



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2023 – 07:52 AM EDT

PDB ID : 4L3H  
Title : Crystal Structure of the E113Q-MauG/pre-Methylamine Dehydrogenase Complex After Treatment with Hydrogen Peroxide  
Authors : Yukl, E.T.; Wilmot, C.M.  
Deposited on : 2013-06-05  
Resolution : 1.79 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

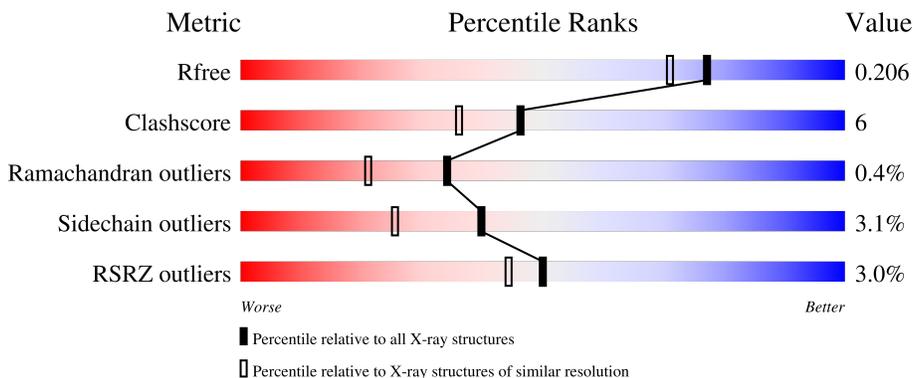
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 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	373	 3% 83% 10% • 5%
1	B	373	 % 85% 10% • •
2	C	137	 6% 78% 13% •• 6%
2	E	137	 % 70% 20% • 9%
3	D	385	 5% 83% 14% ••

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Mol	Chain	Length	Quality of chain
3	F	385	

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	0AF	E	57[B]	-	-	X	-
7	EDO	D	402	-	-	X	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 15313 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 Methylamine utilization protein MauG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	Total	C	N	O	S	0	10	0
			2828	1761	515	541	11			
1	B	357	Total	C	N	O	S	0	5	0
			2807	1747	506	543	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLN	GLU	engineered mutation	UNP Q51658
A	368	HIS	-	expression tag	UNP Q51658
A	369	HIS	-	expression tag	UNP Q51658
A	370	HIS	-	expression tag	UNP Q51658
A	371	HIS	-	expression tag	UNP Q51658
A	372	HIS	-	expression tag	UNP Q51658
A	373	HIS	-	expression tag	UNP Q51658
B	113	GLN	GLU	engineered mutation	UNP Q51658
B	368	HIS	-	expression tag	UNP Q51658
B	369	HIS	-	expression tag	UNP Q51658
B	370	HIS	-	expression tag	UNP Q51658
B	371	HIS	-	expression tag	UNP Q51658
B	372	HIS	-	expression tag	UNP Q51658
B	373	HIS	-	expression tag	UNP Q51658

- Molecule 2 is a protein called Methylamine dehydrogenase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	129	Total	C	N	O	S	0	4	0
			1031	641	178	198	14			
2	E	125	Total	C	N	O	S	0	5	0
			998	621	166	196	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	expression tag	UNP A1BBA0
C	133	HIS	-	expression tag	UNP A1BBA0
C	134	HIS	-	expression tag	UNP A1BBA0
C	135	HIS	-	expression tag	UNP A1BBA0
C	136	HIS	-	expression tag	UNP A1BBA0
C	137	HIS	-	expression tag	UNP A1BBA0
E	132	HIS	-	expression tag	UNP A1BBA0
E	133	HIS	-	expression tag	UNP A1BBA0
E	134	HIS	-	expression tag	UNP A1BBA0
E	135	HIS	-	expression tag	UNP A1BBA0
E	136	HIS	-	expression tag	UNP A1BBA0
E	137	HIS	-	expression tag	UNP A1BBA0

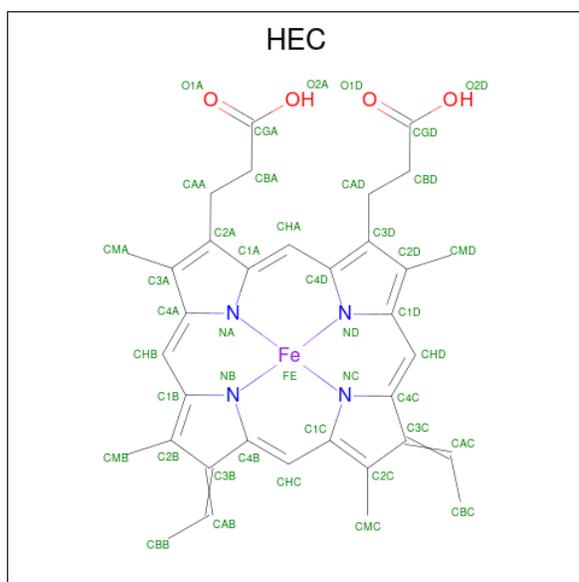
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	376	Total	C	N	O	S	0	5	0
			2961	1877	508	568	8			
3	F	376	Total	C	N	O	S	0	6	0
			2971	1882	512	568	9			

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

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

- Molecule 5 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).

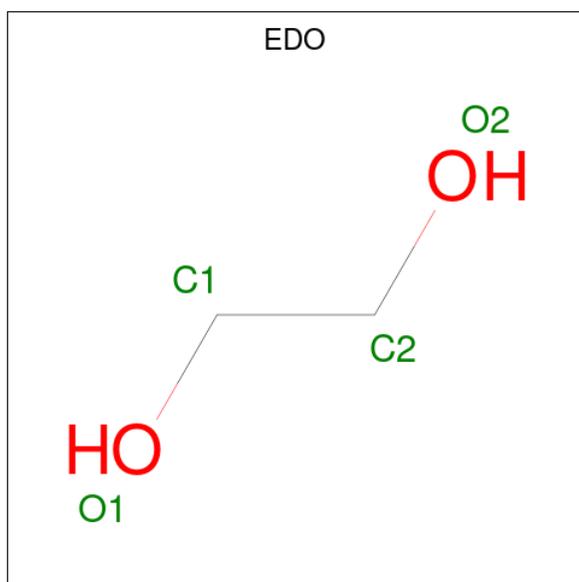


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
5	A	1	43	34	1	4	4	0	0
5	A	1	43	34	1	4	4	0	0
5	B	1	43	34	1	4	4	0	0
5	B	1	43	34	1	4	4	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

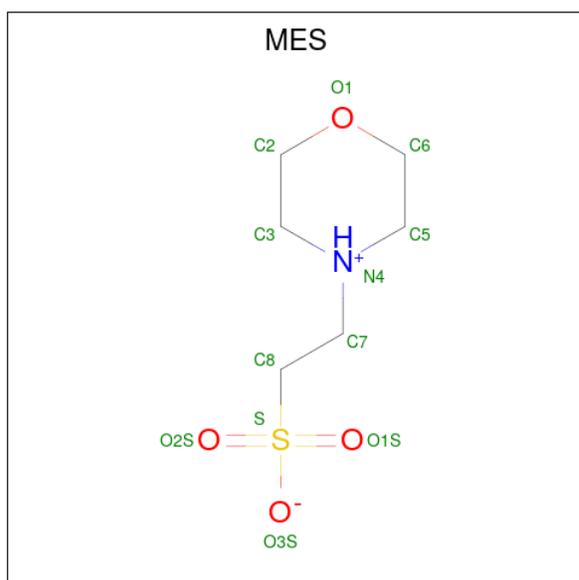
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	A	2	2	2	0	0
6	B	2	2	2	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



