



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:49 AM JST

PDB ID : 5ZE8 / pdb_00005ze8
Title : Crystal structure of a penta-heme cytochrome c552 from *Thermochromatium tepidum*
Authors : Yu, L.-J.; Chen, J.-H.; Shen, J.-R.
Deposited on : 2018-02-27
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

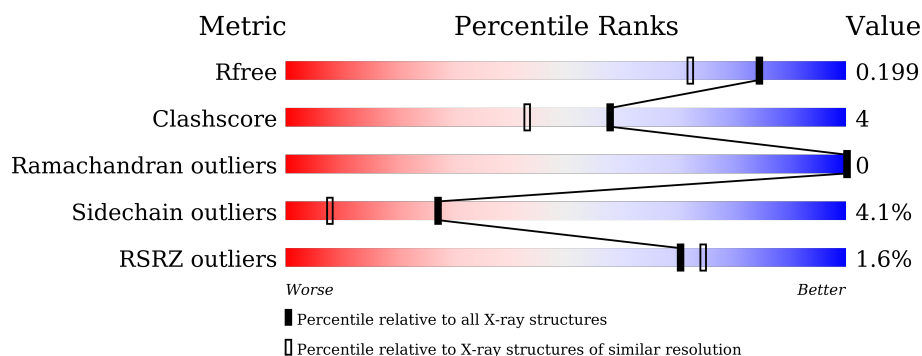
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	435	

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	501	X	-	-	-
2	HEC	A	502	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	503	X	-	-	-
2	HEC	A	504	X	-	-	-
2	HEC	A	505	X	-	-	-

2 Entry composition [i](#)

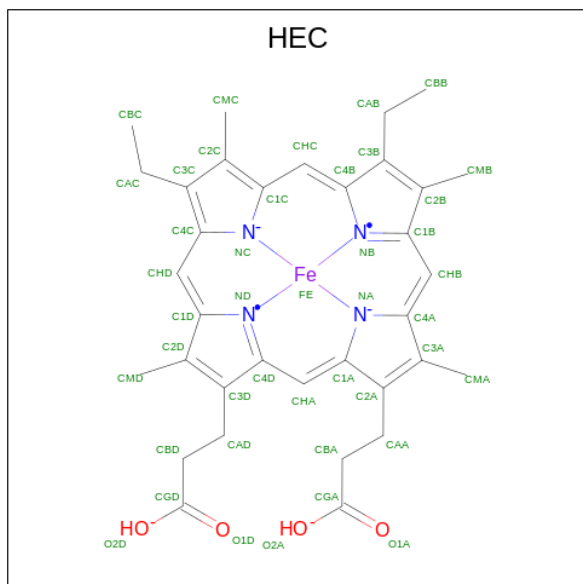
There are 5 unique types of molecules in this entry. The entry contains 3560 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called cytochrome c552.

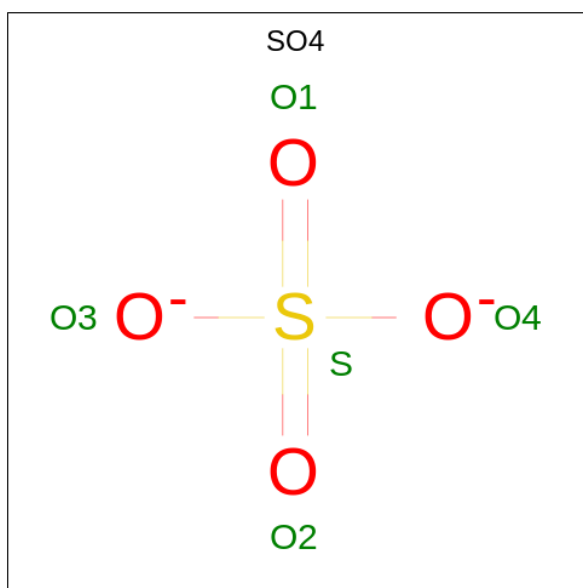
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	1	0
			2983	1874	529	561	19			

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



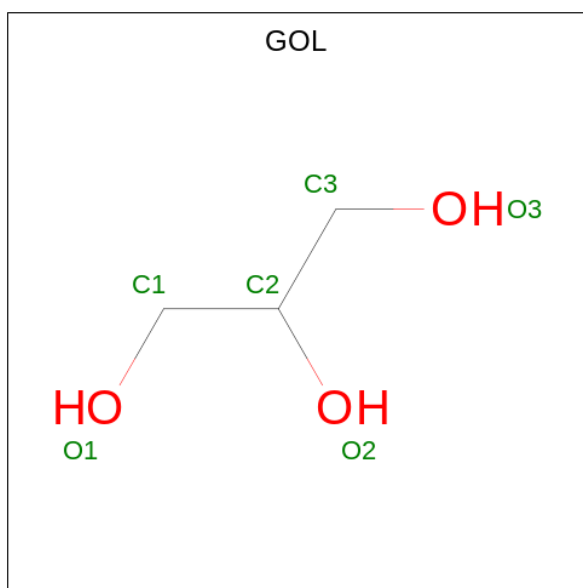
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	351	Total 351	O 351	0	0

- Molecule 1: cytochrome c552



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.70Å 39.10Å 68.65Å 90.00° 109.31° 90.00°	Depositor
Resolution (Å)	68.28 – 1.60 68.28 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.28-1.60) 99.9 (68.28-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.158 , 0.191 0.170 , 0.199	Depositor DCC
R_{free} test set	2437 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3560	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 10.13% 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: SO4, GOL, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.40	15/3061 (0.5%)	1.26	11/4160 (0.3%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	LYS	N-CA	6.93	1.54	1.46
1	A	283	ARG	CA-C	-6.80	1.43	1.52
1	A	92	LYS	CA-C	-6.24	1.45	1.52
1	A	422	LEU	CA-C	-6.11	1.45	1.52
1	A	54	ARG	CD-NE	-5.86	1.38	1.46
1	A	371	LYS	CA-C	5.74	1.59	1.52
1	A	230	ASP	N-CA	5.69	1.53	1.46
1	A	35	GLU	C-N	5.42	1.40	1.33
1	A	77	GLN	C-O	5.27	1.30	1.24
1	A	300	ALA	C-O	-5.25	1.17	1.24
1	A	339	ALA	CA-C	-5.19	1.46	1.52
1	A	375	ASP	CA-C	-5.17	1.46	1.52
1	A	281	LEU	C-O	-5.14	1.18	1.24
1	A	280	MET	N-CA	-5.03	1.40	1.46
1	A	211	THR	N-CA	-5.01	1.40	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	GLY	N-CA-C	6.86	120.95	112.73
1	A	238	VAL	CA-C-N	-6.40	113.36	119.76
1	A	238	VAL	C-N-CA	-6.40	113.36	119.76
1	A	163	ILE	CB-CA-C	-5.76	105.27	110.91
1	A	226	MET	CG-SD-CE	-5.69	88.39	100.90
1	A	207	ILE	CA-C-N	-5.37	114.72	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ILE	C-N-CA	-5.37	114.72	120.03
1	A	434	PRO	N-CA-C	5.26	119.44	111.19
1	A	54	ARG	NE-CZ-NH1	5.18	126.68	121.50
1	A	278	GLU	O-C-N	-5.15	116.66	122.12
1	A	198	GLU	N-CA-C	5.01	114.06	108.25

