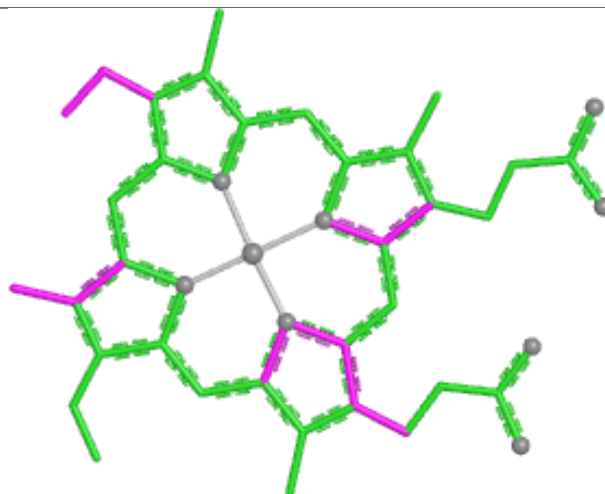


Rings

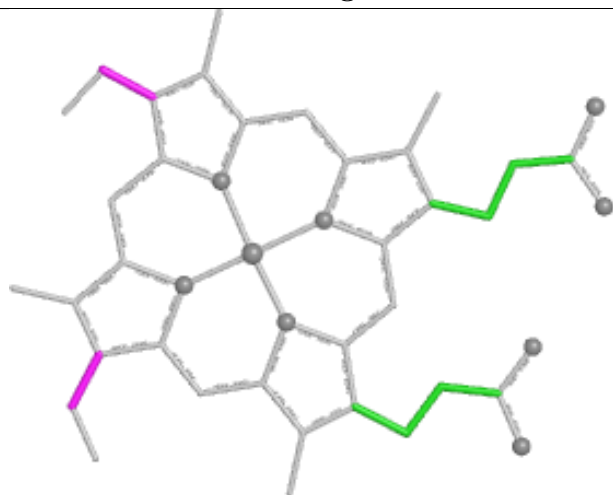
Ligand HEC B 1006



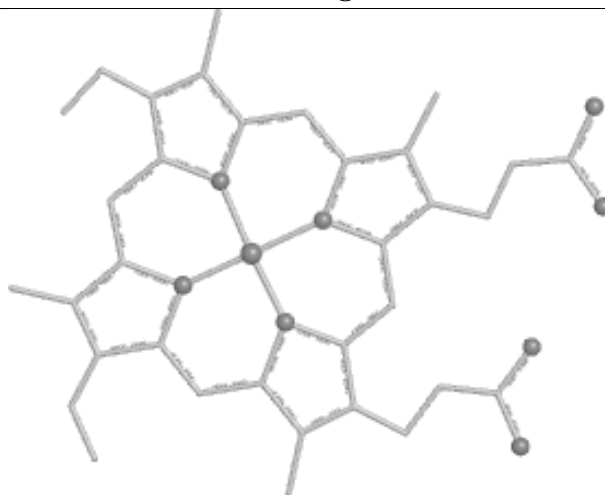
Bond lengths



Bond angles

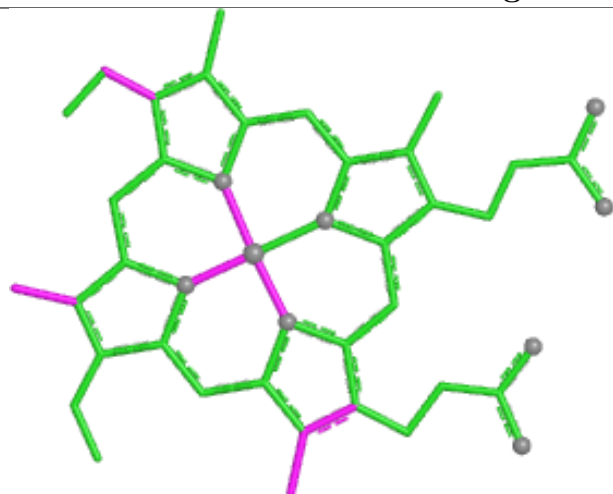


Torsions

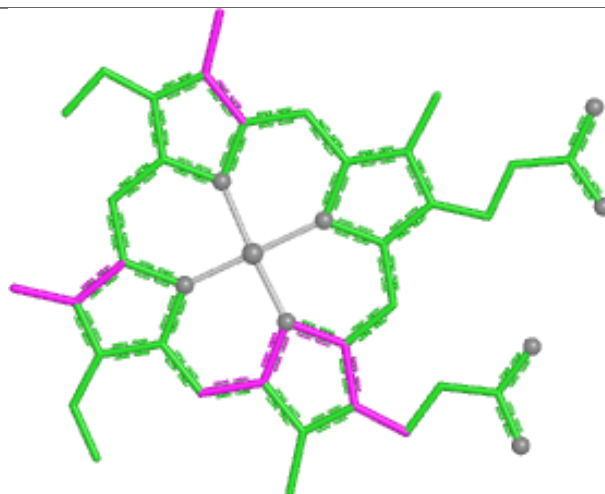


Rings

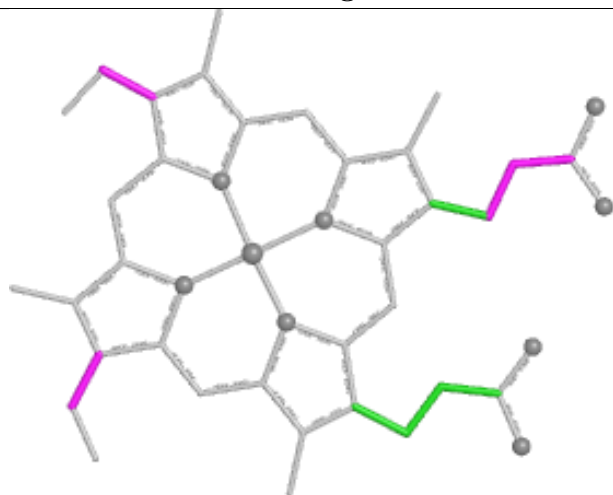
Ligand HEC A 1004



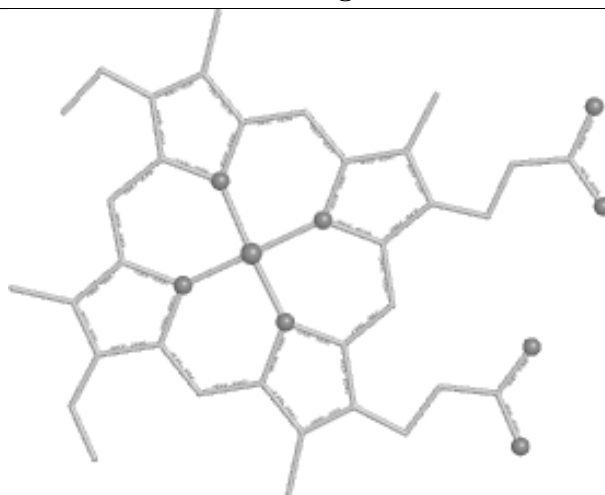
