



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 30, 2023 – 08:49 AM EST

PDB ID : 4K3I  
Title : Crystal Structure of the Quinol Form of Methylamine Dehydrogenase in Complex with the Diferrous Form of MauG, C2 Space Group  
Authors : Yukl, E.Y.; Wilmot, C.M.  
Deposited on : 2013-04-10  
Resolution : 2.00 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 : 2.36  
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) : 2.36

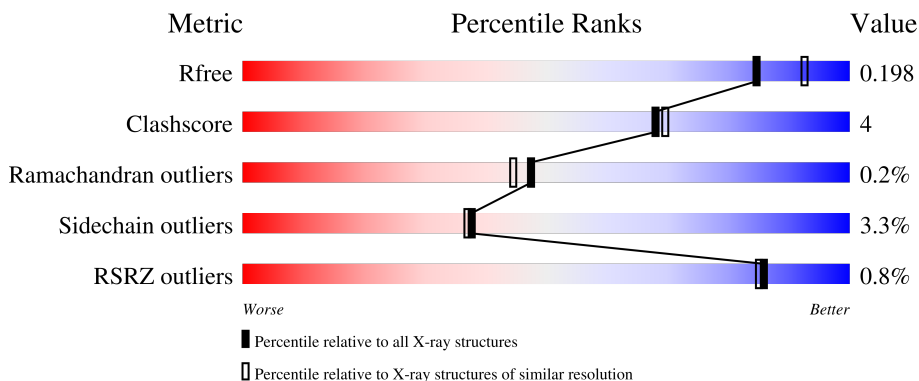
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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.



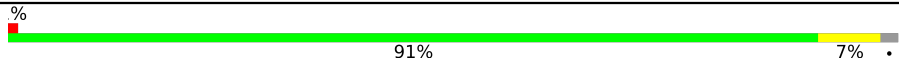
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	
1	B	373	
2	C	137	
2	E	137	
3	D	385	

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Mol	Chain	Length	Quality of chain
3	F	385	 <p>A horizontal bar chart representing the quality of chain. The bar is primarily green, indicating a high quality score of 91%. A small yellow segment at the end indicates a lower quality score of 7%. The bar is labeled with a '%' symbol at the start and a '%' symbol at the end. The text '91%' is centered below the green portion, and '7%' is centered below the yellow portion.</p>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 15344 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	7	0
			2800	1745	509	535	11			
1	B	357	Total	C	N	O	S	0	1	0
			2770	1727	500	532	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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	125	Total	C	N	O	S	0	2	0
			967	597	163	193	14			
2	E	125	Total	C	N	O	S	0	3	0
			964	596	161	191	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	expression tag	UNP P22619
C	133	HIS	-	expression tag	UNP P22619
C	134	HIS	-	expression tag	UNP P22619
C	135	HIS	-	expression tag	UNP P22619
C	136	HIS	-	expression tag	UNP P22619
C	137	HIS	-	expression tag	UNP P22619
E	132	HIS	-	expression tag	UNP P22619
E	133	HIS	-	expression tag	UNP P22619
E	134	HIS	-	expression tag	UNP P22619
E	135	HIS	-	expression tag	UNP P22619
E	136	HIS	-	expression tag	UNP P22619
E	137	HIS	-	expression tag	UNP P22619

- 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
			2965	1876	512	568	9			
3	F	376	Total	C	N	O	S	0	5	0
			2961	1875	508	569	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).

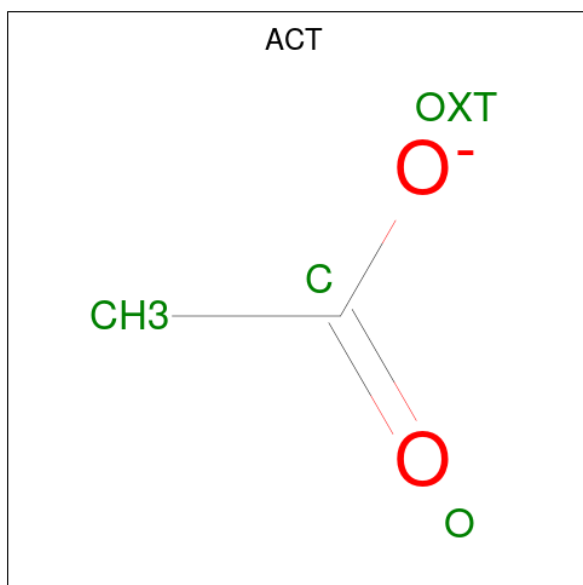
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	A	2	2	2	0	0
6	B	2	2	2	0	0

- 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	A	1	Total	C O	0	0
			4	2 2		
7	A	1	Total	C O	0	0
			4	2 2		
7	A	1	Total	C O	0	0
			4	2 2		
7	B	1	Total	C O	0	0
			4	2 2		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2^-$ ).