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	2983	0	2900	27	0
2	A	215	0	150	3	0
3	A	5	0	0	0	0
4	A	6	0	8	0	0
5	A	351	0	0	13	0
All	All	3560	0	3058	28	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLU:OE2	5:A:601:HOH:O	1.98	0.81
1:A:341:ASP:OD1	5:A:602:HOH:O	2.01	0.79
1:A:163:ILE:HD11	1:A:220:ARG:HH21	1.55	0.71
1:A:371:LYS:HD2	5:A:640:HOH:O	1.93	0.68
1:A:163:ILE:HD11	1:A:220:ARG:NH2	2.11	0.65
1:A:50:GLU:HG3	5:A:867:HOH:O	1.99	0.62
1:A:385:GLU:HG3	5:A:806:HOH:O	2.00	0.61
1:A:301:GLN:HB3	5:A:806:HOH:O	2.03	0.58
1:A:397:LEU:HG	5:A:620:HOH:O	2.02	0.58
1:A:226:MET:HA	1:A:226:MET:HE2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:MET:HA	1:A:88:MET:HE2	1.90	0.54
1:A:245:LYS:NZ	5:A:610:HOH:O	2.43	0.51
1:A:43:GLU:OE2	1:A:53:TYR:OH	2.28	0.50
1:A:201:GLU:OE1	1:A:206:THR:HG22	2.12	0.50
1:A:284:SER:HB2	1:A:308:GLN:NE2	2.27	0.49
1:A:326:THR:N	5:A:605:HOH:O	2.45	0.48
2:A:505:HEC:CGD	2:A:505:HEC:HHA	2.44	0.48
1:A:78:GLN:HG2	1:A:79:GLU:HG3	1.96	0.47
1:A:74:LEU:HD11	1:A:415:PHE:CD1	2.50	0.46
1:A:226:MET:HE1	2:A:505:HEC:HBB3	1.96	0.46
1:A:301:GLN:HG2	5:A:806:HOH:O	2.15	0.46
1:A:163:ILE:CD1	1:A:220:ARG:HH21	2.26	0.46
1:A:37:ILE:HG22	5:A:859:HOH:O	2.16	0.45
1:A:341:ASP:CG	5:A:602:HOH:O	2.59	0.43
1:A:82:ASP:OD1	1:A:84:THR:OG1	2.26	0.42
1:A:309:PRO:HD3	2:A:505:HEC:HBC2	2.02	0.41
1:A:301:GLN:CG	5:A:806:HOH:O	2.68	0.41
1:A:278:GLU:OE1	1:A:282:LYS:NZ	2.30	0.40

There are no symmetry-related clashes.

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	A	382/435 (88%)	370 (97%)	12 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	316/352 (90%)	303 (96%)	13 (4%)	27 8

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	50	GLU
1	A	78	GLN
1	A	203	ASP
1	A	206	THR
1	A	217	ARG
1	A	241	CYS
1	A	285	ILE
1	A	292	LYS
1	A	318	PHE
1	A	321	LEU
1	A	417	GLN
1	A	434	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	106	ASN
1	A	111	GLN
1	A	215	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	A	501	1	50,50,50	1.47	8 (16%)	68,82,82	1.88	18 (26%)
2	HEC	A	503	1	50,50,50	1.29	7 (14%)	68,82,82	1.64	12 (17%)
2	HEC	A	505	1	50,50,50	1.36	7 (14%)	68,82,82	1.82	14 (20%)
2	HEC	A	504	1	50,50,50	1.31	6 (12%)	68,82,82	1.47	12 (17%)
4	GOL	A	507	-	5,5,5	0.44	0	5,5,5	0.46	0
2	HEC	A	502	1	50,50,50	1.34	7 (14%)	68,82,82	1.60	16 (23%)
3	SO4	A	506	-	4,4,4	0.72	0	6,6,6	0.67	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
2	HEC	A	501	1	1/1/3/7	9/14/54/54	-
2	HEC	A	503	1	1/1/3/7	6/14/54/54	-
2	HEC	A	505	1	1/1/3/7	7/14/54/54	-
2	HEC	A	504	1	1/1/3/7	8/14/54/54	-
4	GOL	A	507	-	-	2/4/4/4	-
2	HEC	A	502	1	1/1/3/7	4/14/54/54	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEC	C4B-NB	-3.93	1.33	1.40
2	A	501	HEC	FE-NB	3.66	2.06	1.94
2	A	502	HEC	C1B-NB	-3.32	1.32	1.38
2	A	501	HEC	FE-NC	3.23	2.06	1.95
2	A	505	HEC	C4B-NB	-3.13	1.34	1.40
2	A	503	HEC	FE-NB	3.10	2.04	1.94
2	A	502	HEC	FE-NB	3.08	2.04	1.94
2	A	504	HEC	C1C-NC	-3.07	1.33	1.39
2	A	505	HEC	FE-NB	3.06	2.04	1.94
2	A	501	HEC	CBC-CAC	-3.05	1.37	1.51
2	A	503	HEC	C1B-NB	-2.89	1.32	1.38
2	A	501	HEC	C4D-C3D	2.77	1.49	1.45
2	A	505	HEC	C4D-C3D	2.77	1.49	1.45
2	A	504	HEC	FE-NB	2.69	2.03	1.94
2	A	502	HEC	C4B-C3B	2.63	1.49	1.45
2	A	503	HEC	C1D-C2D	2.63	1.49	1.44
2	A	504	HEC	CHD-C1D	2.55	1.43	1.38
2	A	501	HEC	CMB-C2B	2.51	1.56	1.50
2	A	503	HEC	O2D-CGD	-2.50	1.22	1.30
2	A	504	HEC	C1C-C2C	2.47	1.49	1.43
2	A	505	HEC	FE-NC	2.45	2.03	1.95
2	A	503	HEC	CBB-CAB	-2.45	1.40	1.51
2	A	501	HEC	C4B-C3B	2.41	1.49	1.45
2	A	504	HEC	CBC-CAC	-2.41	1.40	1.51
2	A	505	HEC	O2D-CGD	-2.40	1.22	1.30
2	A	505	HEC	CBB-CAB	-2.40	1.40	1.51
2	A	503	HEC	C4D-C3D	2.39	1.49	1.45
2	A	502	HEC	CHD-C1D	2.39	1.43	1.38
2	A	504	HEC	C4D-C3D	2.39	1.49	1.45
2	A	502	HEC	C1D-ND	-2.36	1.36	1.40
2	A	501	HEC	C4D-ND	-2.29	1.34	1.38
2	A	503	HEC	C4A-C3A	-2.27	1.40	1.45
2	A	505	HEC	CBC-CAC	-2.23	1.41	1.51
2	A	502	HEC	O1A-CGA	2.13	1.29	1.22
2	A	502	HEC	CBB-CAB	-2.11	1.42	1.51