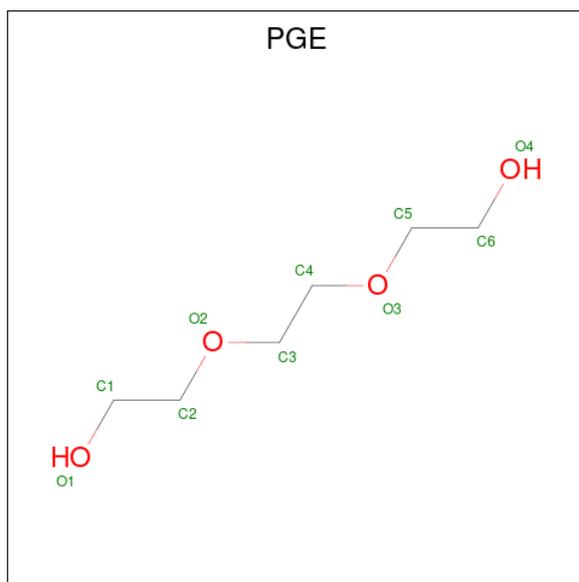
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
8	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is water.

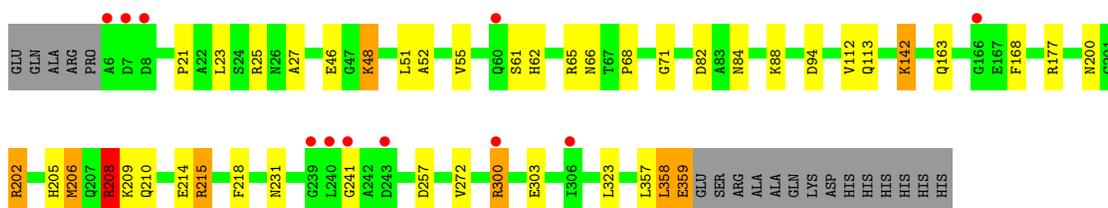
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	232	Total	O	0	3
			235	235		
10	B	372	Total	O	0	6
			378	378		
10	C	82	Total	O	0	1
			83	83		
10	D	255	Total	O	0	3
			258	258		
10	E	117	Total	O	0	2
			119	119		
10	F	408	Total	O	0	8
			416	416		

### 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.

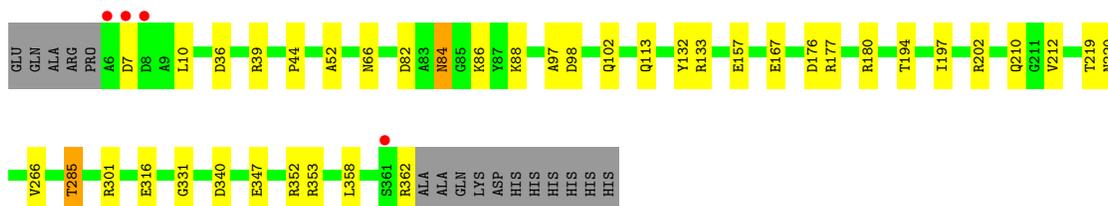
- Molecule 1: Methylamine utilization protein MauG

Chain A: 



- Molecule 1: Methylamine utilization protein MauG

Chain B: 



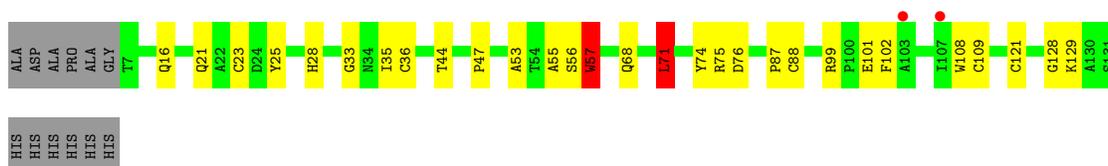
- Molecule 2: Methylamine dehydrogenase light chain

Chain C: 

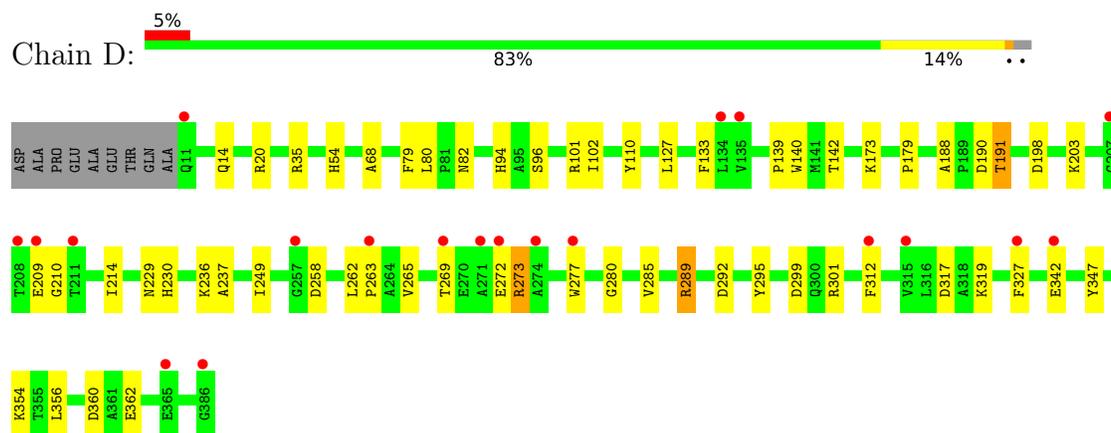


- Molecule 2: Methylamine dehydrogenase light chain

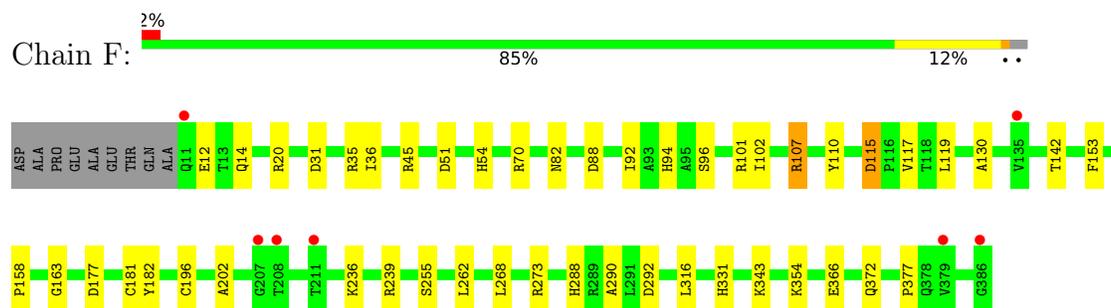
Chain E: 