Bond lengths



Bond angles

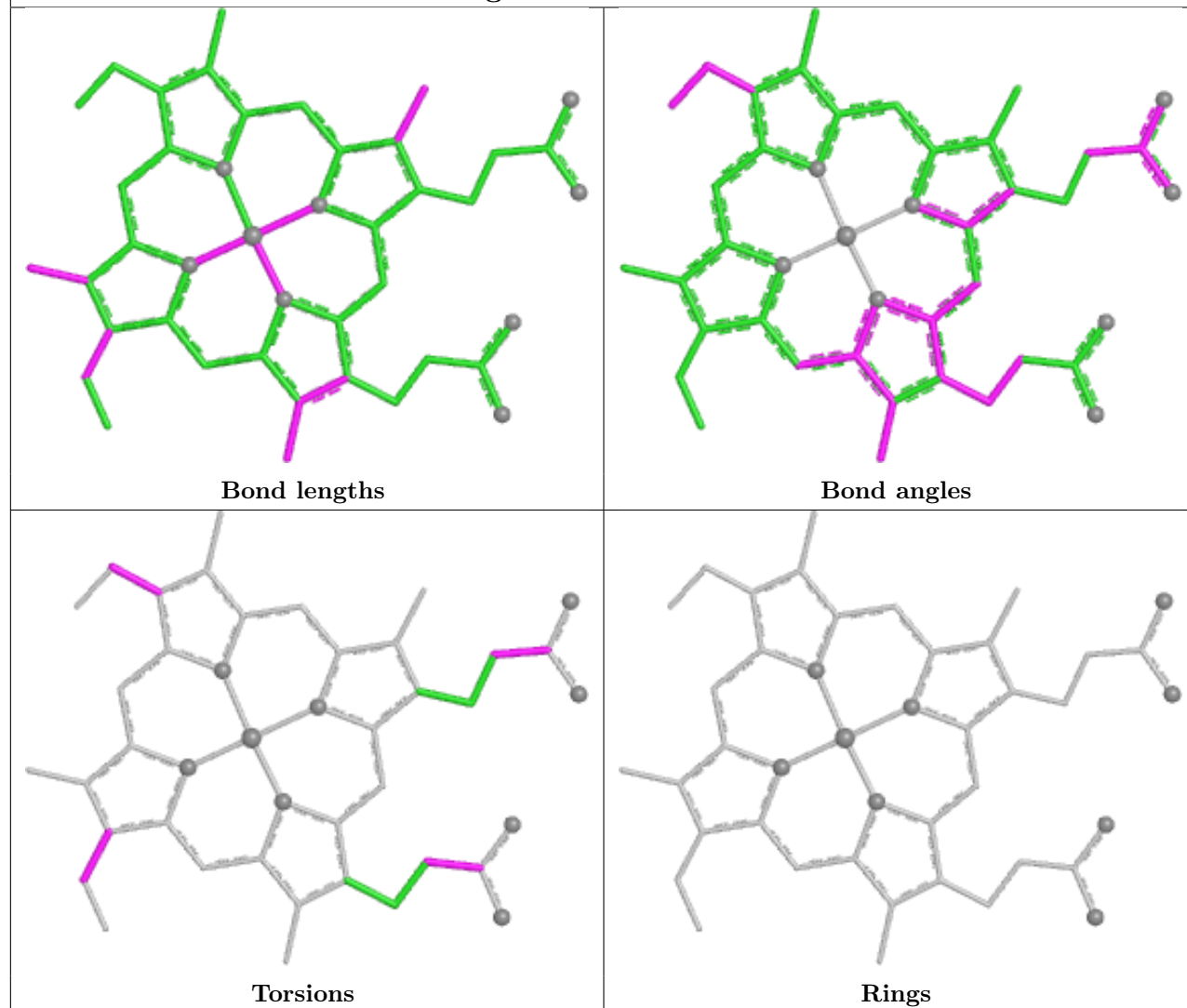


Torsions

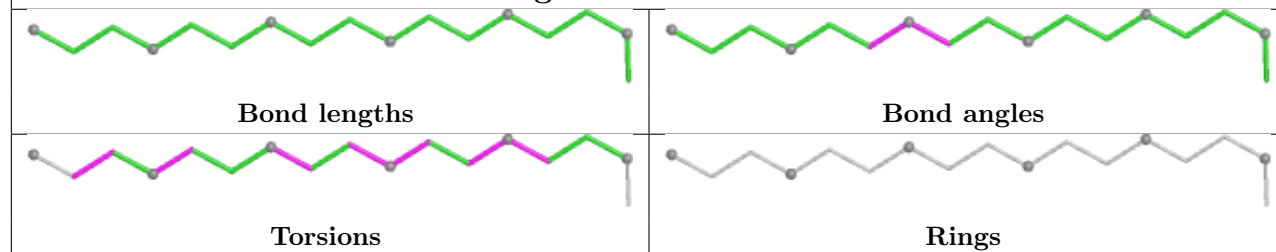


Rings

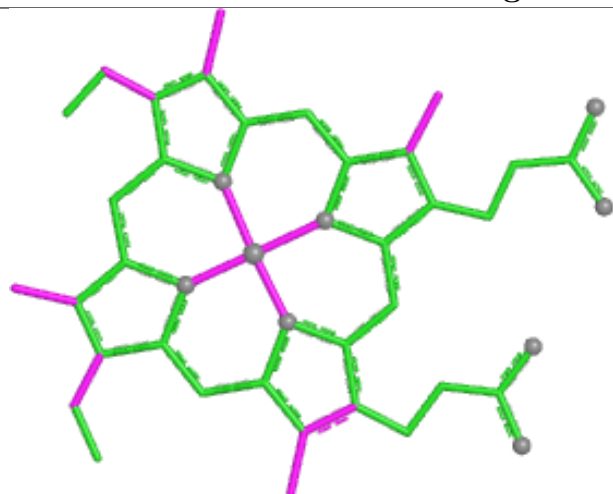
Ligand HEC B 1008



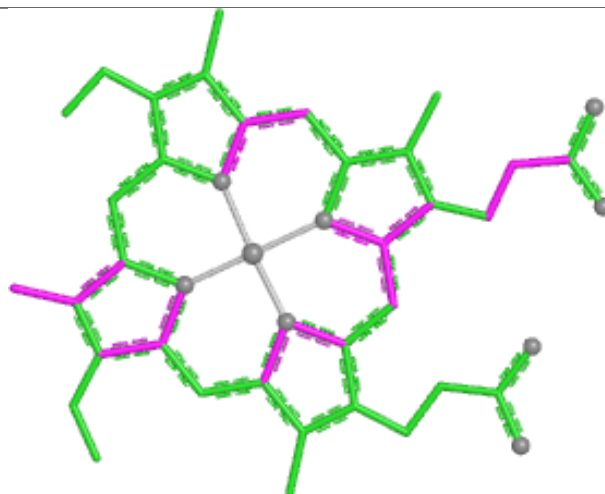
Ligand PG6 B 531



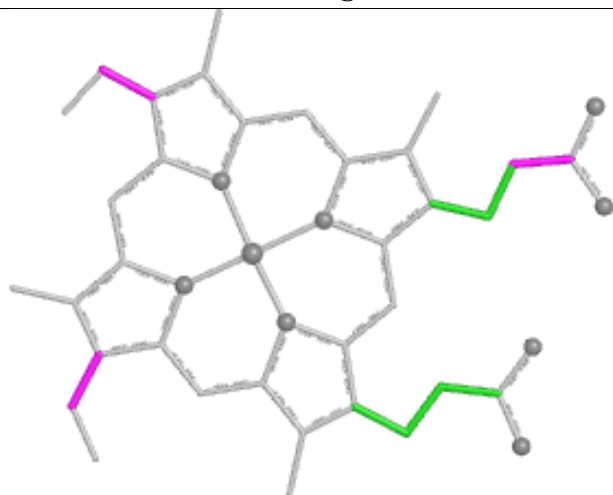
Ligand HEC A 1002



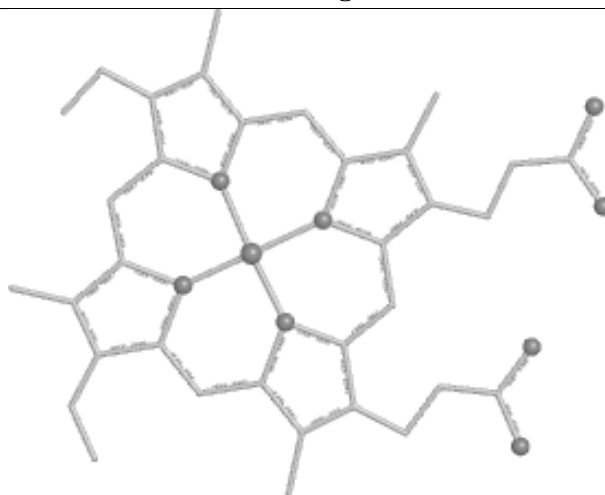
Bond lengths



Bond angles