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	505	HEC	C3D-C4D-ND	6.35	116.51	110.36
2	A	503	HEC	CHB-C1B-NB	5.01	129.86	124.42
2	A	501	HEC	CHA-C4D-ND	4.71	129.53	124.42
2	A	503	HEC	C4B-NB-C1B	4.64	109.86	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEC	CAA-CBA-CGA	-4.38	104.19	113.60
2	A	501	HEC	CAD-CBD-CGD	4.30	122.85	113.60
2	A	505	HEC	CHB-C1B-NB	4.27	129.05	124.42
2	A	505	HEC	C4C-NC-C1C	4.06	109.32	105.35
2	A	501	HEC	CHD-C1D-ND	3.88	129.16	124.37
2	A	502	HEC	CHB-C4A-NA	-3.70	120.44	124.44
2	A	505	HEC	C1D-ND-C4D	-3.55	101.41	105.07
2	A	501	HEC	CMB-C2B-C1B	-3.51	119.69	125.04
2	A	505	HEC	CAC-C3C-C2C	3.48	132.44	126.86
2	A	505	HEC	C4D-C3D-C2D	-3.43	101.90	106.90
2	A	502	HEC	C1B-C2B-C3B	3.35	110.48	106.96
2	A	502	HEC	O2A-CGA-O1A	-3.28	115.13	123.30
2	A	503	HEC	C1A-CHA-C4D	-3.26	119.03	126.06
2	A	502	HEC	C4A-NA-C1A	-3.25	102.17	105.35
2	A	502	HEC	C4B-NB-C1B	3.23	108.41	105.07
2	A	501	HEC	C1B-C2B-C3B	3.23	110.35	106.96
2	A	501	HEC	CBC-CAC-C3C	3.15	121.11	112.43
2	A	501	HEC	C1A-CHA-C4D	-3.11	119.35	126.06
2	A	503	HEC	CAB-C3B-C2B	3.07	132.77	127.53
2	A	504	HEC	CHC-C4B-NB	3.05	128.13	124.37
2	A	501	HEC	CHA-C1A-NA	3.03	127.72	124.44
2	A	502	HEC	C4B-C3B-C2B	-3.02	102.49	106.90
2	A	505	HEC	CAB-C3B-C2B	3.00	132.66	127.53
2	A	501	HEC	C4B-NB-C1B	2.99	108.16	105.07
2	A	505	HEC	C4B-NB-C1B	2.96	108.13	105.07
2	A	503	HEC	CHA-C1A-NA	2.95	127.63	124.44
2	A	502	HEC	CAB-C3B-C2B	2.93	132.54	127.53
2	A	503	HEC	CBC-CAC-C3C	2.83	120.24	112.43
2	A	501	HEC	CHA-C4D-C3D	-2.83	120.69	124.84
2	A	502	HEC	CBD-CAD-C3D	-2.83	104.78	112.63
2	A	504	HEC	C1C-C2C-C3C	-2.80	103.55	106.83
2	A	503	HEC	CAB-C3B-C4B	-2.80	121.18	124.81
2	A	505	HEC	CHA-C4D-C3D	-2.74	120.82	124.84
2	A	505	HEC	CHC-C1C-NC	2.73	128.87	123.85
2	A	504	HEC	CBC-CAC-C3C	2.68	119.82	112.43
2	A	503	HEC	CBA-CAA-C2A	-2.63	105.31	112.63
2	A	501	HEC	C4B-C3B-C2B	-2.63	103.06	106.90
2	A	504	HEC	CHB-C4A-NA	2.60	127.25	124.44
2	A	501	HEC	O2A-CGA-CBA	2.56	122.24	114.03
2	A	504	HEC	CHC-C1C-C2C	-2.55	120.03	127.24
2	A	502	HEC	C4C-NC-C1C	-2.53	102.87	105.35
2	A	504	HEC	C2C-C1C-NC	2.50	113.88	110.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	504	HEC	C4B-NB-C1B	2.48	107.63	105.07
2	A	505	HEC	CHB-C1B-C2B	-2.45	121.15	124.98
2	A	503	HEC	CHC-C4B-NB	2.42	127.36	124.37
2	A	502	HEC	CHC-C1C-NC	-2.37	119.49	123.85
2	A	502	HEC	O2A-CGA-CBA	2.36	121.62	114.03
2	A	505	HEC	C4A-C3A-C2A	2.35	110.37	106.94
2	A	501	HEC	CHC-C4B-NB	2.31	127.22	124.37
2	A	504	HEC	O2A-CGA-O1A	-2.28	117.61	123.30
2	A	503	HEC	CHA-C4D-ND	2.28	126.89	124.42
2	A	505	HEC	C1C-C2C-C3C	2.26	109.47	106.83
2	A	504	HEC	CAC-C3C-C4C	-2.24	121.80	124.92
2	A	501	HEC	O2A-CGA-O1A	-2.23	117.73	123.30
2	A	501	HEC	CAC-C3C-C2C	2.22	130.41	126.86
2	A	501	HEC	CBB-CAB-C3B	2.22	118.55	112.43
2	A	502	HEC	C2D-C1D-ND	2.21	112.45	109.84
2	A	502	HEC	CHA-C4D-ND	2.18	126.79	124.42
2	A	502	HEC	C1A-CHA-C4D	-2.18	121.36	126.06
2	A	502	HEC	C3C-C4C-NC	2.16	112.56	110.15
2	A	503	HEC	C1C-CHC-C4B	-2.16	121.22	126.34
2	A	504	HEC	CHA-C4D-ND	2.13	126.73	124.42
2	A	502	HEC	O2D-CGD-O1D	-2.13	117.99	123.30
2	A	504	HEC	C4C-CHD-C1D	-2.10	121.36	126.34
2	A	505	HEC	C4B-C3B-C2B	-2.07	103.89	106.90
2	A	501	HEC	CHD-C1D-C2D	-2.05	121.03	126.73
2	A	504	HEC	CAD-C3D-C4D	2.03	128.20	124.66
2	A	503	HEC	C2B-C1B-NB	-2.02	107.47	109.88

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	HEC	NA
2	A	502	HEC	NA
2	A	503	HEC	NA
2	A	504	HEC	NA
2	A	505	HEC	NA