- Molecule 3: Methylamine dehydrogenase heavy chain



- Molecule 3: Methylamine dehydrogenase heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.53Å 83.52Å 107.78Å 109.94° 91.54° 105.78°	Depositor
Resolution (Å)	44.49 – 1.79 44.49 – 1.79	Depositor EDS
% Data completeness (in resolution range)	97.0 (44.49-1.79) 97.0 (44.49-1.79)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.154 , 0.198 0.162 , 0.206	Depositor DCC
$R_{free}$ test set	7881 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtrriage
Anisotropy	0.192	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15313	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, CA, MES, HEC, OAF, PGE, 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	0.82	0/2895	0.93	3/3922 (0.1%)
1	B	1.01	2/2871 (0.1%)	1.00	9/3893 (0.2%)
2	C	0.91	0/1034	0.96	2/1413 (0.1%)
2	E	1.07	0/1000	1.05	2/1366 (0.1%)
3	D	0.86	0/3038	0.97	4/4140 (0.1%)
3	F	1.03	0/3051	1.06	8/4155 (0.2%)
All	All	0.94	2/13889 (0.0%)	0.99	28/18889 (0.1%)

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
2	C	0	6
2	E	0	1
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	THR	CB-CG2	-5.49	1.34	1.52
1	B	132	TYR	CE1-CZ	-5.07	1.31	1.38

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	129	LYS	O-C-N	-6.84	111.76	122.70
1	B	177	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	B	98	ASP	CB-CG-OD1	5.89	123.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	101	ARG	NE-CZ-NH1	5.83	123.21	120.30
3	F	88	ASP	CB-CG-OD1	5.78	123.50	118.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	129	LYS	Peptide,Mainchain
2	C	130[A]	ALA	Peptide
2	C	130[B]	ALA	Peptide
2	C	57[B]	0AF	Mainchain
2	E	57[B]	0AF	Mainchain

## 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	2828	0	2703	37	0
1	B	2807	0	2667	23	0
2	C	1031	0	911	23	0
2	E	998	0	890	28	0
3	D	2961	0	2842	39	0
3	F	2971	0	2857	25	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	86	0	60	5	0
5	B	86	0	60	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	B	12	0	18	5	0
7	D	4	0	6	8	0
8	D	12	0	13	0	0
8	F	12	0	13	0	0
9	F	10	0	14	1	0
10	A	235	0	0	4	0
10	B	378	0	0	6	0
10	C	83	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	258	0	0	3	0
10	E	119	0	0	2	0
10	F	416	0	0	3	0
All	All	15313	0	13054	168	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 6.

The worst 5 of 168 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:215[A]:ARG:HG3	1:A:215[A]:ARG:HH11	0.97	1.08
1:A:215[A]:ARG:HG3	1:A:215[A]:ARG:NH1	1.72	0.96
1:A:206:MET:HA	1:A:206:MET:HE2	1.46	0.96
3:D:230:HIS:HA	7:D:402:EDO:H11	1.52	0.90
2:E:57[B]:0AF:HBC1	2:E:108[B]:TRP:NE1	1.87	0.90

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	362/373 (97%)	353 (98%)	8 (2%)	1 (0%)	41 27
1	B	360/373 (96%)	351 (98%)	9 (2%)	0	100 100
2	C	129/137 (94%)	123 (95%)	3 (2%)	3 (2%)	6 1
2	E	126/137 (92%)	123 (98%)	3 (2%)	0	100 100
3	D	379/385 (98%)	366 (97%)	11 (3%)	2 (0%)	29 15
3	F	380/385 (99%)	368 (97%)	11 (3%)	1 (0%)	41 27
All	All	1736/1790 (97%)	1684 (97%)	45 (3%)	7 (0%)	34 21

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	130[A]	ALA
2	C	130[B]	ALA
2	C	131	SER
1	A	358	LEU
3	D	102	ILE

### 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	286/292 (98%)	265 (93%)	21 (7%)	14 4
1	B	284/292 (97%)	278 (98%)	6 (2%)	53 42
2	C	110/112 (98%)	108 (98%)	2 (2%)	59 48
2	E	108/112 (96%)	105 (97%)	3 (3%)	43 30
3	D	308/310 (99%)	299 (97%)	9 (3%)	42 29
3	F	310/310 (100%)	304 (98%)	6 (2%)	57 46
All	All	1406/1428 (98%)	1359 (97%)	47 (3%)	40 23

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	71	LEU
3	D	258	ASP
3	D	20	ARG
3	D	173	LYS
3	D	354	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	163	GLN
3	F	30	GLN

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Mol	Chain	Res	Type
1	B	210	GLN
3	F	54	HIS
3	D	331	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	0AF	E	57[B]	2	13,16,17	1.22	1 (7%)	11,22,24	2.88	6 (54%)
2	0AF	C	57[A]	2	13,16,17	1.24	1 (7%)	11,22,24	1.22	1 (9%)
2	0AF	C	57[B]	2	13,16,17	0.87	0	11,22,24	1.65	1 (9%)
2	0AF	E	57[A]	2	13,16,17	1.10	1 (7%)	11,22,24	2.29	3 (27%)

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	0AF	E	57[B]	2	-	0/4/6/8	0/2/2/2
2	0AF	C	57[A]	2	-	0/4/6/8	0/2/2/2
2	0AF	C	57[B]	2	-	0/4/6/8	0/2/2/2
2	0AF	E	57[A]	2	-	0/4/6/8	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57[A]	0AF	CZ2-CE2	-2.20	1.39	1.42
2	E	57[A]	0AF	CZ2-CE2	-2.14	1.39	1.42
2	E	57[B]	0AF	CD1-NE1	-2.13	1.32	1.36

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57[B]	0AF	CB-CG-CD1	-7.01	119.30	127.97
2	E	57[A]	0AF	CG-CB-CA	5.51	123.05	114.53
2	C	57[B]	0AF	CB-CG-CD1	-3.96	123.07	127.97
2	E	57[B]	0AF	CH2-CZ2-CE2	3.29	124.04	120.12
2	E	57[A]	0AF	CB-CA-C	-3.12	105.62	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	57[B]	0AF	6	0
2	C	57[A]	0AF	4	0
2	C	57[B]	0AF	2	0
2	E	57[A]	0AF	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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
5	HEC	A	403	1	32,50,50	1.56	6 (18%)	24,82,82	2.05	7 (29%)
7	EDO	B	404	-	3,3,3	0.59	0	2,2,2	0.51	0
7	EDO	B	406	-	3,3,3	0.45	0	2,2,2	0.23	0
5	HEC	B	402	10,1	32,50,50	1.66	8 (25%)	24,82,82	2.54	11 (45%)
8	MES	D	401	-	12,12,12	1.76	1 (8%)	14,16,16	6.37	9 (64%)
5	HEC	B	403	1	32,50,50	1.61	7 (21%)	24,82,82	2.81	11 (45%)
9	PGE	F	402	-	9,9,9	0.46	0	8,8,8	0.61	0
7	EDO	D	402	-	3,3,3	0.48	0	2,2,2	0.90	0
8	MES	F	401	-	12,12,12	1.48	1 (8%)	14,16,16	6.84	8 (57%)
5	HEC	A	402	1	32,50,50	1.64	8 (25%)	24,82,82	2.46	13 (54%)
7	EDO	B	405	-	3,3,3	0.53	0	2,2,2	0.56	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
5	HEC	A	403	1	-	2/10/54/54	-
7	EDO	B	404	-	-	1/1/1/1	-
7	EDO	B	406	-	-	1/1/1/1	-
5	HEC	B	402	10,1	-	3/10/54/54	-
8	MES	D	401	-	-	4/6/14/14	0/1/1/1
5	HEC	B	403	1	-	2/10/54/54	-
9	PGE	F	402	-	-	5/7/7/7	-
7	EDO	D	402	-	-	0/1/1/1	-
8	MES	F	401	-	-	3/6/14/14	0/1/1/1
5	HEC	A	402	1	-	0/10/54/54	-
7	EDO	B	405	-	-	1/1/1/1	-