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

- Molecule 9 is water.

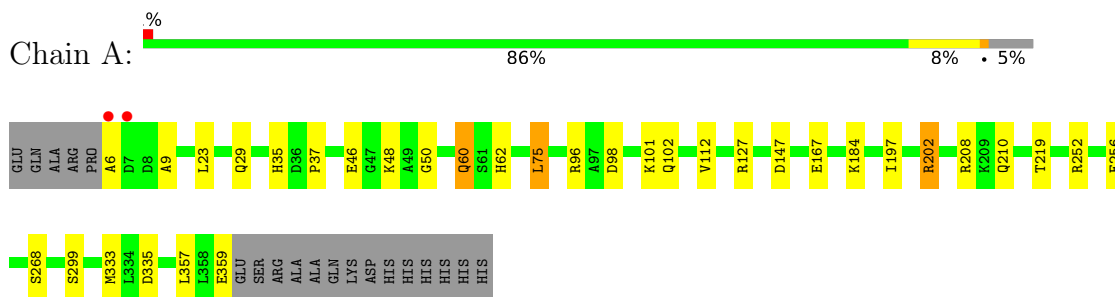
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	392	Total	O	0	5
			397	397		
9	B	290	Total	O	0	2
			292	292		
9	C	127	Total	O	0	1
			128	128		
9	D	442	Total	O	0	2
			444	444		
9	E	96	Total	O	0	0
			96	96		
9	F	360	Total	O	0	2
			362	362		



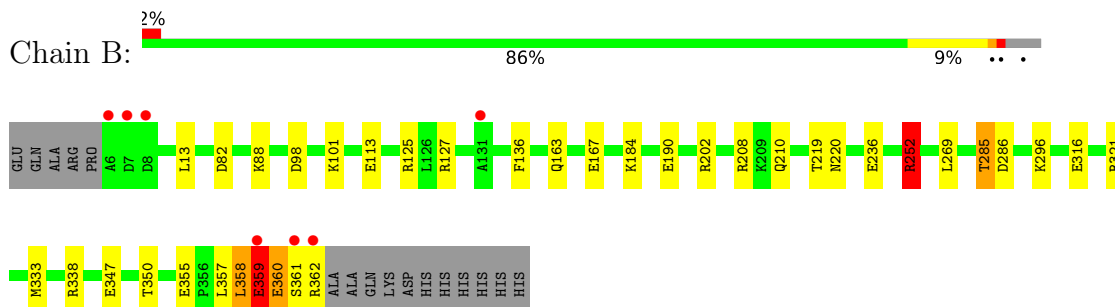
### 3 Residue-property plots i

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.

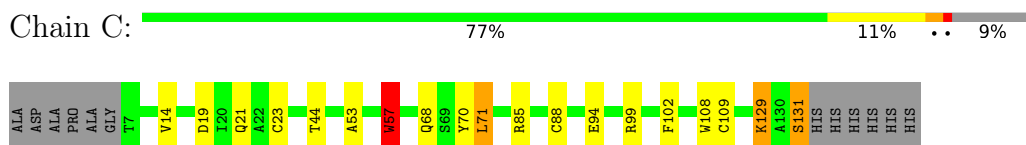
- Molecule 1: Methylamine utilization protein MauG



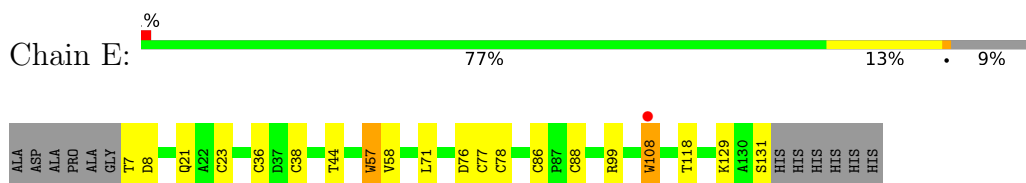
- Molecule 1: Methylamine utilization protein MauG