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	507	GOL	O1-C1-C2-C3
2	A	501	HEC	C2C-C3C-CAC-CBC
2	A	501	HEC	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	504	HEC	C4C-C3C-CAC-CBC
2	A	504	HEC	C2C-C3C-CAC-CBC
2	A	502	HEC	C2B-C3B-CAB-CBB
2	A	501	HEC	C2B-C3B-CAB-CBB
2	A	504	HEC	C2B-C3B-CAB-CBB
2	A	502	HEC	C4B-C3B-CAB-CBB
2	A	503	HEC	C2B-C3B-CAB-CBB
2	A	505	HEC	C2B-C3B-CAB-CBB
2	A	501	HEC	C3D-CAD-CBD-CGD
2	A	503	HEC	C2C-C3C-CAC-CBC
2	A	505	HEC	C2C-C3C-CAC-CBC
2	A	502	HEC	C2C-C3C-CAC-CBC
2	A	505	HEC	C3D-CAD-CBD-CGD
4	A	507	GOL	O1-C1-C2-O2
2	A	503	HEC	C4C-C3C-CAC-CBC
2	A	502	HEC	C4C-C3C-CAC-CBC
2	A	505	HEC	C4C-C3C-CAC-CBC
2	A	504	HEC	C4B-C3B-CAB-CBB
2	A	503	HEC	C4B-C3B-CAB-CBB
2	A	501	HEC	C4B-C3B-CAB-CBB
2	A	505	HEC	C4B-C3B-CAB-CBB
2	A	503	HEC	CAD-CBD-CGD-O1D
2	A	501	HEC	CAD-CBD-CGD-O1D
2	A	503	HEC	CAD-CBD-CGD-O2D
2	A	505	HEC	CAA-CBA-CGA-O2A
2	A	505	HEC	CAA-CBA-CGA-O1A
2	A	501	HEC	CAA-CBA-CGA-O1A
2	A	501	HEC	CAA-CBA-CGA-O2A
2	A	501	HEC	CAD-CBD-CGD-O2D
2	A	504	HEC	C4D-C3D-CAD-CBD
2	A	504	HEC	CAA-CBA-CGA-O2A
2	A	504	HEC	CAA-CBA-CGA-O1A
2	A	504	HEC	C2D-C3D-CAD-CBD

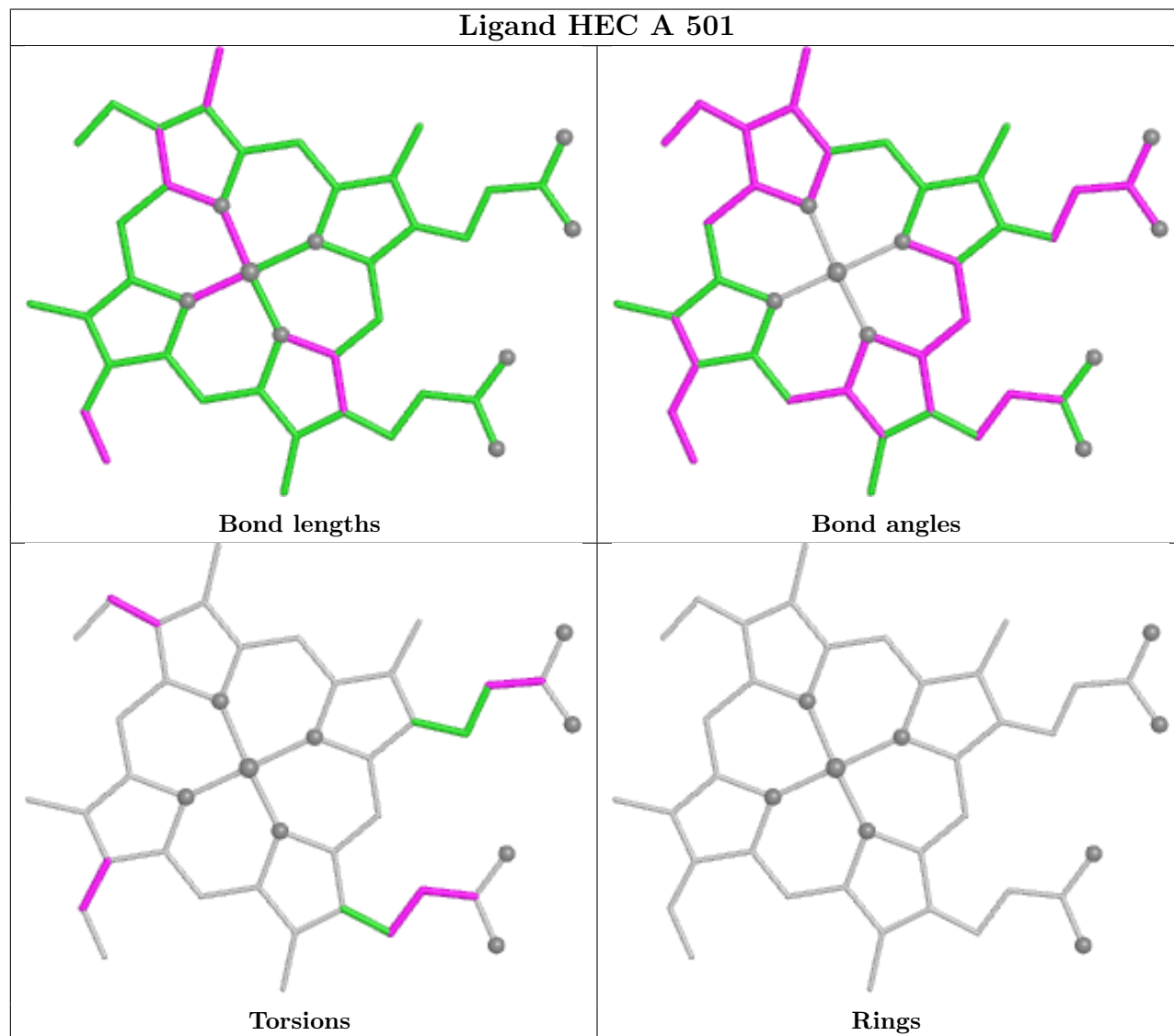
There are no ring outliers.

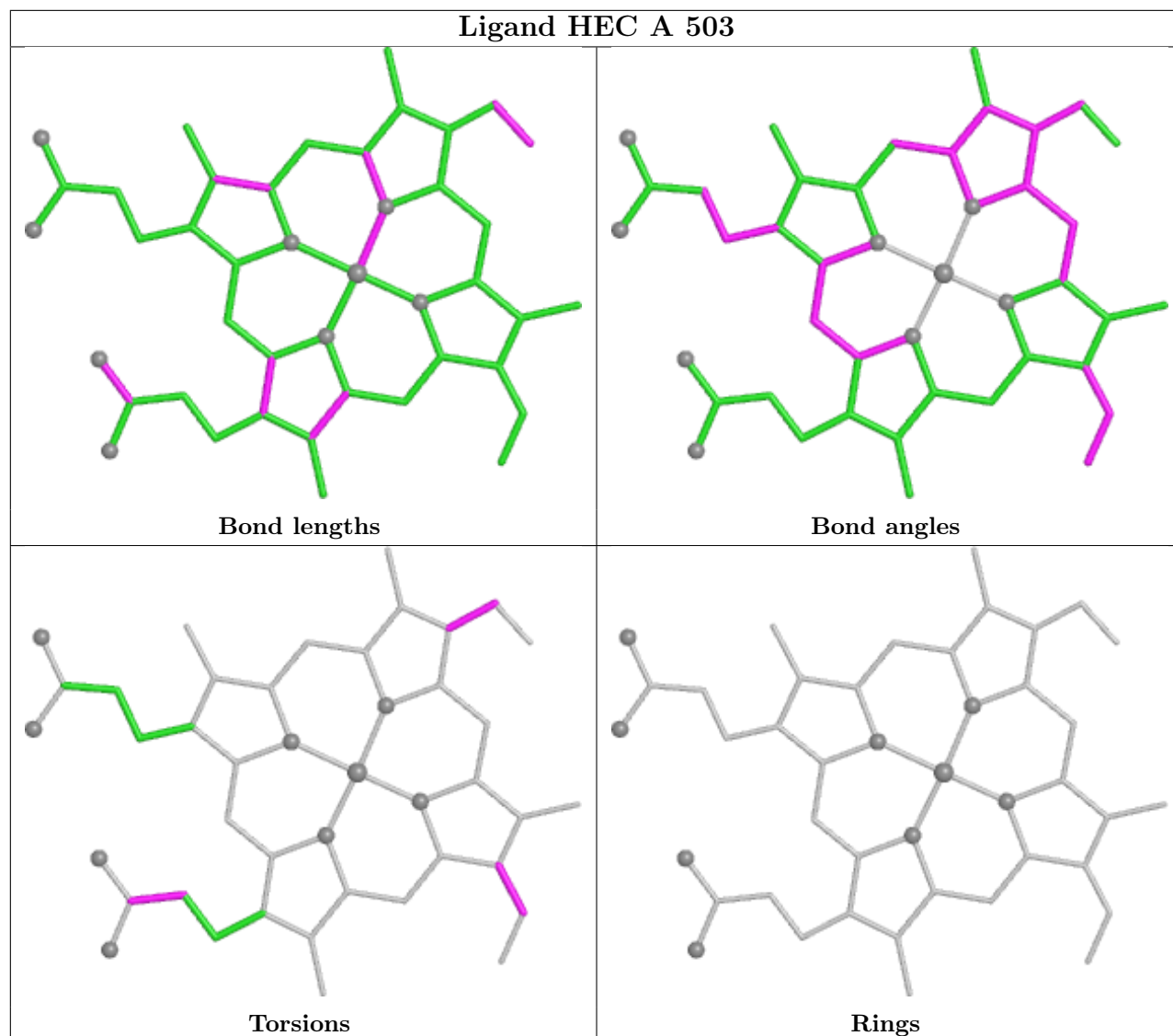
1 monomer is involved in 3 short contacts:

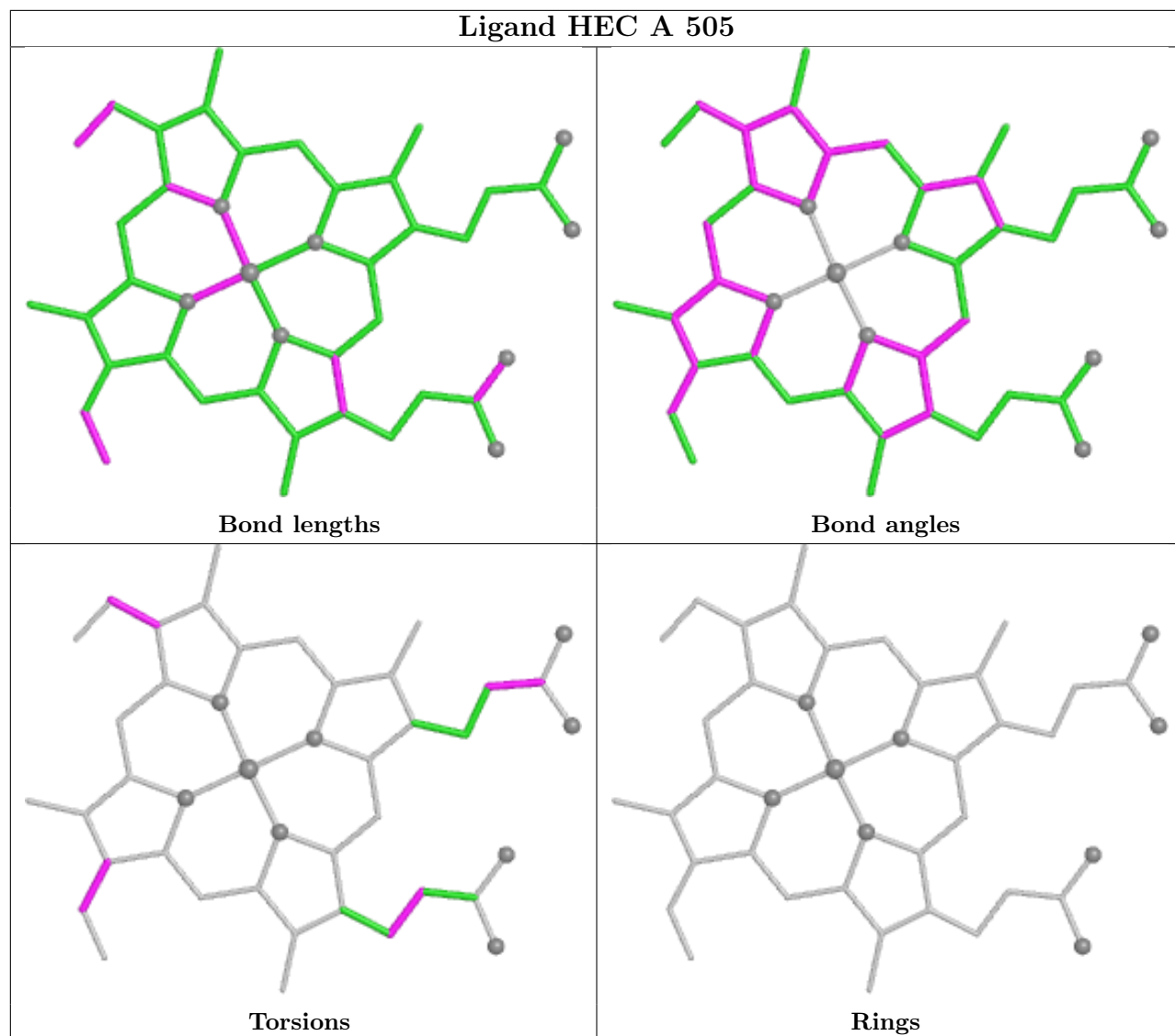
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	505	HEC	3	0