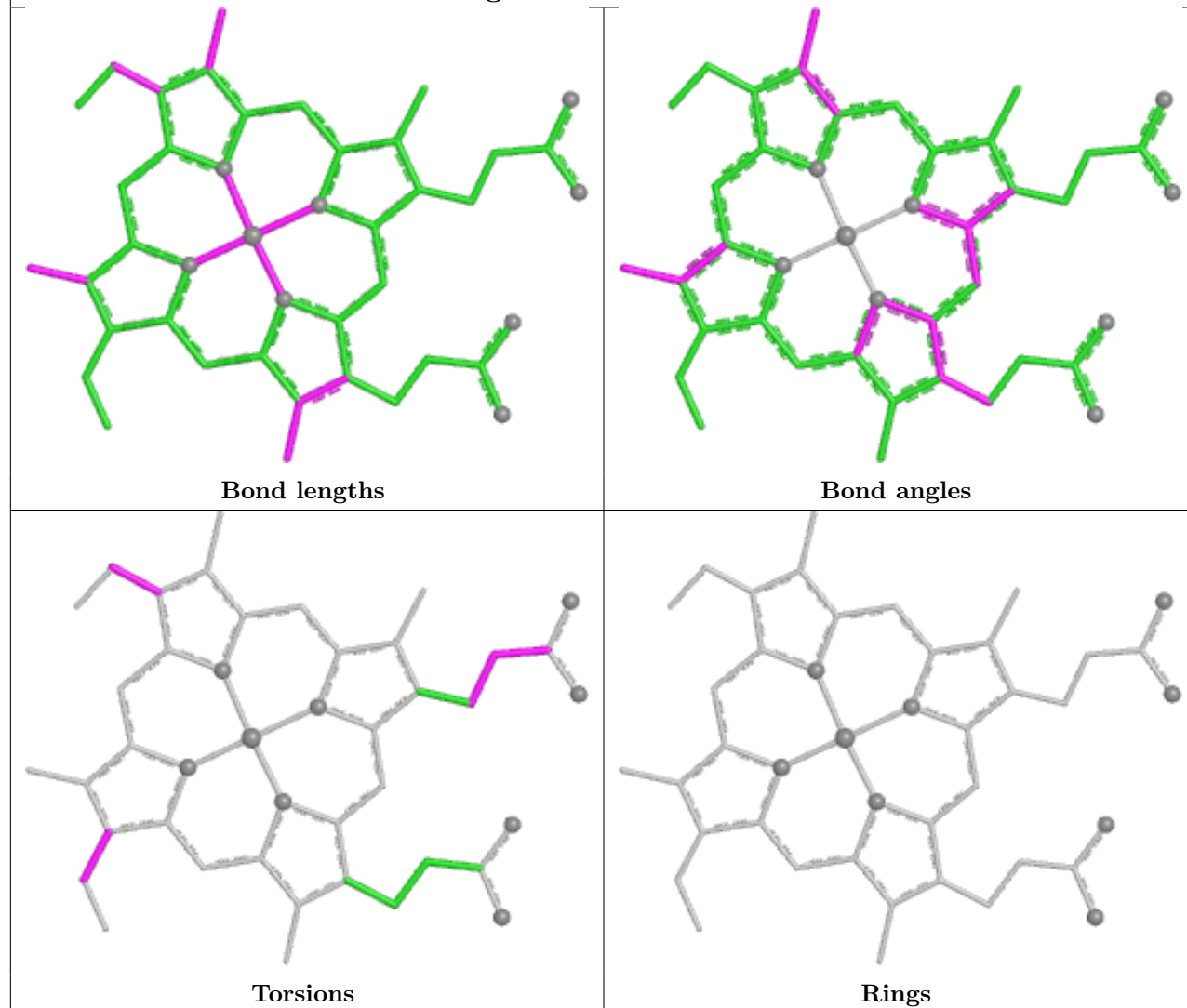


Torsions

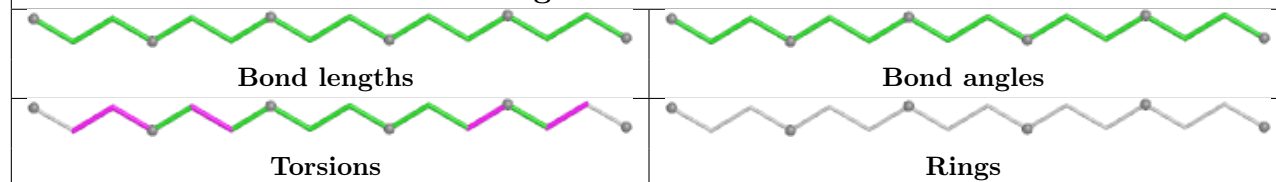


Rings

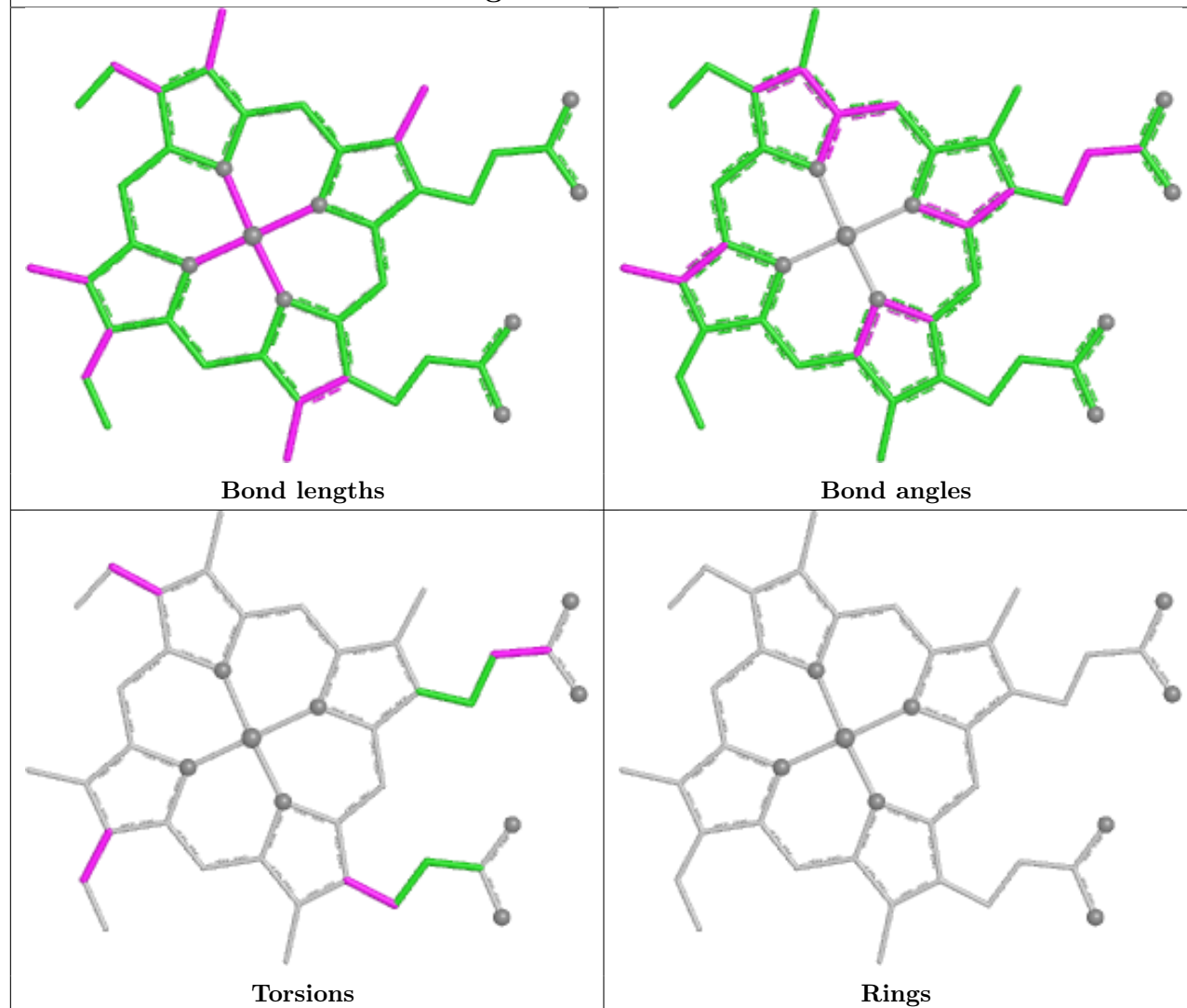
Ligand HEC B 1004



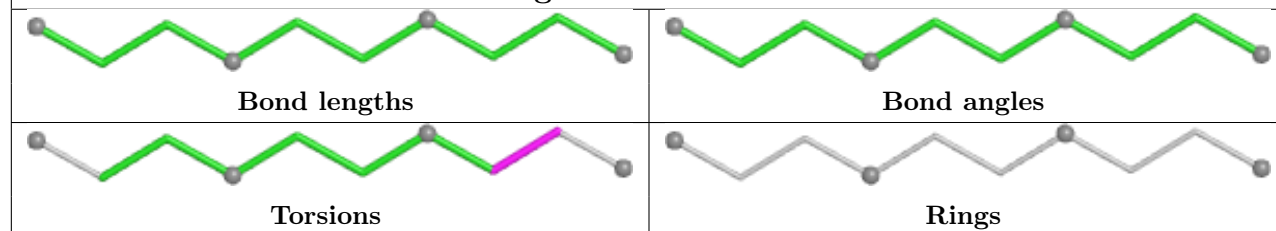
Ligand PG6 A 542



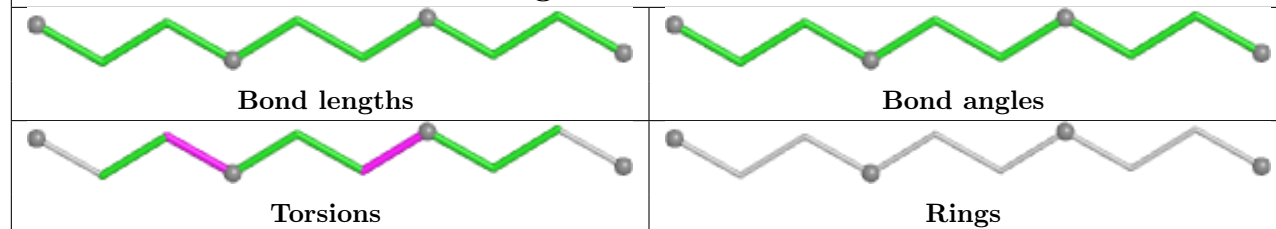
Ligand HEC B 1002

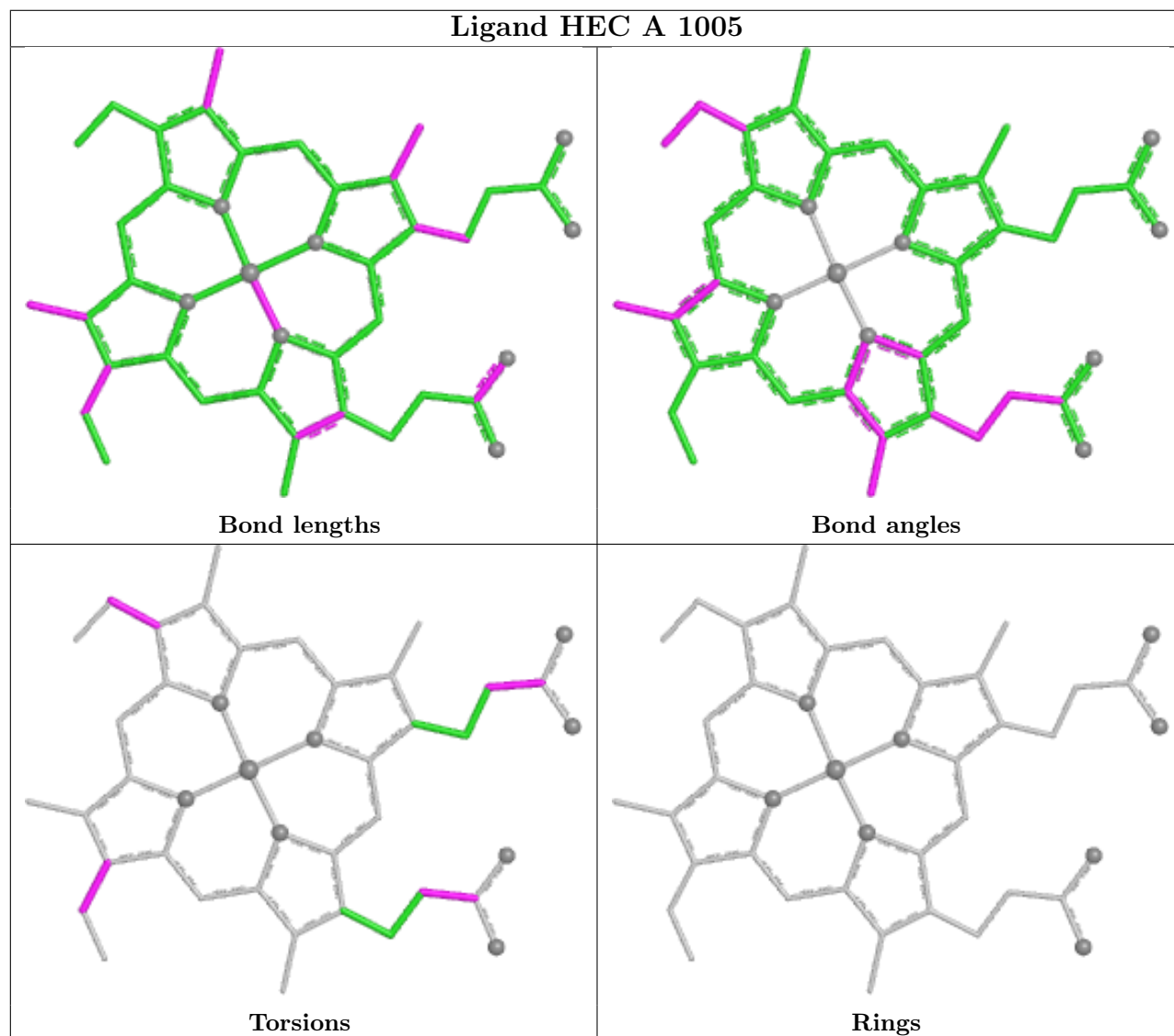
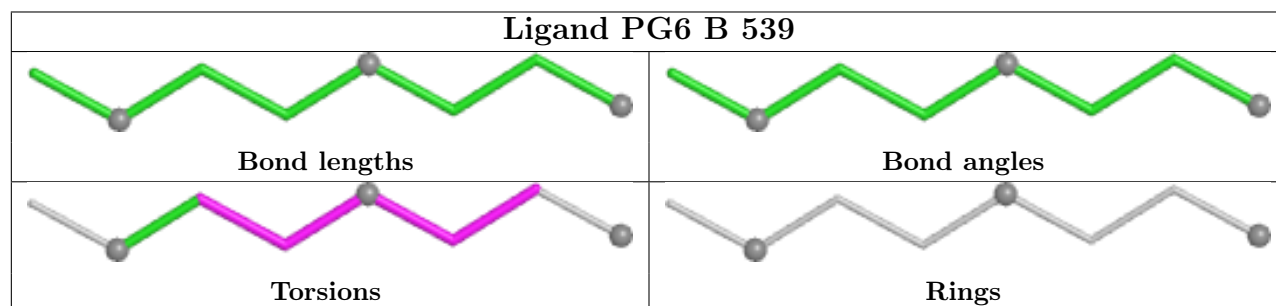
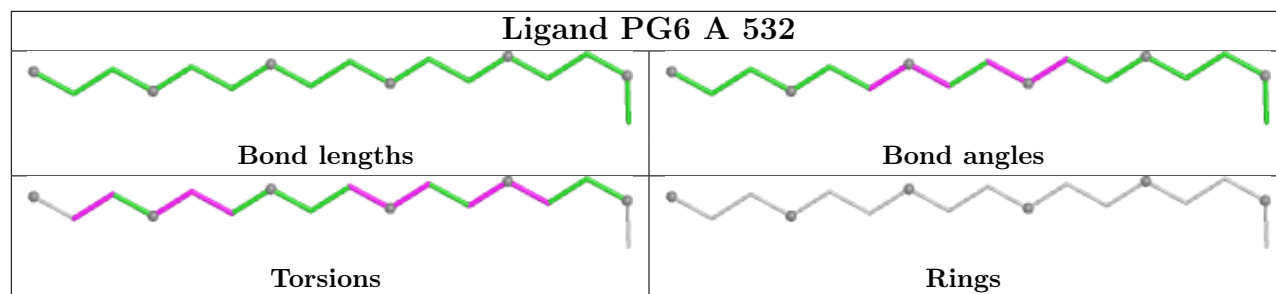