- Molecule 2: Methylamine dehydrogenase light chain

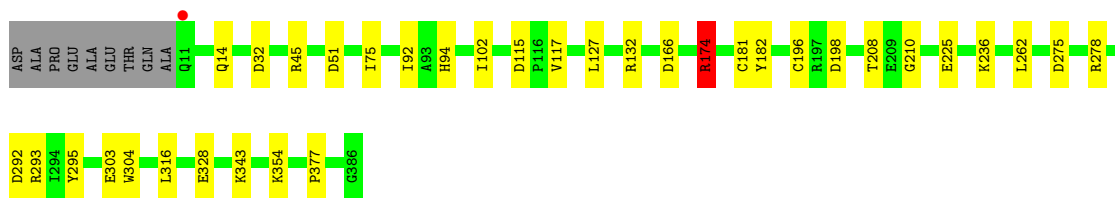


- Molecule 2: Methylamine dehydrogenase light chain




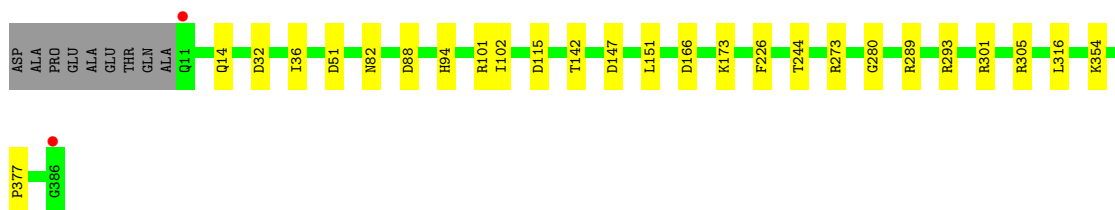
- Molecule 3: Methylamine dehydrogenase heavy chain

Chain D:  89% 9%



• Molecule 3: Methylamine dehydrogenase heavy chain

Chain F:  91% 7%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	346.36Å 55.56Å 112.55Å 90.00° 106.55° 90.00°	Depositor
Resolution (Å)	43.06 – 2.00 43.06 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.06-2.00) 99.6 (43.06-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.144 , 0.190 0.155 , 0.198	Depositor DCC
$R_{free}$ test set	6968 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtrriage
Anisotropy	0.400	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.014 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15344	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: TOQ, EDO, NA, CA, HEC, ACT

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	1.00	1/2867 (0.0%)	1.01	6/3888 (0.2%)
1	B	0.86	0/2834	0.94	6/3844 (0.2%)
2	C	1.13	1/978 (0.1%)	1.04	6/1335 (0.4%)
2	E	0.98	1/981 (0.1%)	1.00	6/1340 (0.4%)
3	D	1.05	3/3046 (0.1%)	1.02	11/4148 (0.3%)
3	F	0.93	0/3041	0.95	6/4142 (0.1%)
All	All	0.98	6/13747 (0.0%)	0.99	41/18697 (0.2%)

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	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	225	GLU	CD-OE2	-5.67	1.19	1.25
3	D	295	TYR	CG-CD2	-5.48	1.32	1.39
3	D	32	ASP	CB-CG	-5.19	1.40	1.51
1	A	268	SER	CB-OG	5.16	1.49	1.42
2	E	108	TRP	CD2-CE2	5.13	1.47	1.41

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ARG	NE-CZ-NH2	-9.18	115.71	120.30
3	D	174	ARG	NE-CZ-NH1	-8.12	116.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	147	ASP	CB-CG-OD1	7.18	124.76	118.30
3	D	278	ARG	NE-CZ-NH2	-6.91	116.85	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	57	TOQ	Mainchain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2800	0	2677	15	0
1	B	2770	0	2640	41	0
2	C	967	0	870	12	0
2	E	964	0	872	9	0
3	D	2965	0	2843	12	0
3	F	2961	0	2840	13	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	86	0	60	1	0
5	B	86	0	60	2	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	12	0	18	0	0
7	B	4	0	6	2	0
8	D	4	0	3	0	0
9	A	397	0	0	3	0
9	B	292	0	0	9	0
9	C	128	0	0	2	0
9	D	444	0	0	3	0
9	E	96	0	0	0	0
9	F	362	0	0	3	0
All	All	15344	0	12889	99	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.