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	401	MES	C8-S	-5.45	1.69	1.77
8	F	401	MES	C8-S	-4.62	1.70	1.77
5	B	403	HEC	C3C-C4C	4.52	1.51	1.43
5	A	402	HEC	C2B-C3B	-3.56	1.37	1.40
5	B	403	HEC	CMD-C2D	-3.45	1.44	1.51

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	401	MES	O3S-S-C8	-14.84	81.77	105.77
8	D	401	MES	O3S-S-C8	-13.79	83.46	105.77
8	D	401	MES	O3S-S-O1S	-12.06	81.82	111.27
8	F	401	MES	O1S-S-C8	11.30	120.52	106.92
8	F	401	MES	O2S-S-C8	10.72	119.83	106.92

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

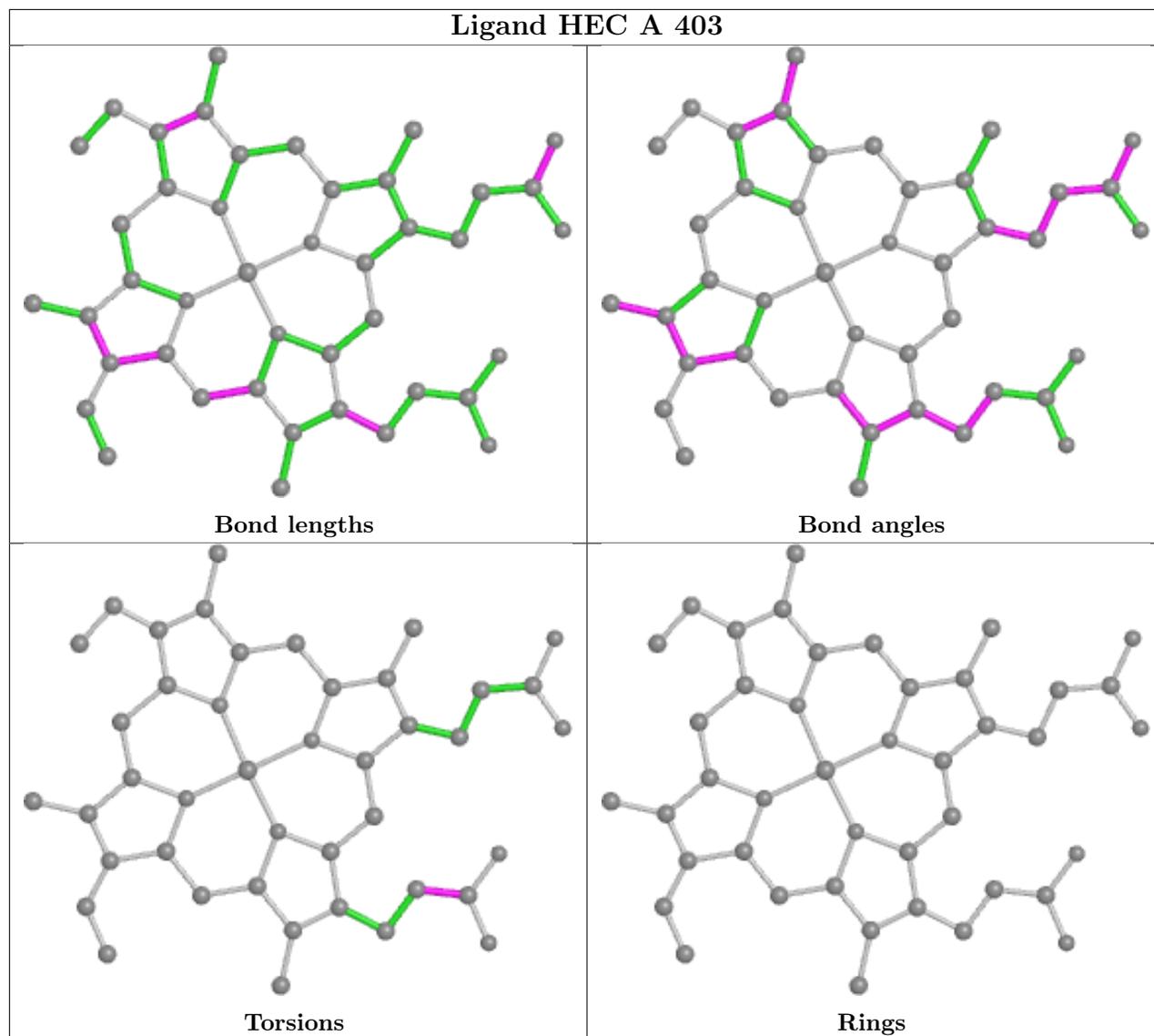
Mol	Chain	Res	Type	Atoms
8	F	401	MES	C7-C8-S-O2S
9	F	402	PGE	C6-C5-O3-C4
9	F	402	PGE	O2-C3-C4-O3
8	D	401	MES	C7-C8-S-O3S
7	B	404	EDO	O1-C1-C2-O2