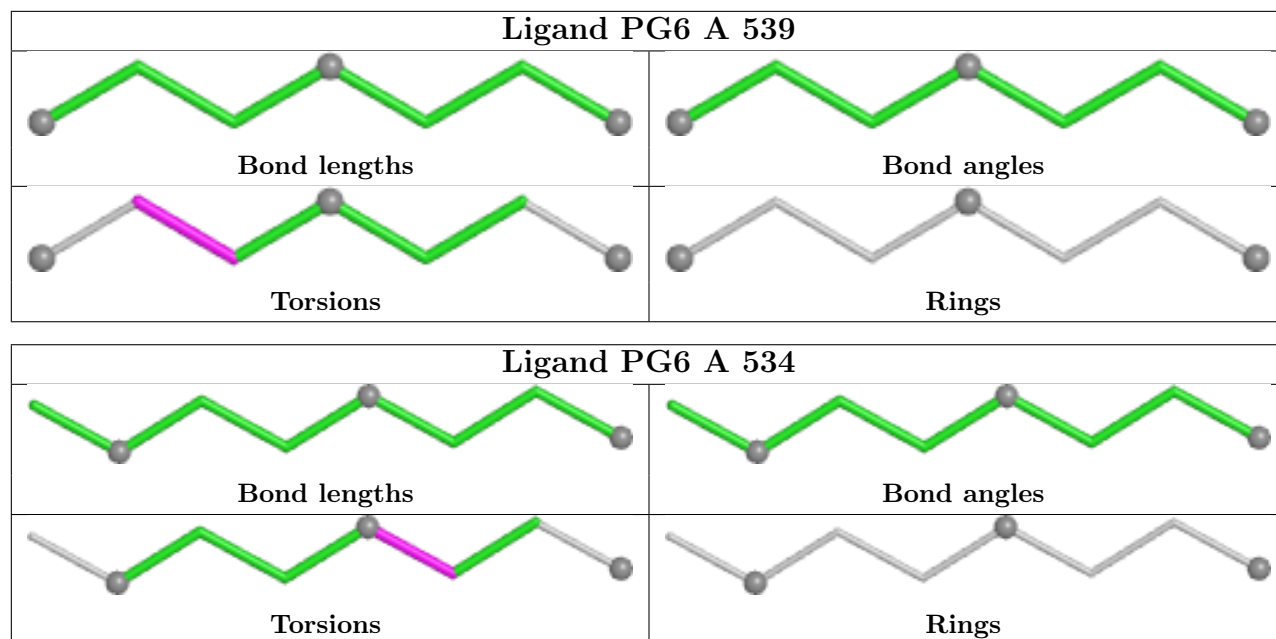
Ligand PG6 B 542



Ligand PG6 B 534







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	519/525 (98%)	-0.51	2 (0%)	88 91	11, 19, 31, 49	10 (1%)
1	B	519/525 (98%)	-0.47	3 (0%)	85 89	11, 19, 32, 49	13 (2%)
All	All	1038/1050 (98%)	-0.49	5 (0%)	87 90	11, 19, 31, 49	23 (2%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	523	ALA	7.6
1	A	522	VAL	3.5
1	B	522	VAL	3.0
1	B	523	ALA	2.4
1	B	51[A]	ARG	2.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PG4	A	546	6/13	0.64	0.58	36,37,37,37	6
7	PG4	B	537	6/13	0.68	0.54	29,30,31,32	6
7	PG4	A	545	7/13	0.69	0.51	32,33,34,35	7
7	PG4	B	540	8/13	0.71	0.26	49,54,59,59	0
7	PG4	A	533	4/13	0.74	0.39	25,27,27,28	4
6	PG6	B	539	8/18	0.76	0.23	51,53,55,56	0
6	PG6	A	543	10/18	0.78	0.30	31,32,35,37	10
7	PG4	A	540	9/13	0.78	0.43	26,28,33,33	9
7	PG4	B	543	5/13	0.78	0.21	58,60,61,62	0
6	PG6	B	534	10/18	0.79	0.35	17,20,32,33	10
6	PG6	B	541	14/18	0.80	0.20	54,61,63,63	0
7	PG4	B	532	5/13	0.81	0.35	31,31,32,33	5
6	PG6	B	531	17/18	0.81	0.18	31,39,45,46	0
6	PG6	A	542	16/18	0.83	0.26	28,35,37,38	16
6	PG6	B	542	10/18	0.83	0.23	27,29,31,32	10
6	PG6	A	544	4/18	0.84	0.18	20,21,23,23	4
5	NA	A	529	1/1	0.84	0.19	28,28,28,28	1
7	PG4	A	538	6/13	0.85	0.18	51,53,53,55	0
6	PG6	A	532	17/18	0.86	0.15	24,34,44,45	2
6	PG6	A	534	8/18	0.87	0.14	33,40,50,50	0
6	PG6	B	538[A]	10/18	0.87	0.14	29,40,47,47	1
7	PG4	A	541	5/13	0.87	0.17	46,47,48,50	0
3	SO3	B	533	4/4	0.91	0.14	44,44,44,45	4
5	NA	A	536	1/1	0.92	0.08	38,38,38,38	0
5	NA	B	535	1/1	0.94	0.20	17,17,17,17	1
6	PG6	A	539	7/18	0.94	0.09	28,31,40,43	0
5	NA	A	535	1/1	0.94	0.12	13,13,13,13	1
3	SO3	B	536	4/4	0.95	0.08	37,37,37,37	4
3	SO3	A	537	4/4	0.96	0.09	38,38,38,38	4
2	HEC	B	1007[A]	43/43	0.97	0.06	10,13,15,16	4
5	NA	A	530	1/1	0.97	0.17	29,29,29,29	0
3	SO3	B	526	4/4	0.97	0.11	12,12,14,14	4
2	HEC	B	1003[A]	43/43	0.97	0.08	12,16,29,35	4
5	NA	B	530	1/1	0.97	0.04	40,40,40,40	1
3	SO3	A	526	4/4	0.97	0.11	13,16,16,18	4
4	CA	A	528	1/1	0.97	0.05	16,16,16,16	1
2	HEC	B	1001	43/43	0.98	0.07	19,23,29,31	0
2	HEC	A	1003[A]	43/43	0.98	0.07	11,14,25,34	4
5	NA	A	531	1/1	0.98	0.06	43,43,43,43	1
2	HEC	A	1001[A]	43/43	0.98	0.07	16,19,21,24	4
2	HEC	B	1005	43/43	0.98	0.06	12,14,20,24	0
5	NA	B	529	1/1	0.98	0.12	29,29,29,29	0
2	HEC	A	1007[A]	43/43	0.98	0.06	11,14,16,17	3

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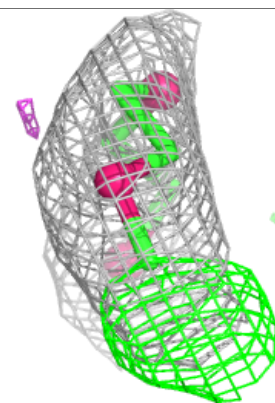
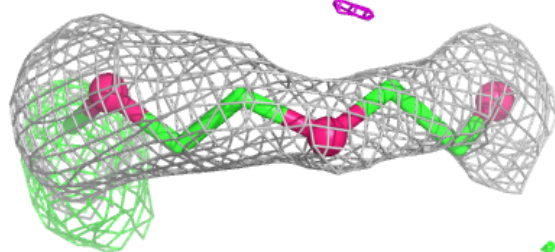
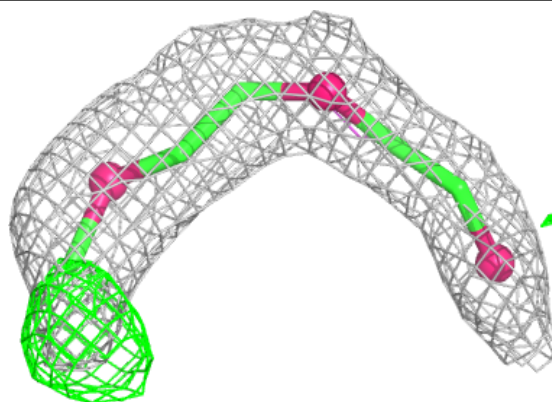
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEC	B	1008	43/43	0.98	0.06	14,18,29,38	0
2	HEC	A	1008	43/43	0.98	0.06	15,19,28,36	0
4	CA	B	528	1/1	0.98	0.05	16,16,16,16	1
2	HEC	A	1006	43/43	0.99	0.05	11,13,15,15	0
2	HEC	B	1002	43/43	0.99	0.05	16,19,22,23	0
4	CA	A	527	1/1	0.99	0.04	19,19,19,19	0
2	HEC	A	1004	43/43	0.99	0.05	11,15,17,17	0
4	CA	B	527	1/1	0.99	0.05	18,18,18,18	0
2	HEC	B	1004	43/43	0.99	0.04	11,14,17,19	0
2	HEC	A	1005	43/43	0.99	0.05	12,13,20,22	0
2	HEC	B	1006	43/43	0.99	0.05	10,14,15,18	0
2	HEC	A	1002	43/43	0.99	0.05	15,17,19,22	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.