The worst 5 of 99 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)
9:C:208:HOH:O	3:F:36:ILE:HD11	1.58	1.02
3:D:208:THR:HG22	3:D:210:GLY:H	1.35	0.91
1:B:359:GLU:HA	1:B:360:GLU:HG3	1.55	0.88
3:D:208:THR:HB	9:D:716[B]:HOH:O	1.75	0.86
1:B:355:GLU:HA	1:B:358:LEU:HD23	1.67	0.76

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	359/373 (96%)	353 (98%)	6 (2%)	0	100	100
1	B	356/373 (95%)	345 (97%)	9 (2%)	2 (1%)	25	19
2	C	124/137 (90%)	122 (98%)	2 (2%)	0	100	100
2	E	125/137 (91%)	121 (97%)	4 (3%)	0	100	100
3	D	379/385 (98%)	367 (97%)	11 (3%)	1 (0%)	41	37
3	F	379/385 (98%)	366 (97%)	12 (3%)	1 (0%)	41	37
All	All	1722/1790 (96%)	1674 (97%)	44 (3%)	4 (0%)	47	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	358	LEU
1	B	359	GLU
3	D	102	ILE

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Mol	Chain	Res	Type
3	F	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	283/292 (97%)	268 (95%)	15 (5%)	22	18
1	B	279/292 (96%)	266 (95%)	13 (5%)	26	22
2	C	106/112 (95%)	103 (97%)	3 (3%)	43	44
2	E	107/112 (96%)	103 (96%)	4 (4%)	34	32
3	D	309/310 (100%)	302 (98%)	7 (2%)	50	53
3	F	309/310 (100%)	305 (99%)	4 (1%)	69	74
All	All	1393/1428 (98%)	1347 (97%)	46 (3%)	38	37

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	71	LEU
3	D	262	LEU
2	C	129	LYS
3	D	117	VAL
3	D	354	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	14	GLN
3	F	14	GLN
3	F	54	HIS
1	A	210	GLN
1	B	29	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 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	TOQ	C	57	2	14,17,18	1.65	2 (14%)	13,24,26	1.65	3 (23%)
2	TOQ	E	57	2	14,17,18	1.91	2 (14%)	13,24,26	1.89	2 (15%)

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	TOQ	C	57	2	-	0/4/6/8	0/2/2/2
2	TOQ	E	57	2	-	0/4/6/8	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	TOQ	CH2-CZ2	5.09	1.46	1.40
2	E	57	TOQ	CE3-CD2	4.17	1.50	1.42
2	C	57	TOQ	CE3-CD2	3.64	1.49	1.42
2	C	57	TOQ	CH2-CZ2	3.62	1.44	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	TOQ	CB-CG-CD1	-4.38	122.55	127.97
2	C	57	TOQ	CE3-CZ3-CH2	3.21	123.50	120.32
2	E	57	TOQ	CE3-CD2-CG	2.87	139.69	134.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	57	TOQ	CB-CA-C	2.58	116.31	111.47
2	C	57	TOQ	CZ3-CE3-CD2	-2.40	117.79	121.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	57	TOQ	2	0
2	E	57	TOQ	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	1.61	7 (21%)	24,82,82	2.66	9 (37%)
7	EDO	B	405	-	3,3,3	0.48	0	2,2,2	0.45	0
7	EDO	A	406	-	3,3,3	0.50	0	2,2,2	0.40	0
5	HEC	B	403	1	32,50,50	2.05	9 (28%)	24,82,82	2.81	9 (37%)
5	HEC	B	402	1	32,50,50	1.61	8 (25%)	24,82,82	2.57	14 (58%)
7	EDO	A	408	-	3,3,3	0.34	0	2,2,2	0.53	0
7	EDO	A	405	-	3,3,3	0.28	0	2,2,2	0.77	0
5	HEC	A	402	1	32,50,50	1.70	7 (21%)	24,82,82	2.85	11 (45%)
8	ACT	D	401	-	3,3,3	0.76	0	3,3,3	0.83	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	405	-	-	0/1/1/1	-
7	EDO	A	406	-	-	0/1/1/1	-
5	HEC	B	403	1	-	2/10/54/54	-
5	HEC	B	402	1	-	0/10/54/54	-
7	EDO	A	408	-	-	1/1/1/1	-
7	EDO	A	405	-	-	1/1/1/1	-
5	HEC	A	402	1	-	3/10/54/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	HEC	C3C-C2C	-5.79	1.34	1.40
5	B	403	HEC	C2B-C3B	-4.98	1.35	1.40
5	A	402	HEC	C1D-CHD	3.92	1.51	1.41
5	A	402	HEC	CAD-C3D	-3.59	1.46	1.52
5	A	402	HEC	C3C-C4C	3.55	1.49	1.43