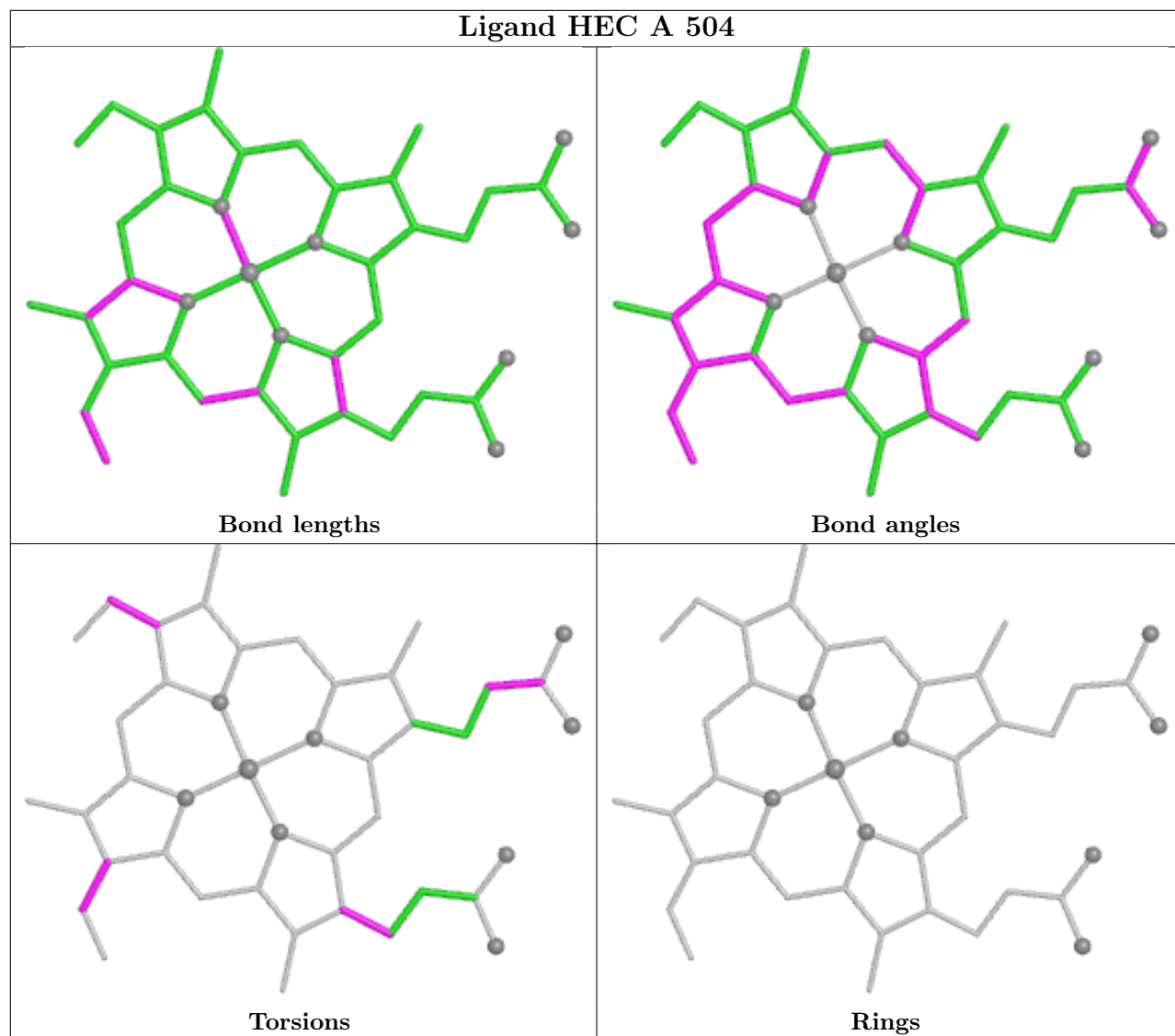
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

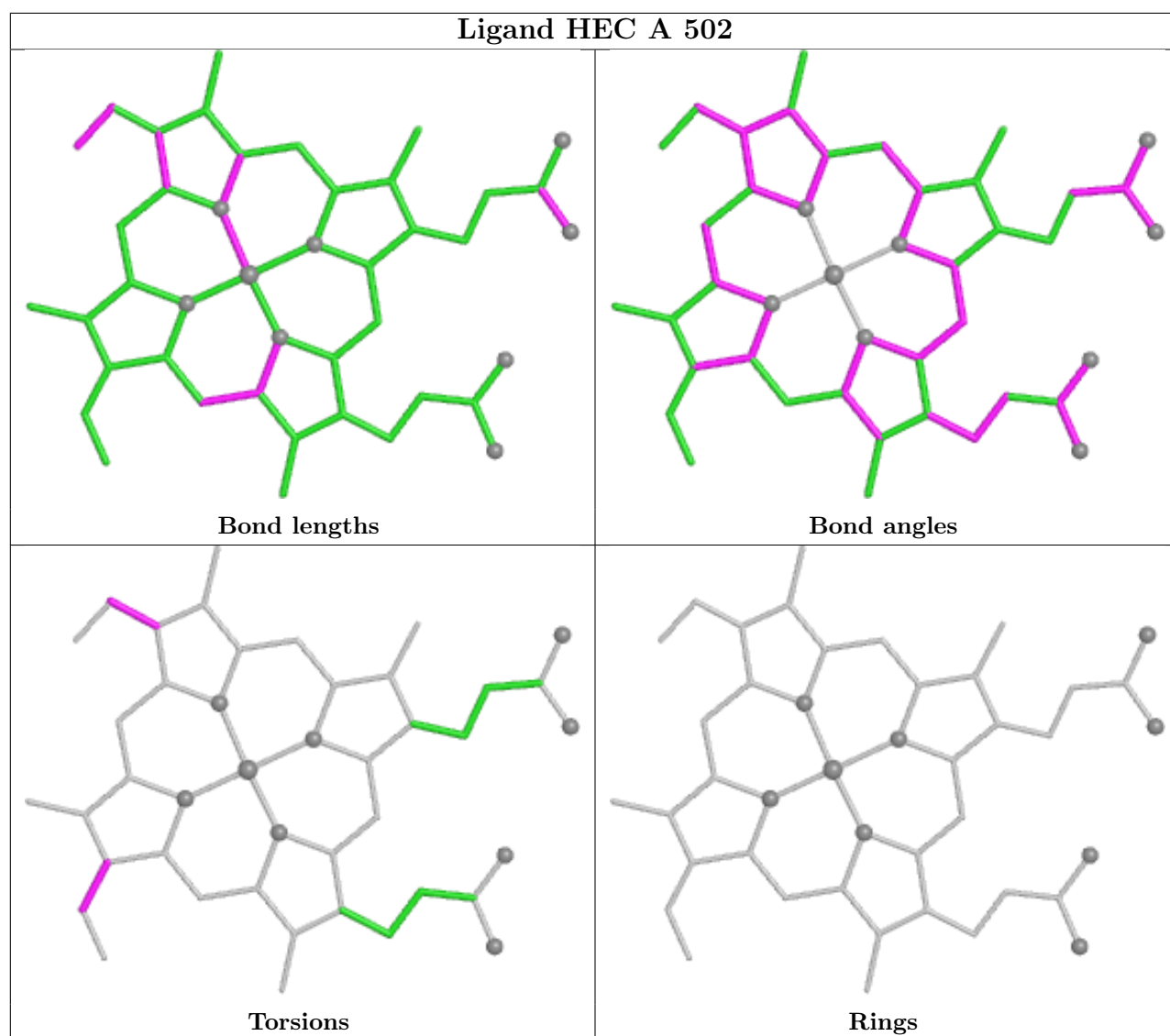
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	385/435 (88%)	0.02	6 (1%) 70 74	9, 18, 36, 54	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	ALA	2.5
1	A	142	ALA	2.4
1	A	303	TRP	2.4
1	A	341	ASP	2.4
1	A	292	LYS	2.1
1	A	249	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