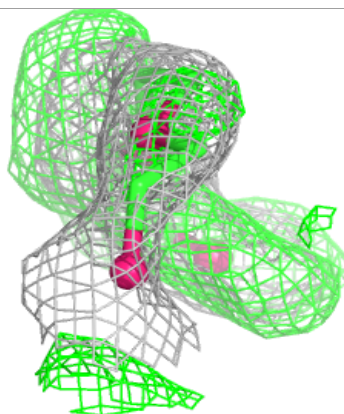
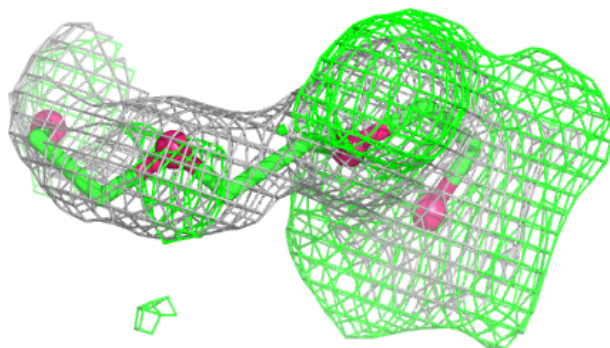
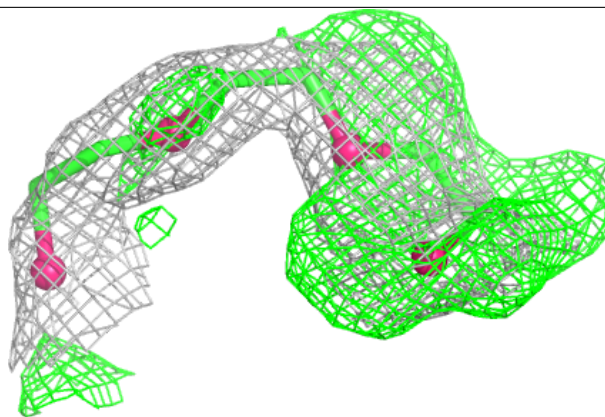
Electron density around PG6 B 539:

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

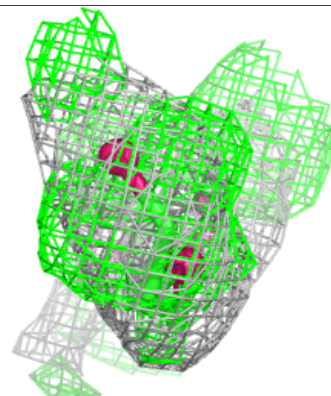
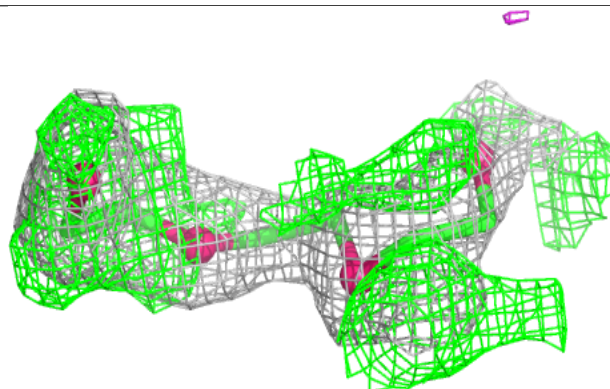
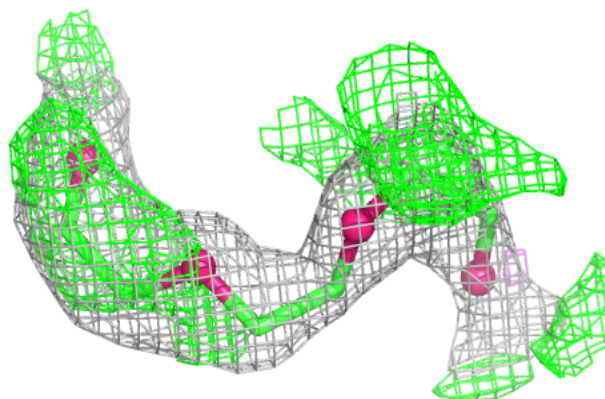


Electron density around PG6 A 543:

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

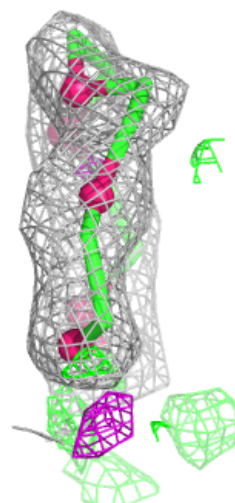
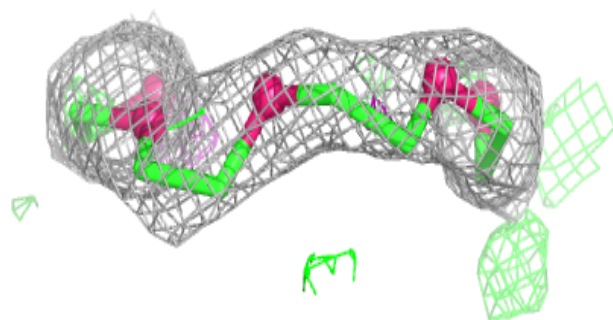
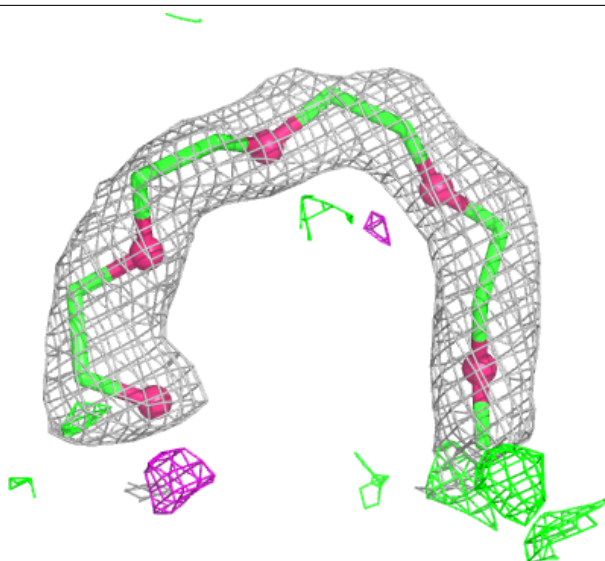
**Electron density around PG6 B 534:**

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



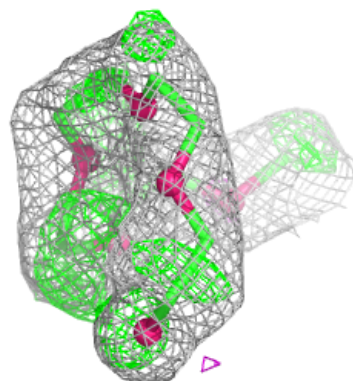
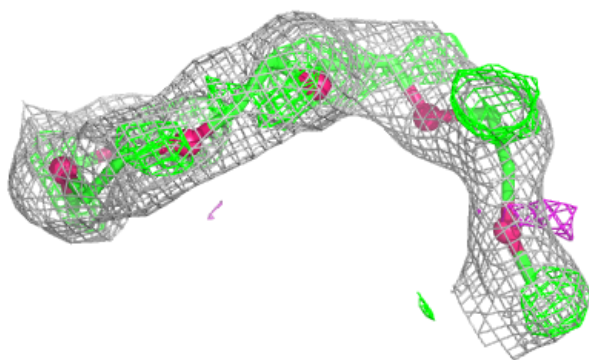
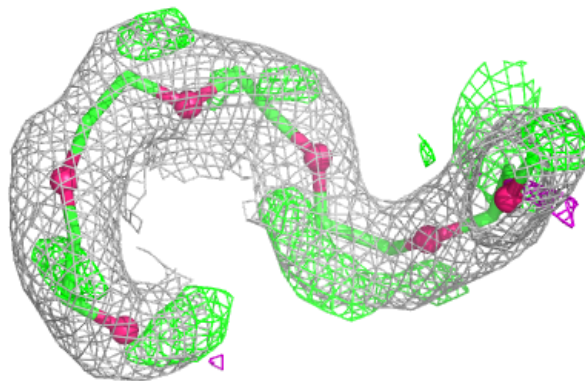
Electron density around PG6 B 541:

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and green (positive)



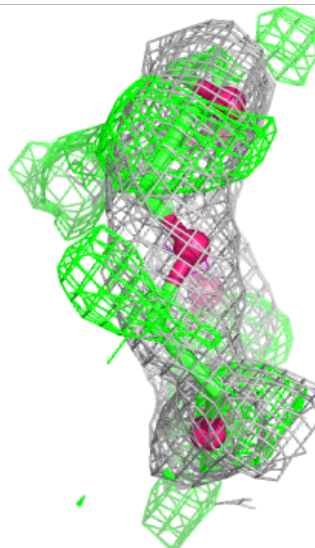
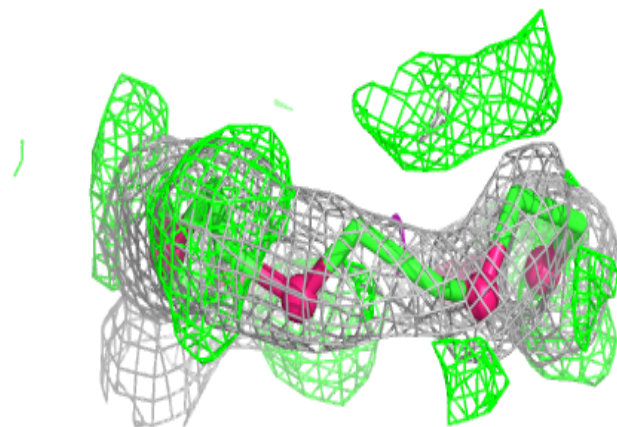
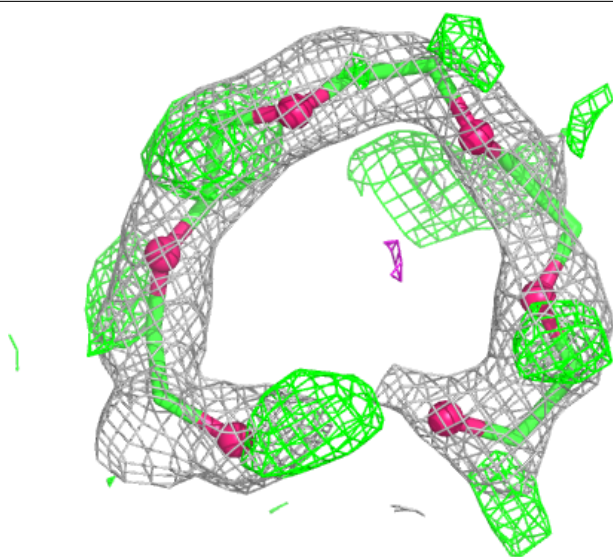
Electron density around PG6 B 531:

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



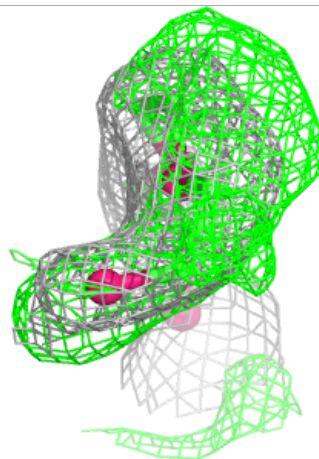
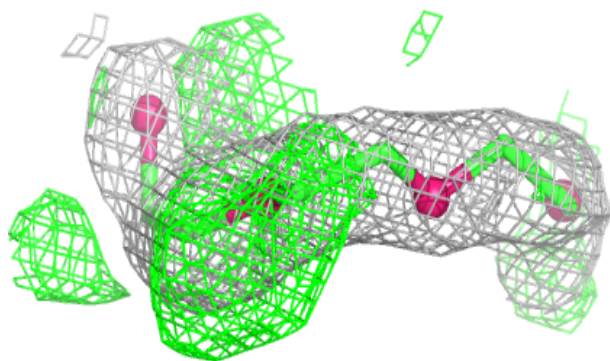
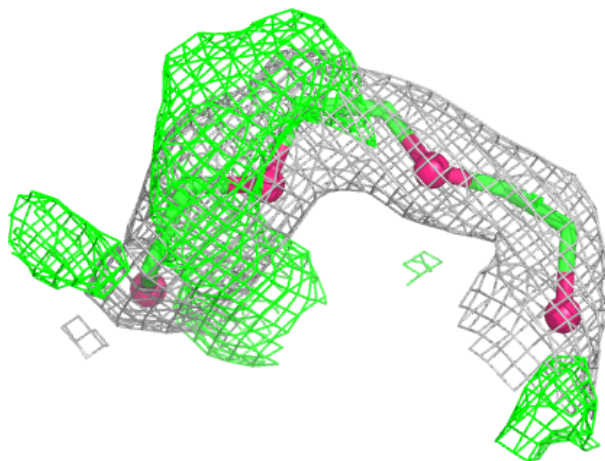
Electron density around PG6 A 542:

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



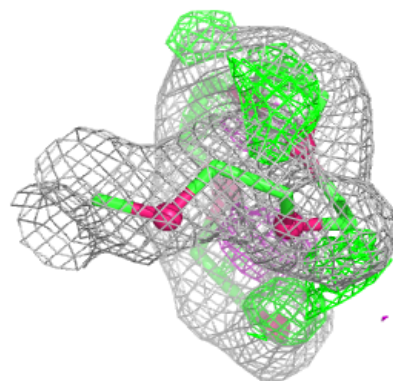
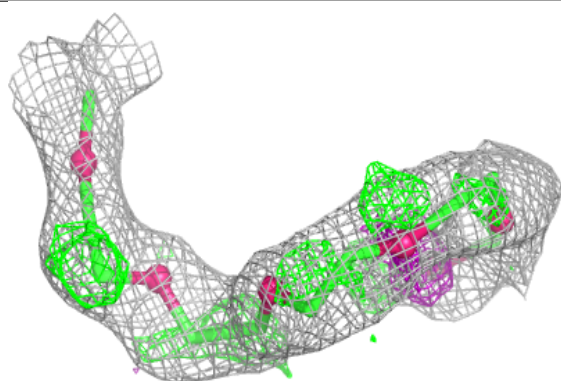
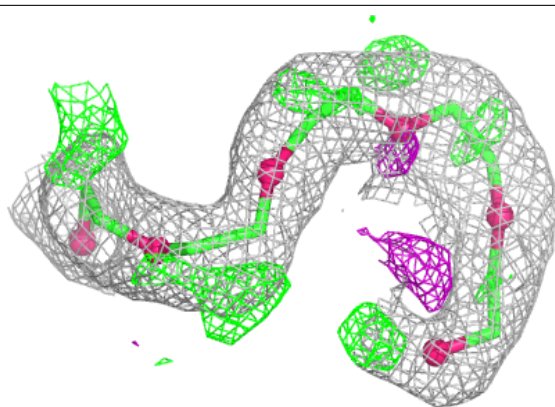
Electron density around PG6 B 542:

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

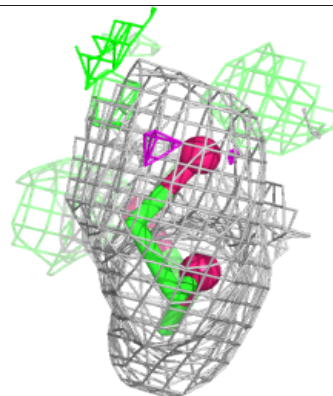
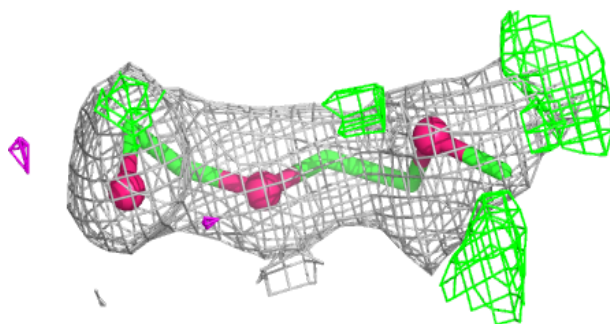
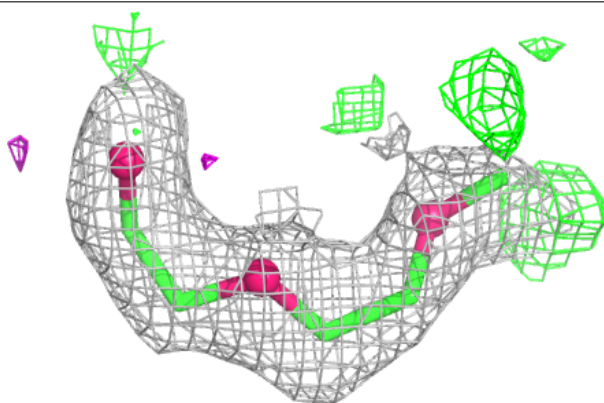


Electron density around PG6 A 532:

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and green (positive)

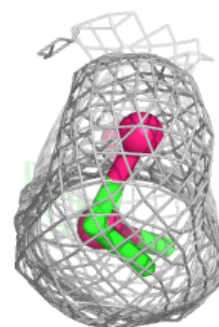
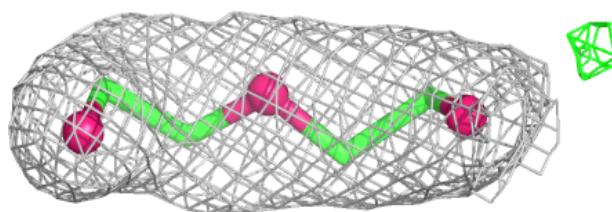
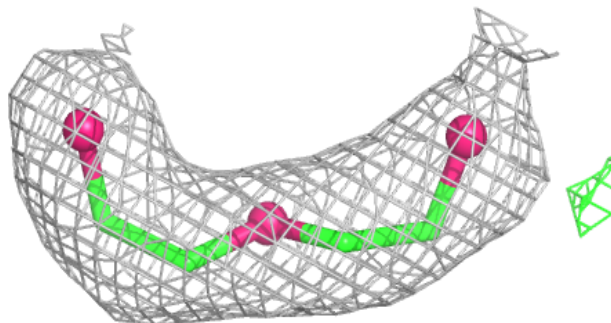
**Electron density around PG6 A 534:**

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



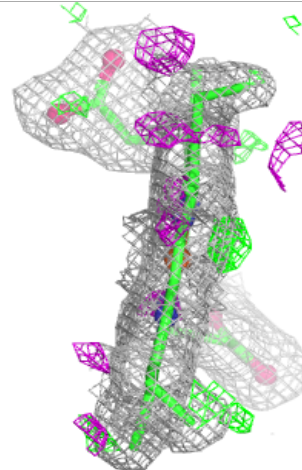
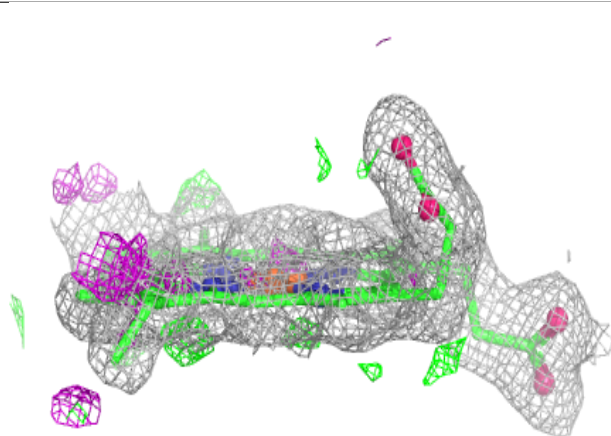
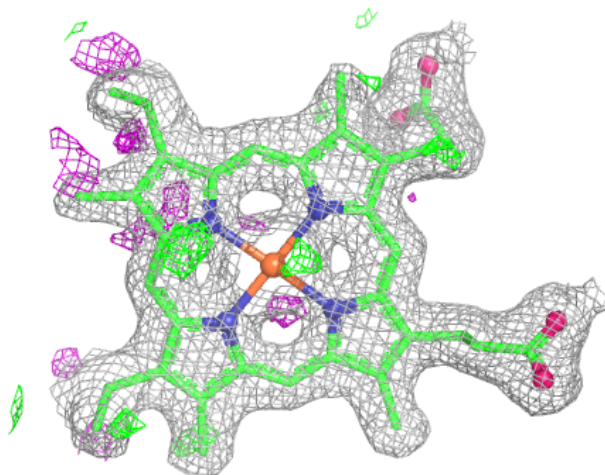
Electron density around PG6 A 539:

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and green (positive)



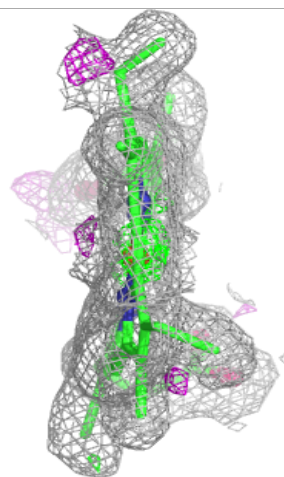
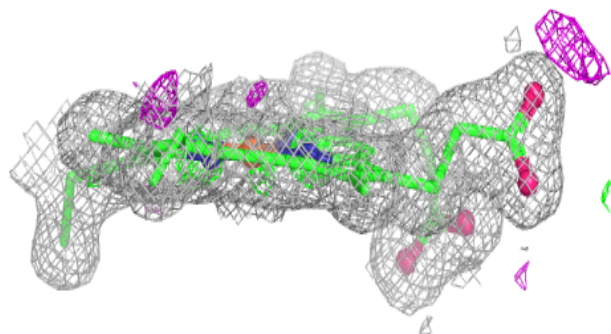
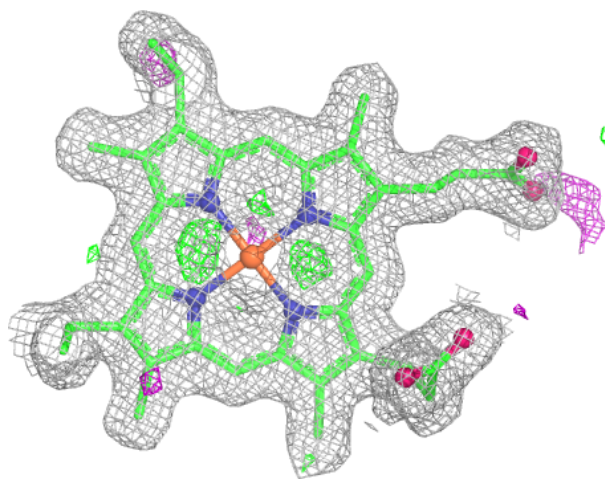
Electron density around HEC B 1001:

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



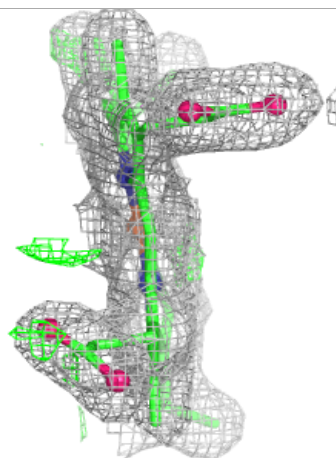
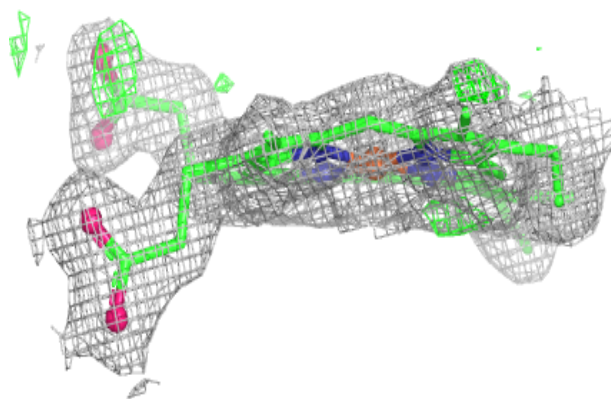
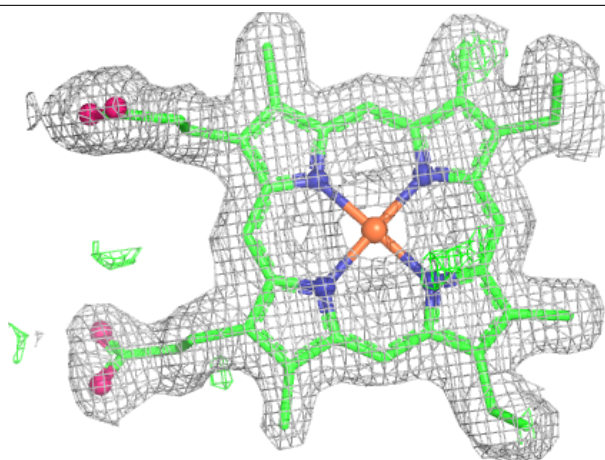
Electron density around HEC B 1005:

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and green (positive)



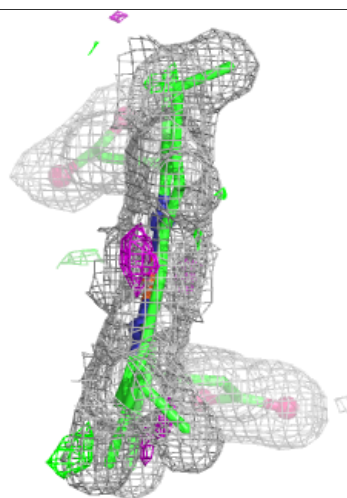
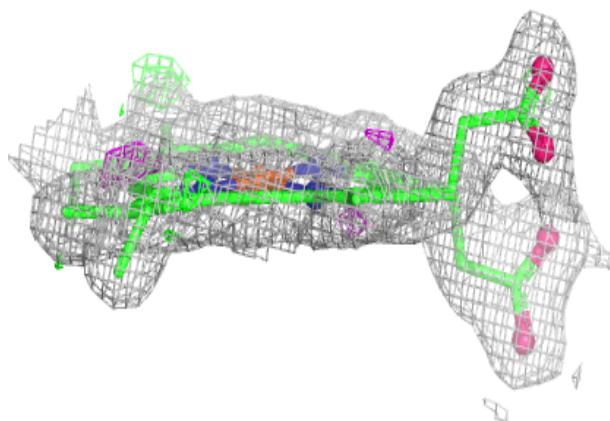
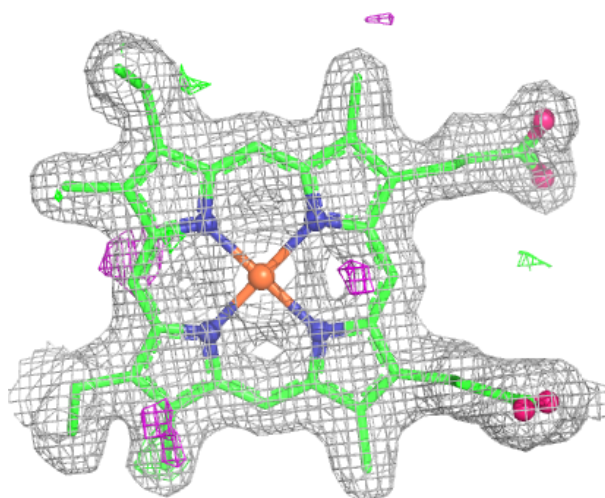
Electron density around HEC B 1008:

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



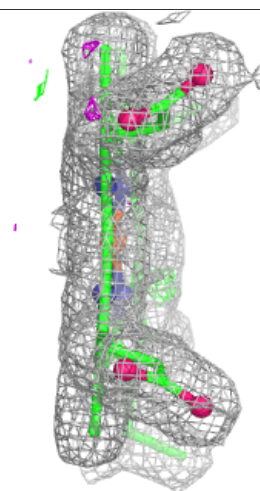
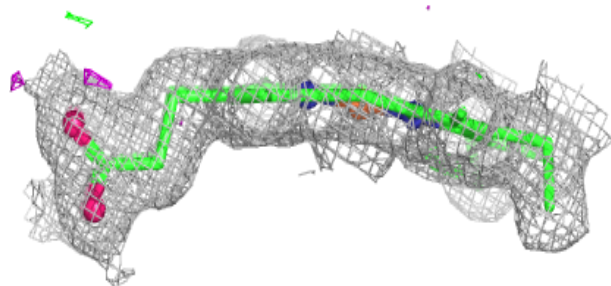
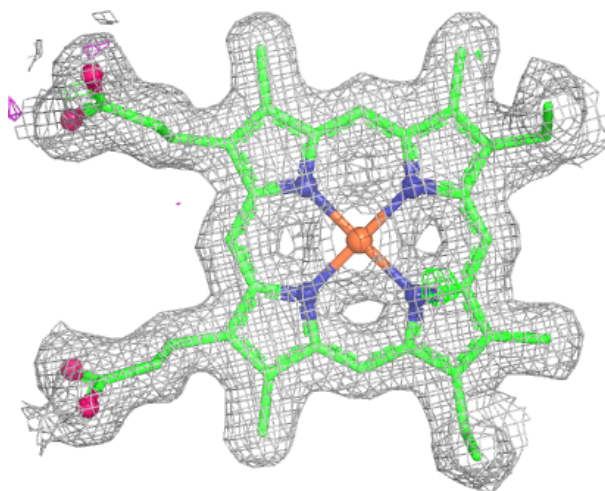
Electron density around HEC A 1008:

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



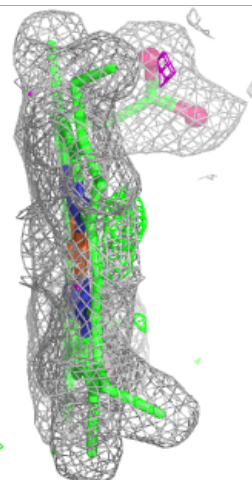
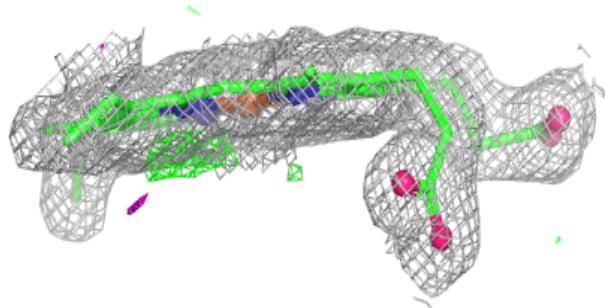
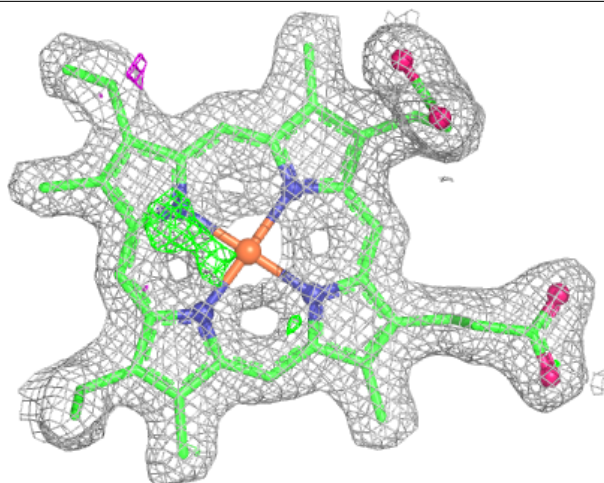
Electron density around HEC A 1006:

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



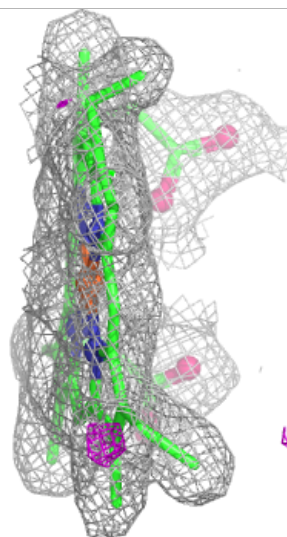
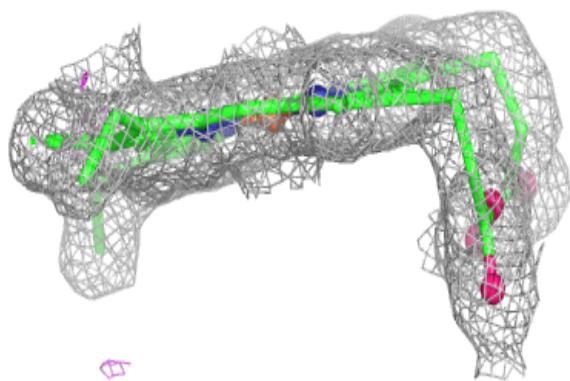
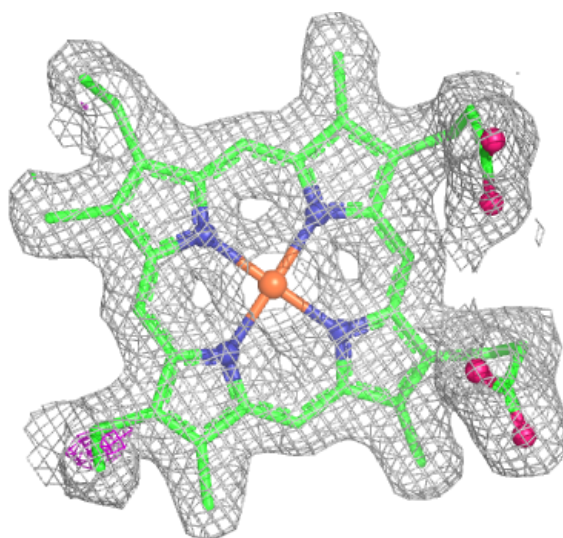
Electron density around HEC B 1002:

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



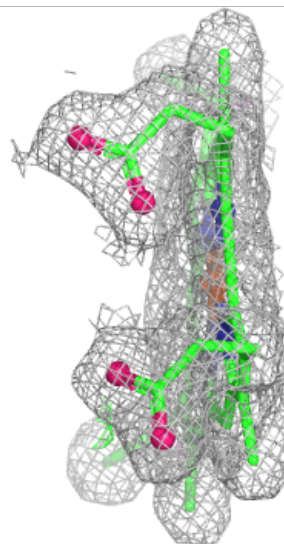
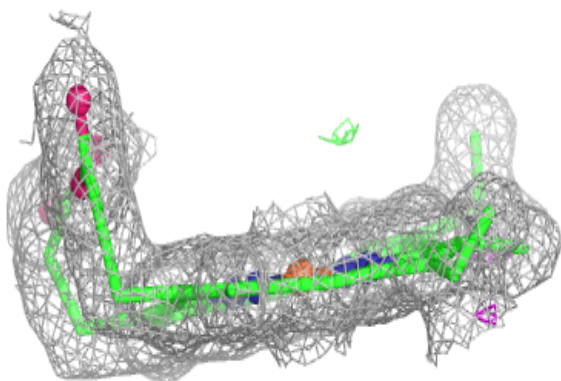
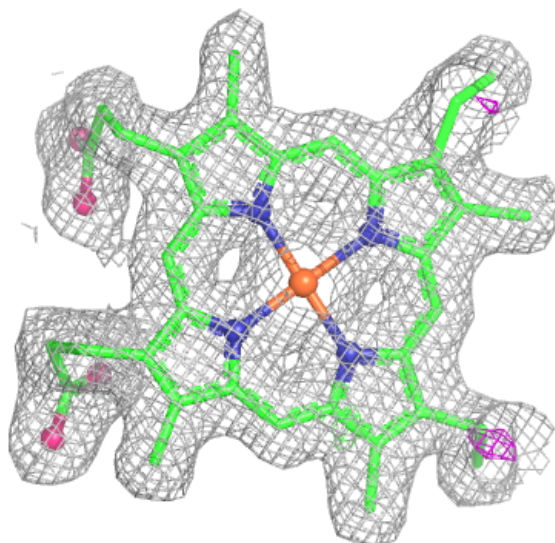
Electron density around HEC A 1004:

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



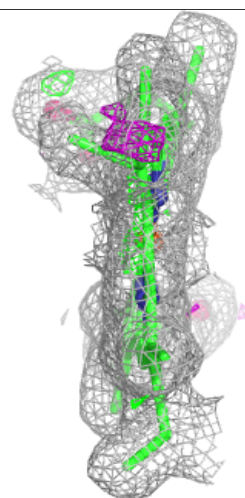
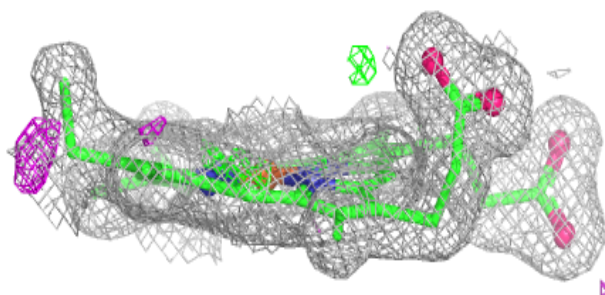
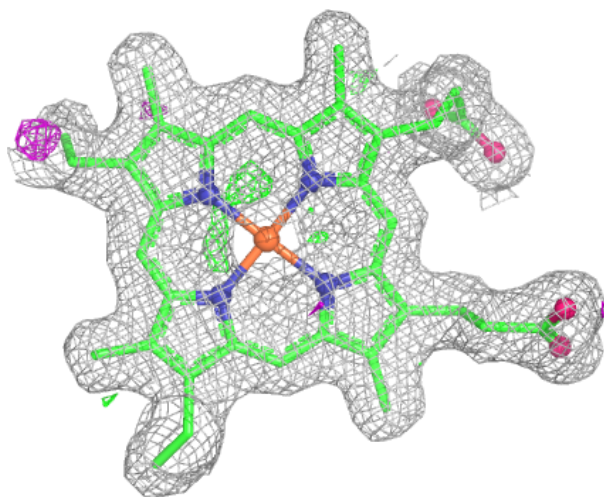
Electron density around HEC B 1004:

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



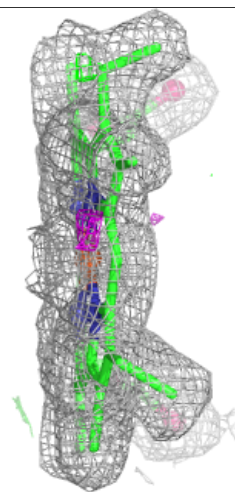
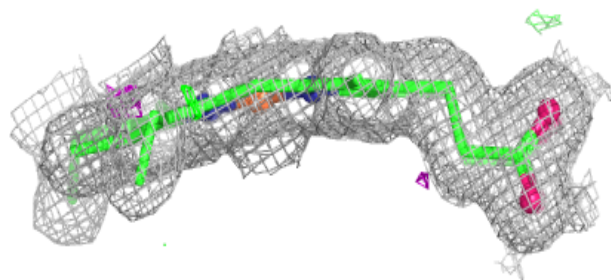
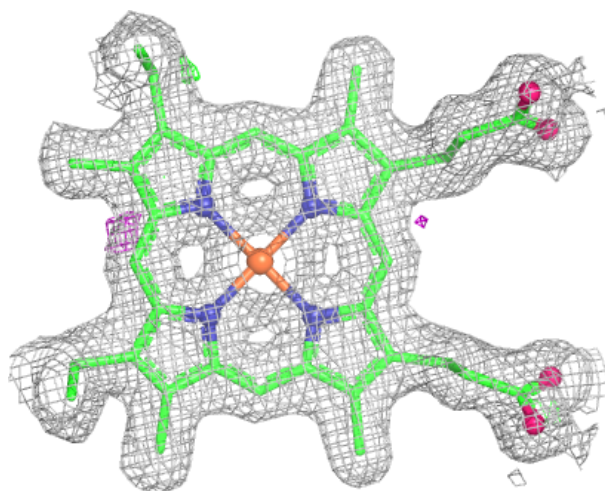
Electron density around HEC A 1005:

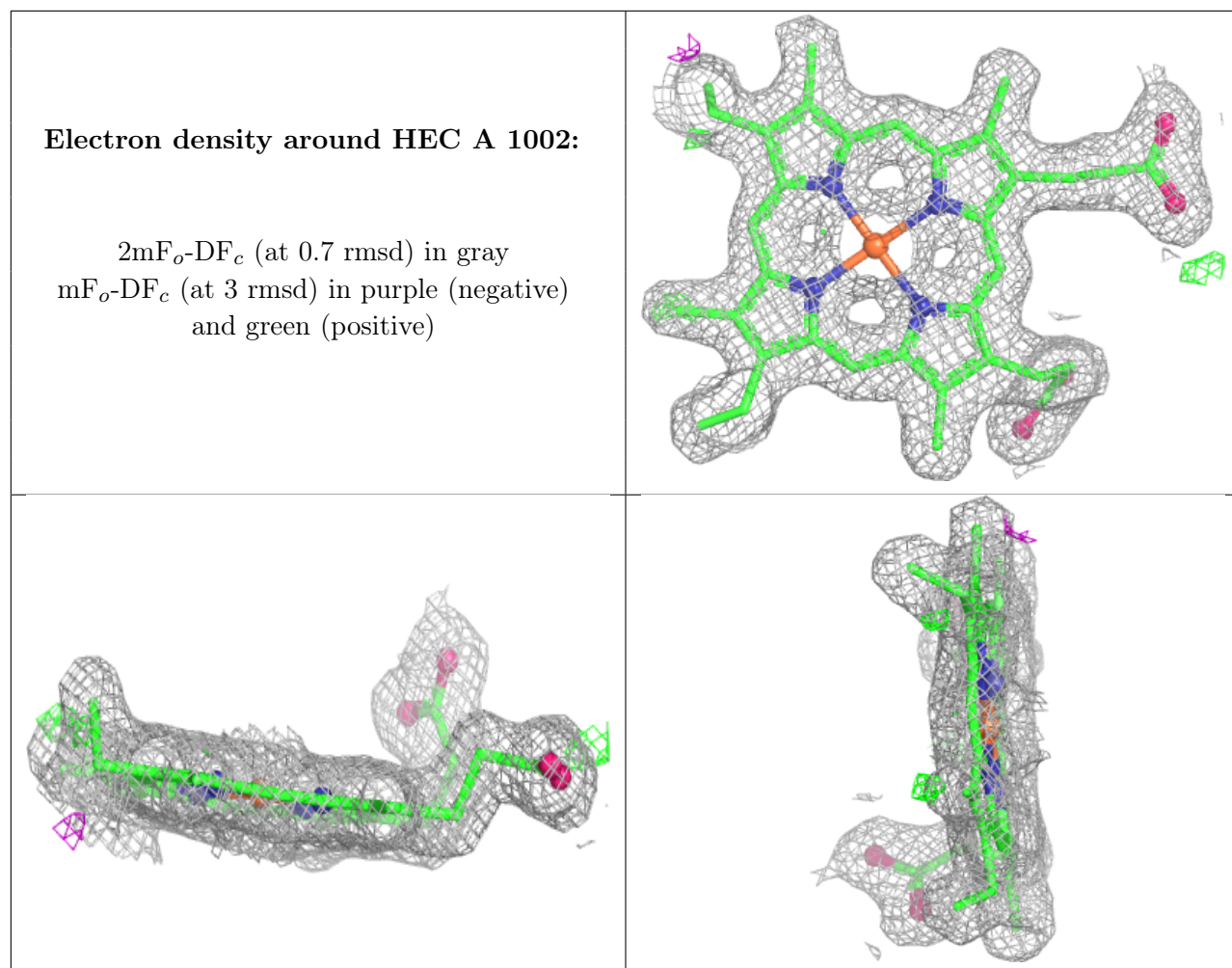
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC B 1006:

$2mF_o-DF_c$ (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.