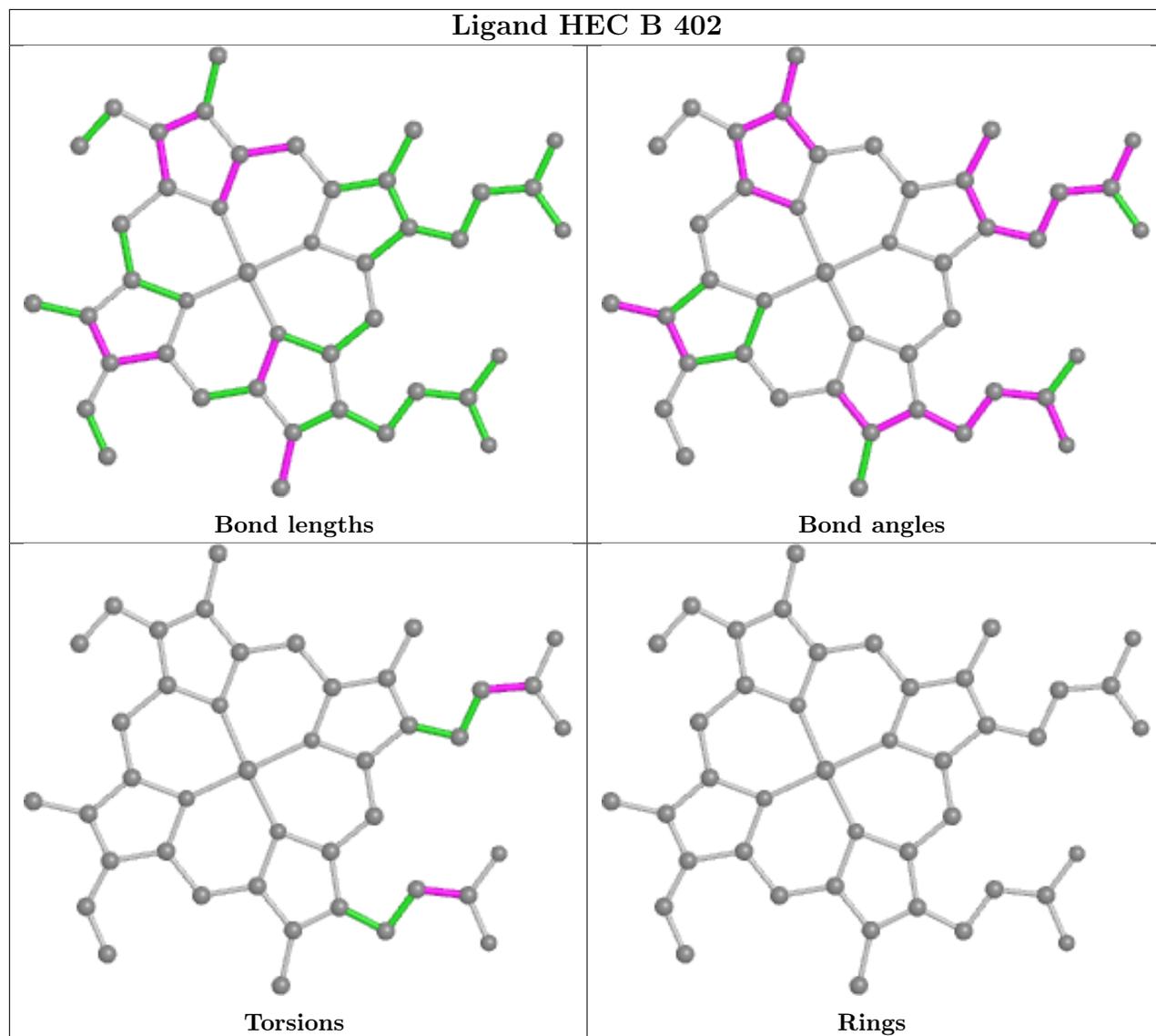
There are no ring outliers.

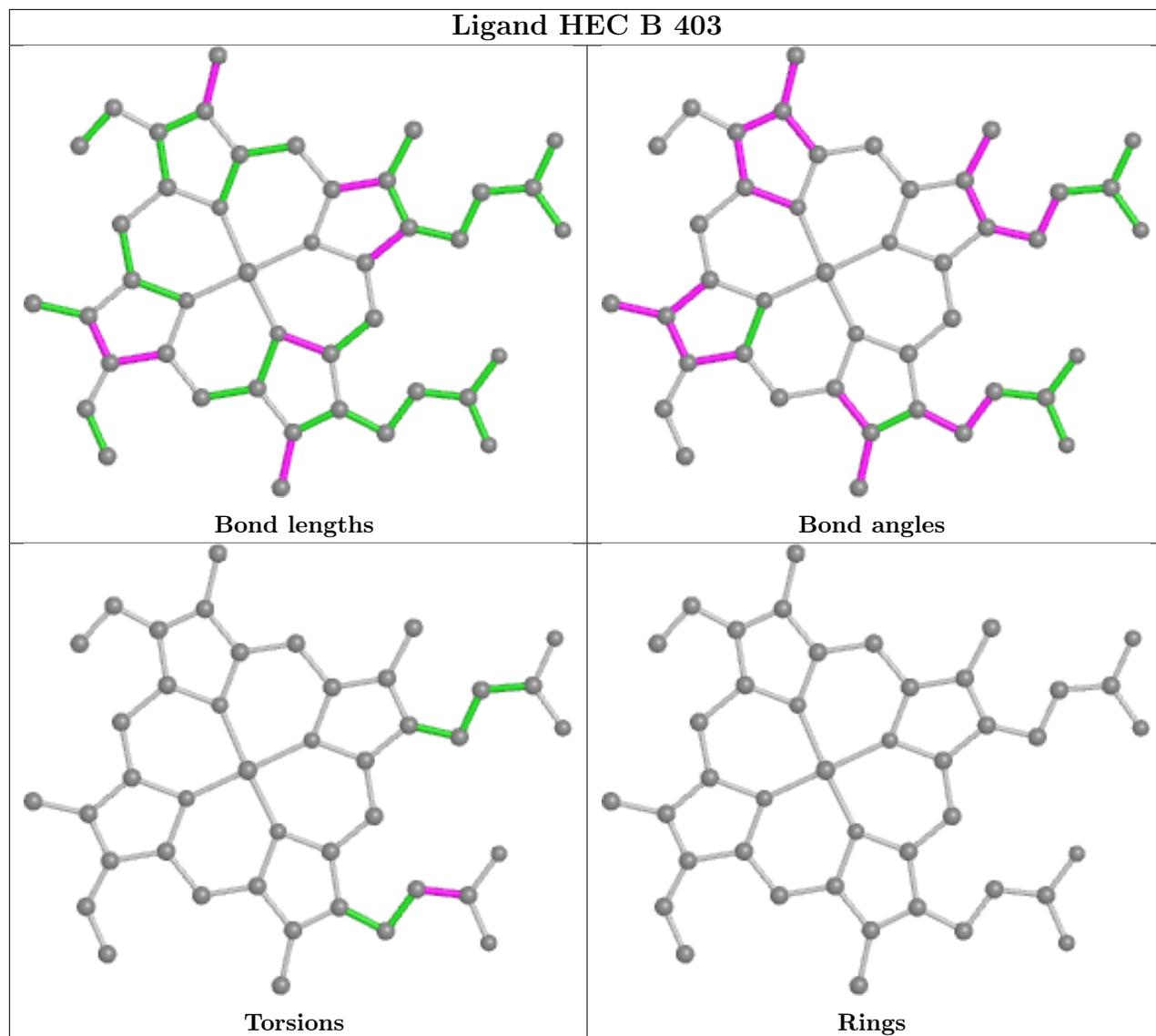
8 monomers are involved in 22 short contacts:

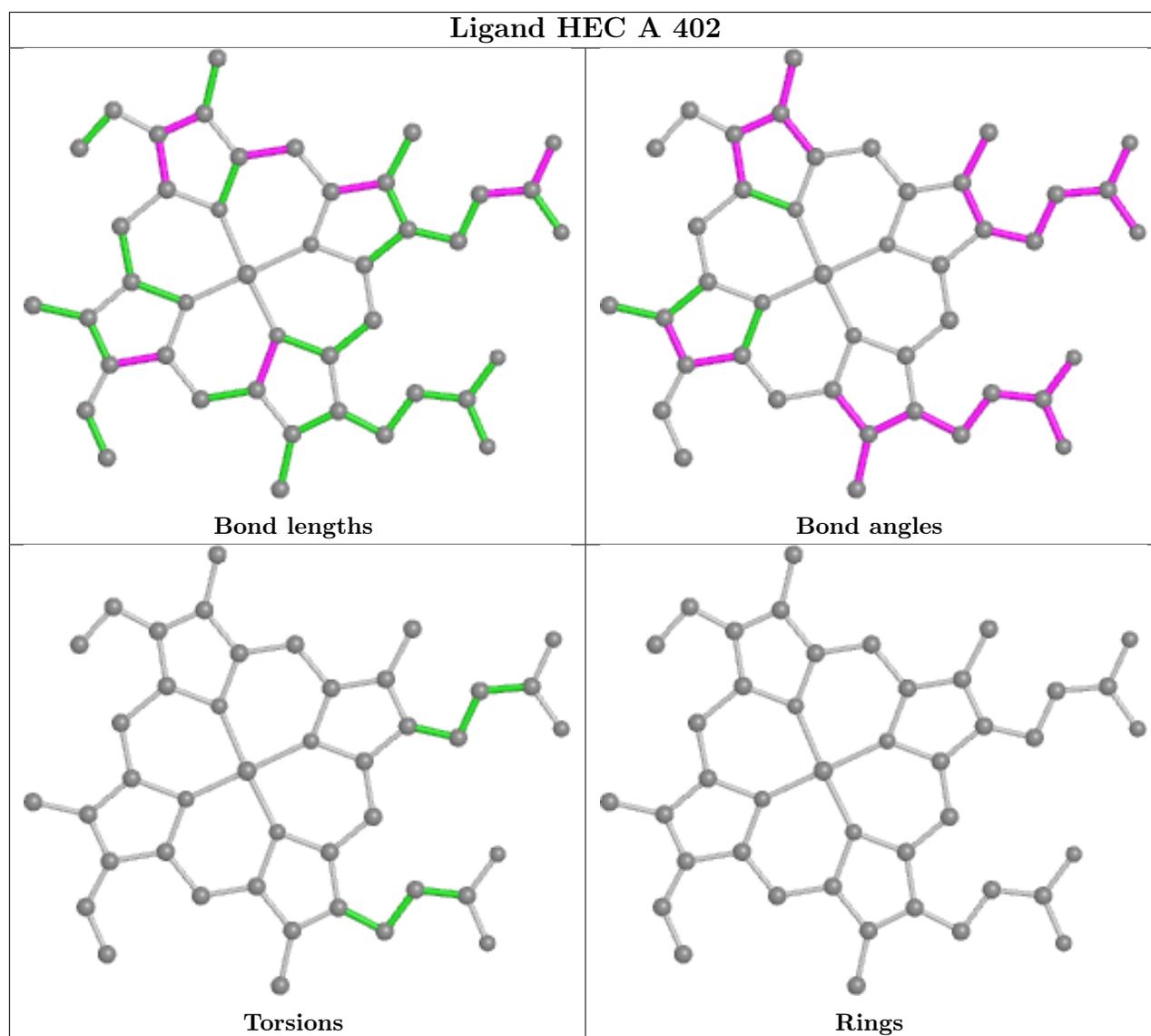
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	403	HEC	2	0
7	B	404	EDO	3	0
5	B	402	HEC	2	0
5	B	403	HEC	1	0
9	F	402	PGE	1	0
7	D	402	EDO	8	0
5	A	402	HEC	3	0
7	B	405	EDO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	354/373 (94%)	-0.13	11 (3%) 49 43	30, 42, 62, 75	0
1	B	357/373 (95%)	-0.36	4 (1%) 80 78	22, 32, 50, 80	0
2	C	128/137 (93%)	0.38	8 (6%) 20 15	26, 39, 69, 103	0
2	E	124/137 (90%)	0.05	2 (1%) 72 68	23, 28, 42, 72	0
3	D	376/385 (97%)	0.22	20 (5%) 26 21	26, 45, 73, 88	0
3	F	376/385 (97%)	-0.16	7 (1%) 66 63	21, 30, 47, 73	0
All	All	1715/1790 (95%)	-0.06	52 (3%) 50 44	21, 36, 64, 103	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	ALA	6.2
3	D	208	THR	6.1
1	A	6	ALA	5.9
3	D	271[A]	ALA	5.5
2	C	131	SER	5.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	0AF	C	57[A]	15/16	0.95	0.22	42,43,44,45	15
2	0AF	C	57[B]	15/16	0.95	0.22	42,43,44,45	15
2	0AF	E	57[A]	15/16	0.95	0.24	31,34,37,41	15
2	0AF	E	57[B]	15/16	0.95	0.24	31,34,37,41	15

### 6.3 Carbohydrates [i](#)

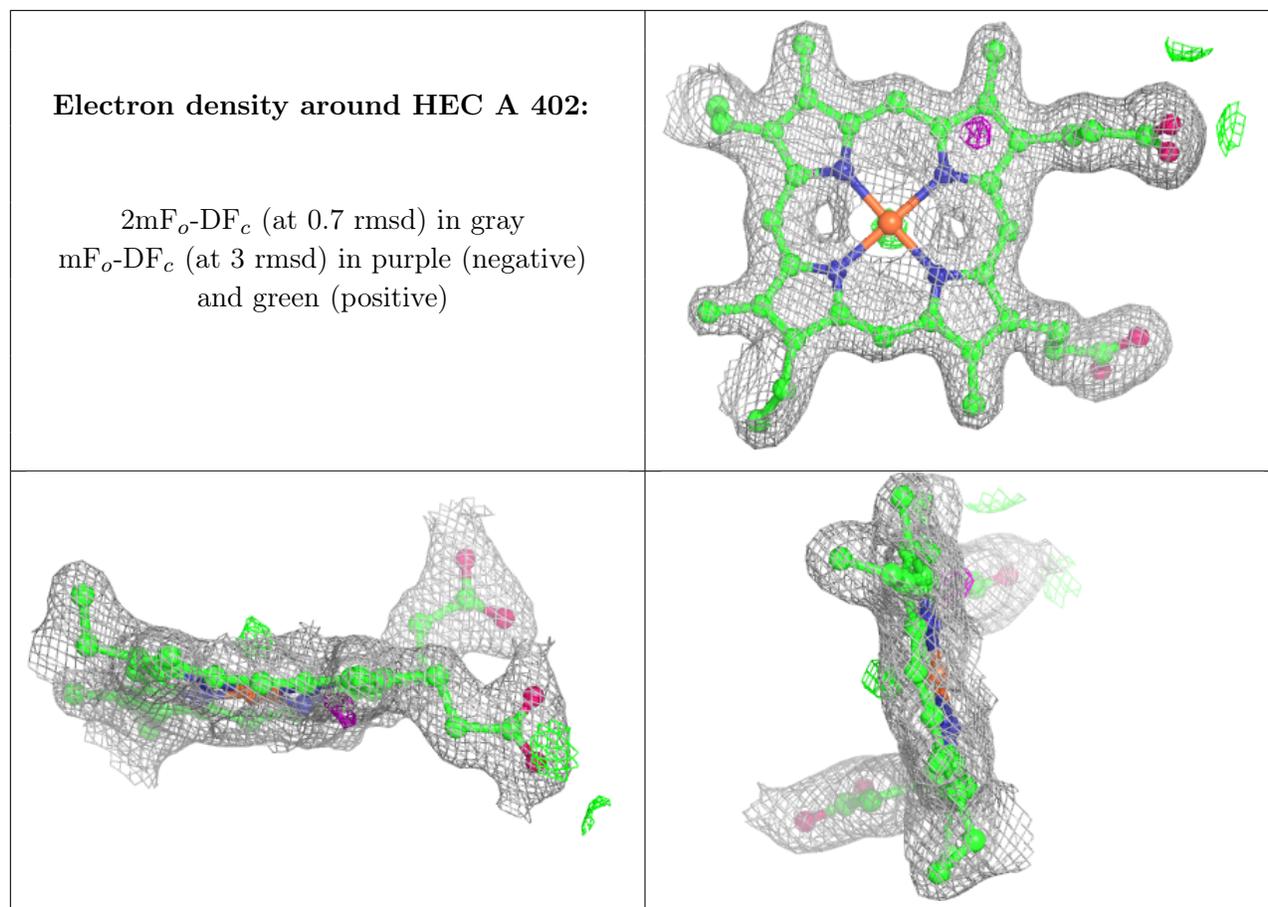
There are no monosaccharides in this entry.