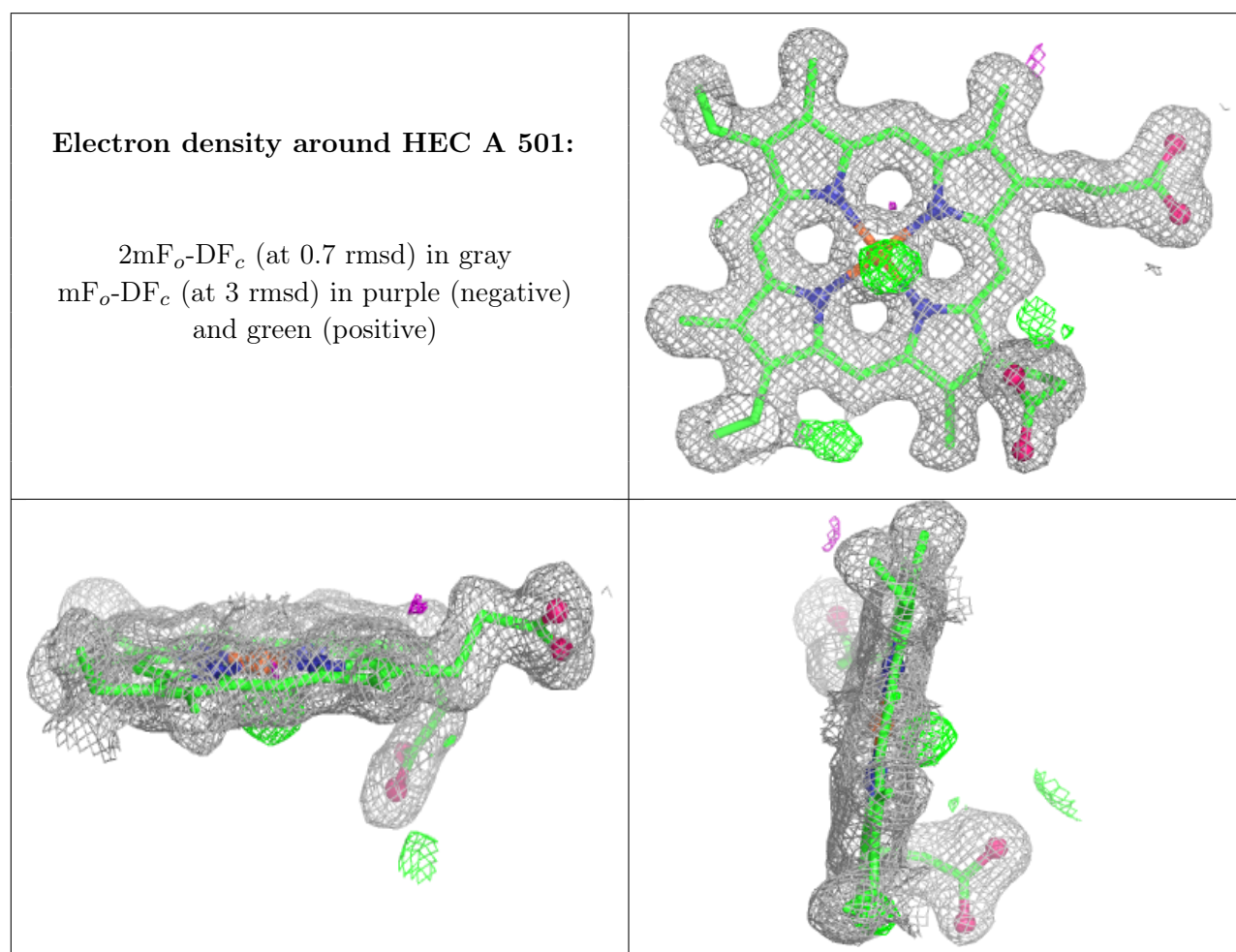
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	506	5/5	0.73	0.13	36,51,55,63	0

Continued on next page...

Continued from previous page...

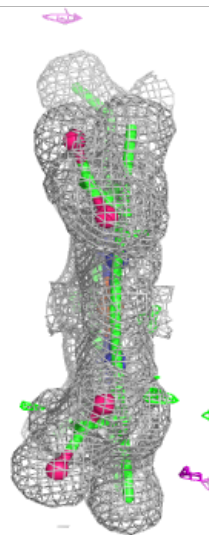
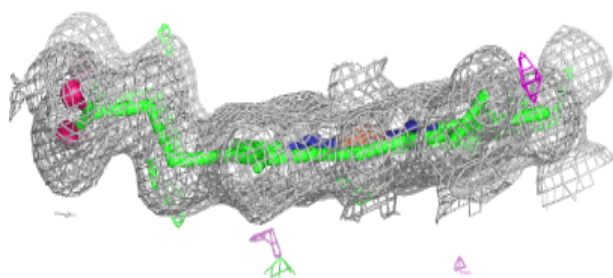
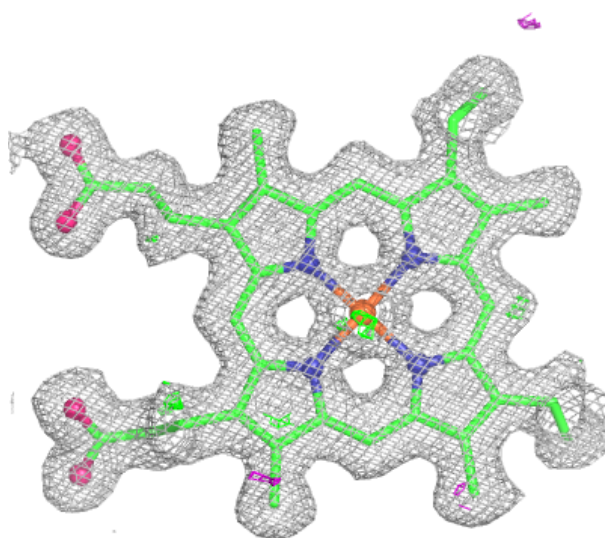
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	507	6/6	0.75	0.14	43,45,48,50	0
2	HEC	A	501	43/43	0.98	0.06	11,14,23,39	0
2	HEC	A	504	43/43	0.99	0.04	7,9,11,13	0
2	HEC	A	505	43/43	0.99	0.04	9,11,13,14	0
2	HEC	A	502	43/43	0.99	0.04	9,11,13,14	0
2	HEC	A	503	43/43	0.99	0.05	8,10,17,21	0

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



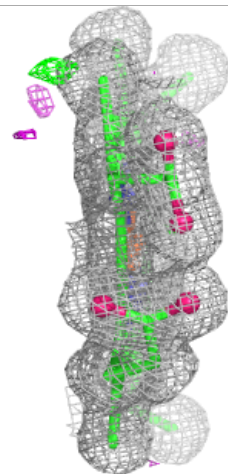
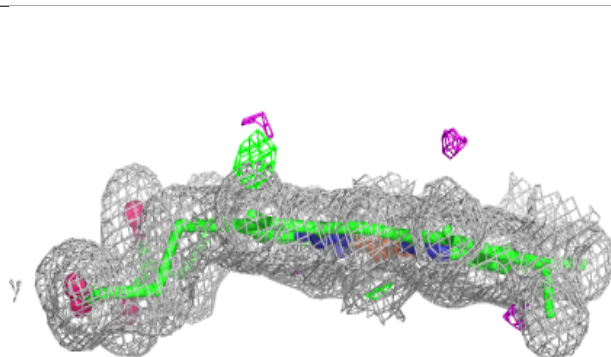
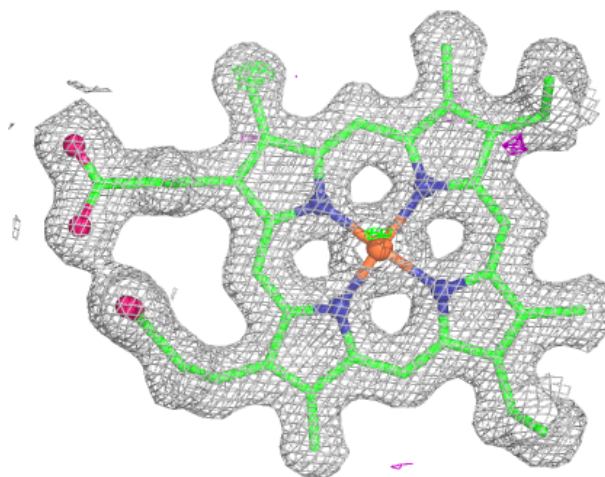
Electron density around HEC A 504:

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



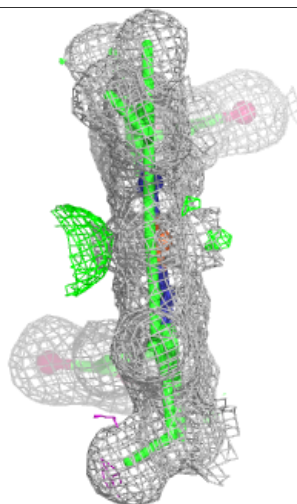
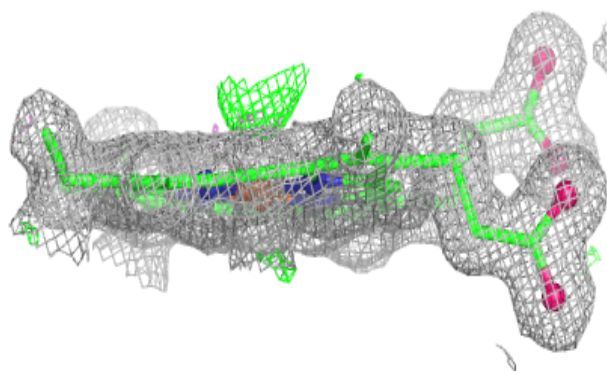
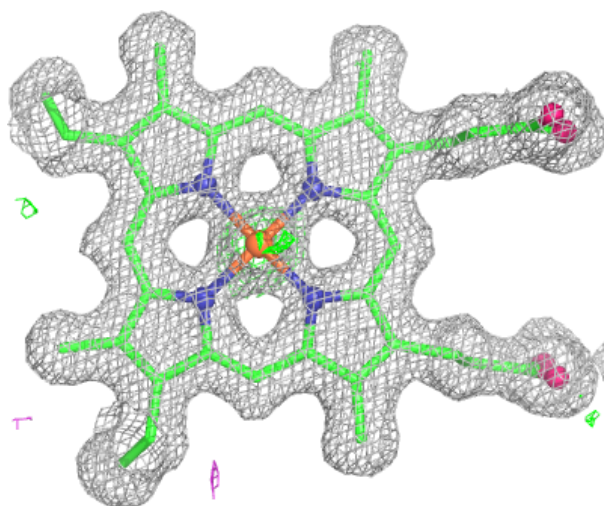
Electron density around HEC A 505:

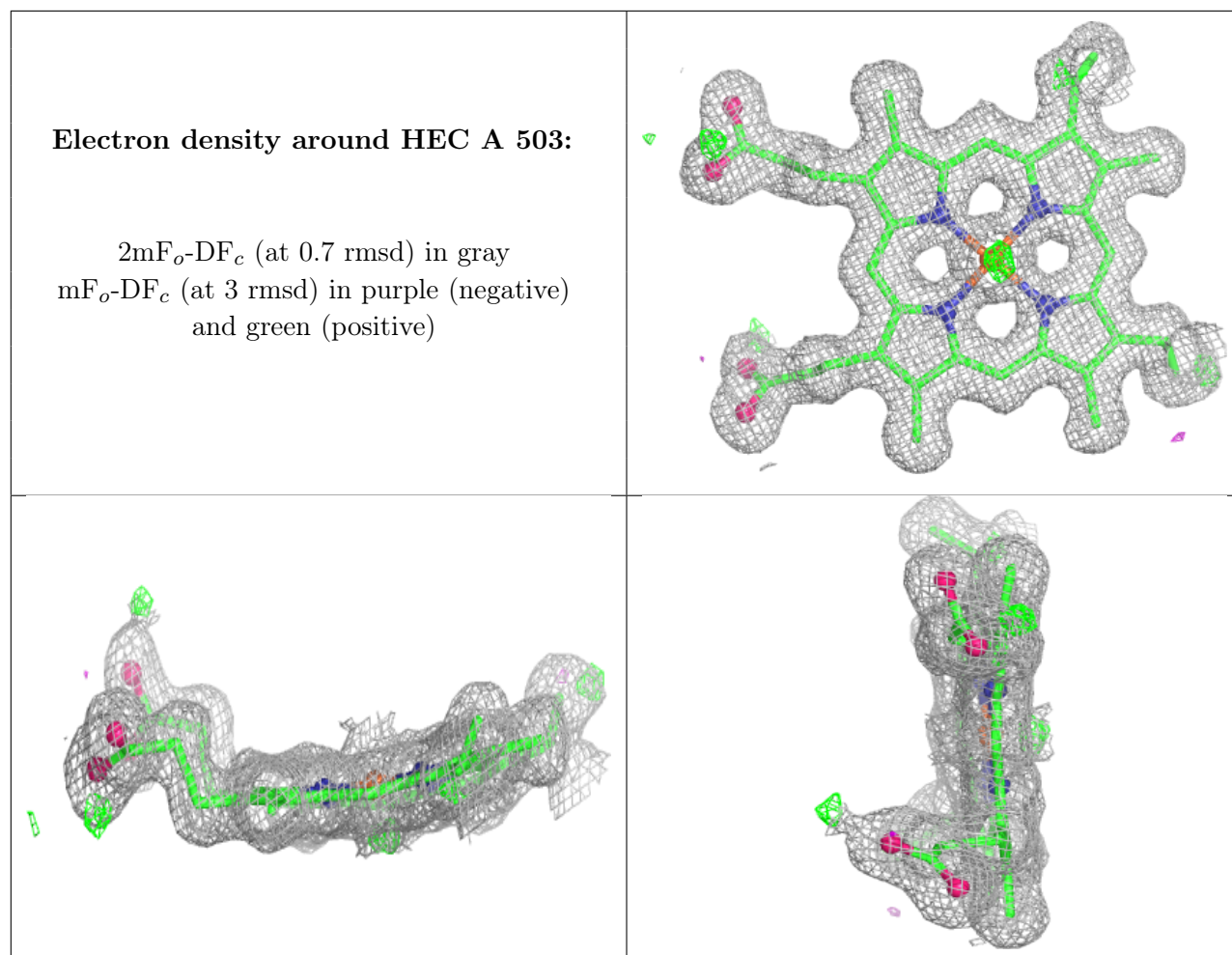
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 502:

$2mF_o-DF_c$ (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.