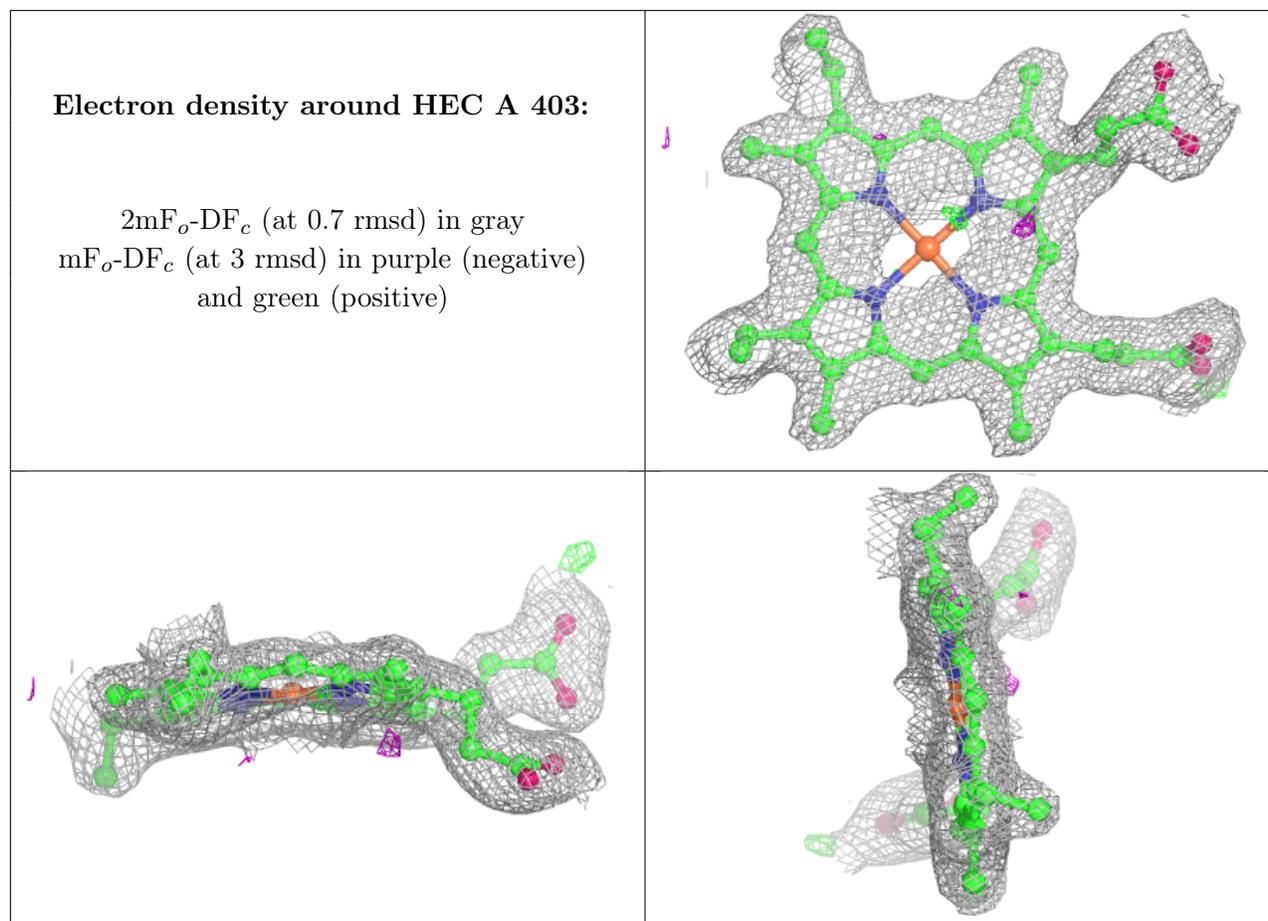
### 6.4 Ligands [i](#)

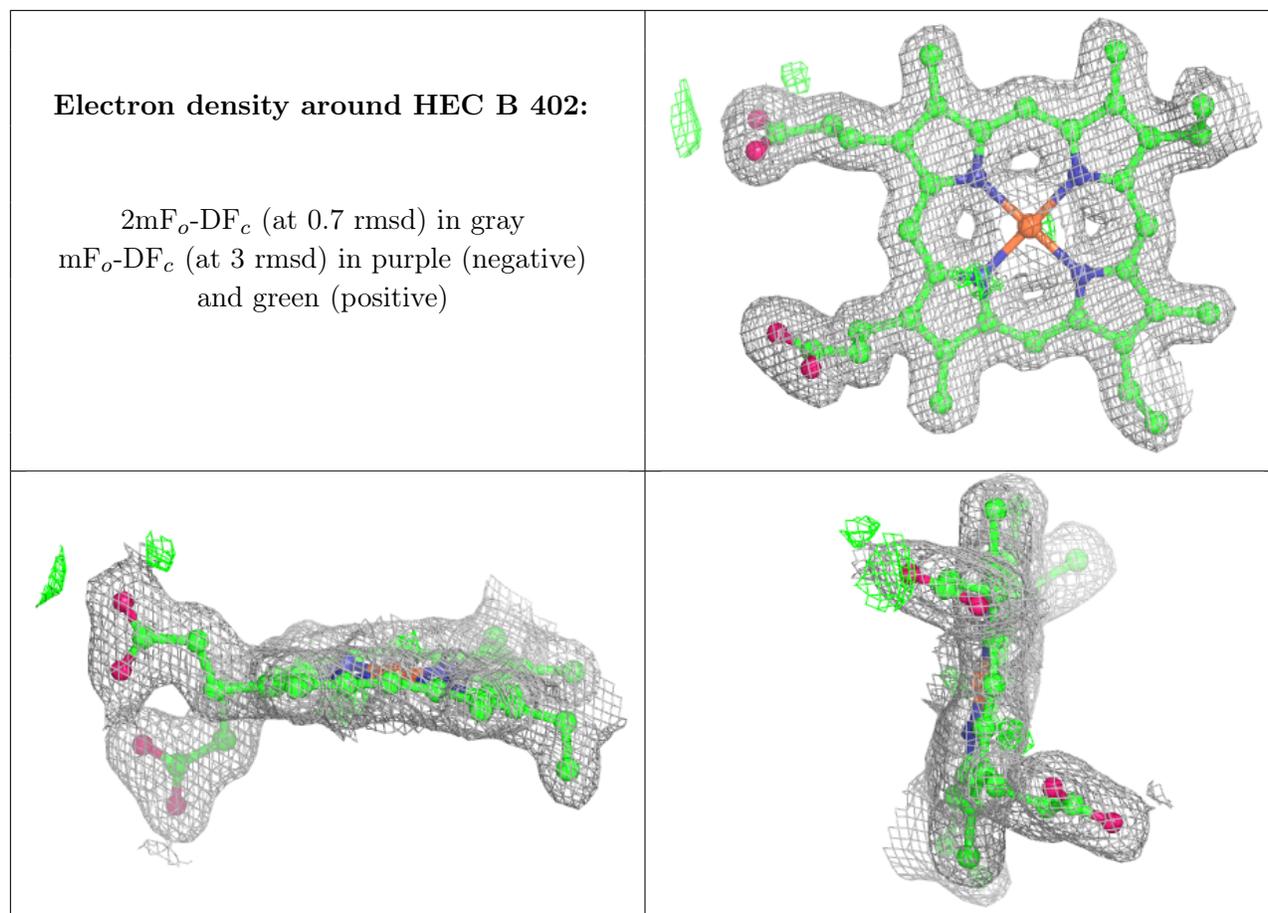
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

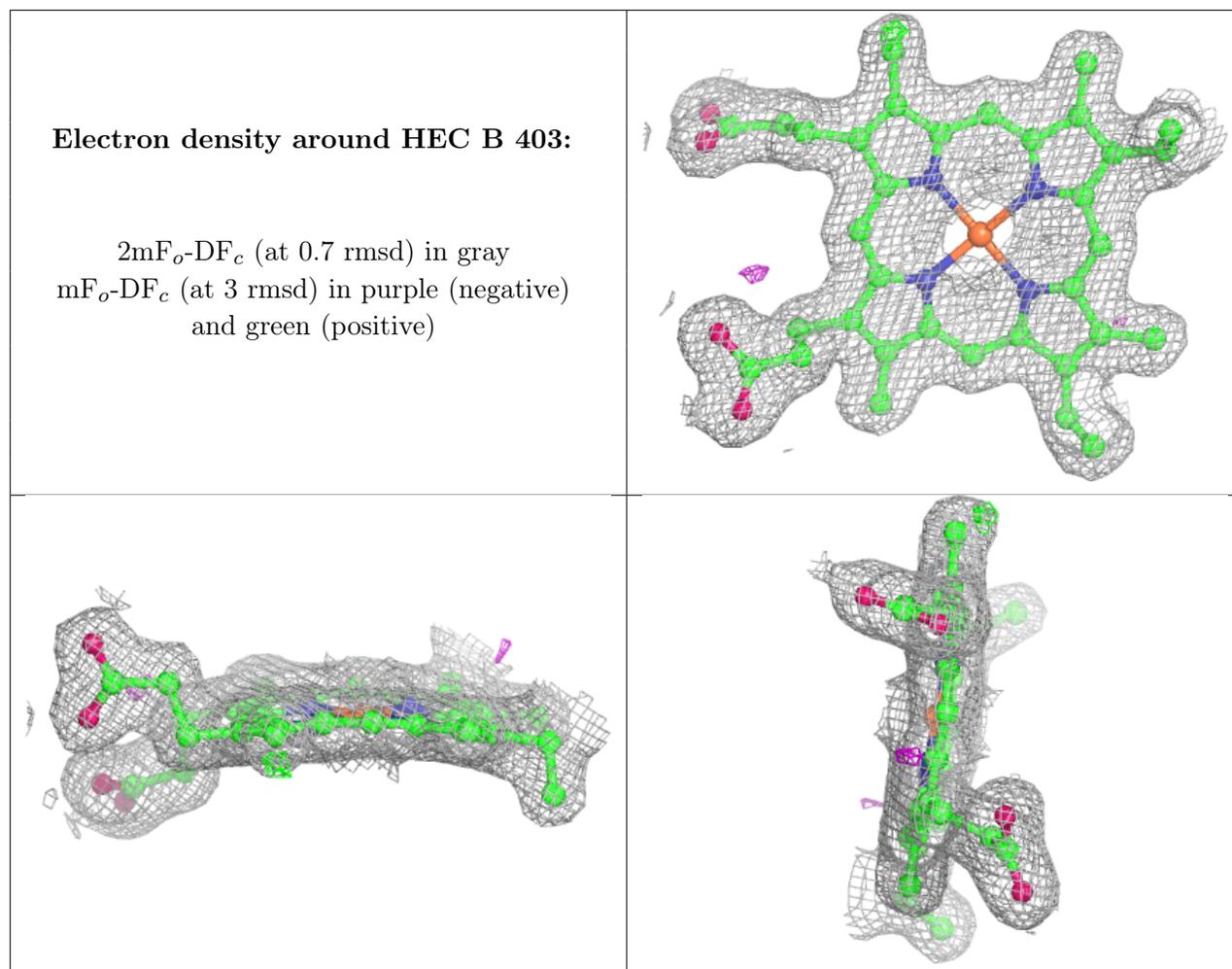
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	PGE	F	402	10/10	0.70	0.23	63,82,98,100	0
7	EDO	B	404	4/4	0.85	0.29	50,55,55,62	0
7	EDO	D	402	4/4	0.87	0.17	35,38,39,46	0
8	MES	F	401	12/12	0.90	0.21	33,51,57,59	12
7	EDO	B	406	4/4	0.93	0.08	50,53,54,57	0
8	MES	D	401	12/12	0.93	0.18	32,55,60,62	12
7	EDO	B	405	4/4	0.94	0.10	36,41,41,41	0
6	NA	A	405	1/1	0.94	0.15	62,62,62,62	0
6	NA	B	407	1/1	0.97	0.11	33,33,33,33	0
5	HEC	A	402	43/43	0.97	0.08	31,36,40,42	0
6	NA	A	404	1/1	0.97	0.09	49,49,49,49	0
4	CA	A	401	1/1	0.97	0.04	37,37,37,37	0
6	NA	B	408	1/1	0.99	0.05	34,34,34,34	0
5	HEC	A	403	43/43	0.99	0.07	31,34,37,39	0
5	HEC	B	402	43/43	0.99	0.06	22,25,29,31	0
5	HEC	B	403	43/43	0.99	0.08	18,22,24,26	0
4	CA	B	401	1/1	1.00	0.07	23,23,23,23	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.









## 6.5 Other polymers [i](#)

There are no such residues in this entry.