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	402	HEC	CMB-C2B-C3B	7.75	134.93	125.82
5	A	403	HEC	C1D-C2D-C3D	-6.58	102.42	107.00
5	B	403	HEC	CMC-C2C-C3C	6.55	133.52	125.82
5	B	403	HEC	CBD-CAD-C3D	-6.25	101.96	112.62
5	A	403	HEC	CMC-C2C-C3C	5.60	132.40	125.82

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

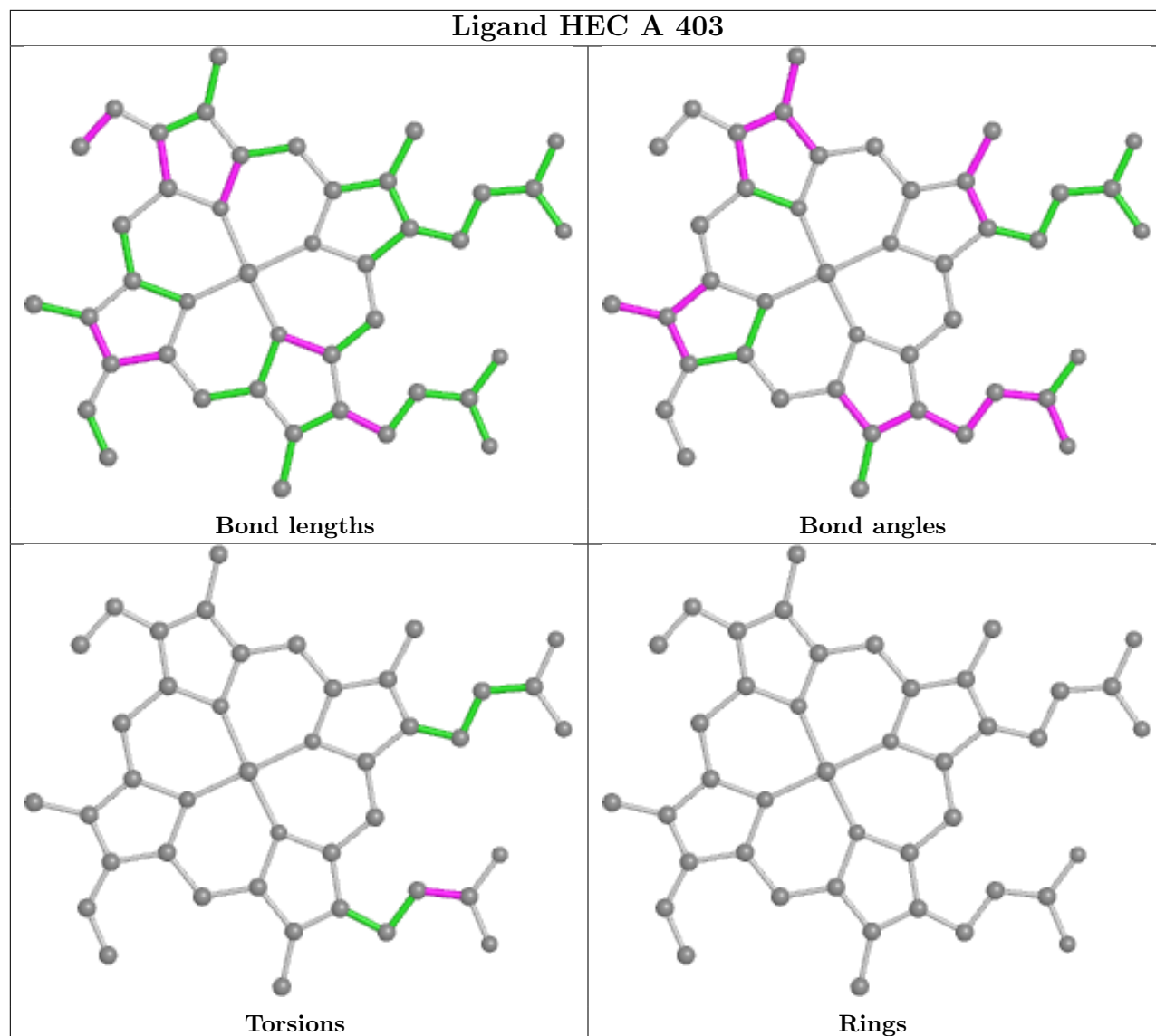
Mol	Chain	Res	Type	Atoms
5	A	402	HEC	CAD-CBD-CGD-O1D
5	A	402	HEC	CAD-CBD-CGD-O2D
5	A	403	HEC	CAD-CBD-CGD-O2D
5	A	403	HEC	CAD-CBD-CGD-O1D
7	A	405	EDO	O1-C1-C2-O2

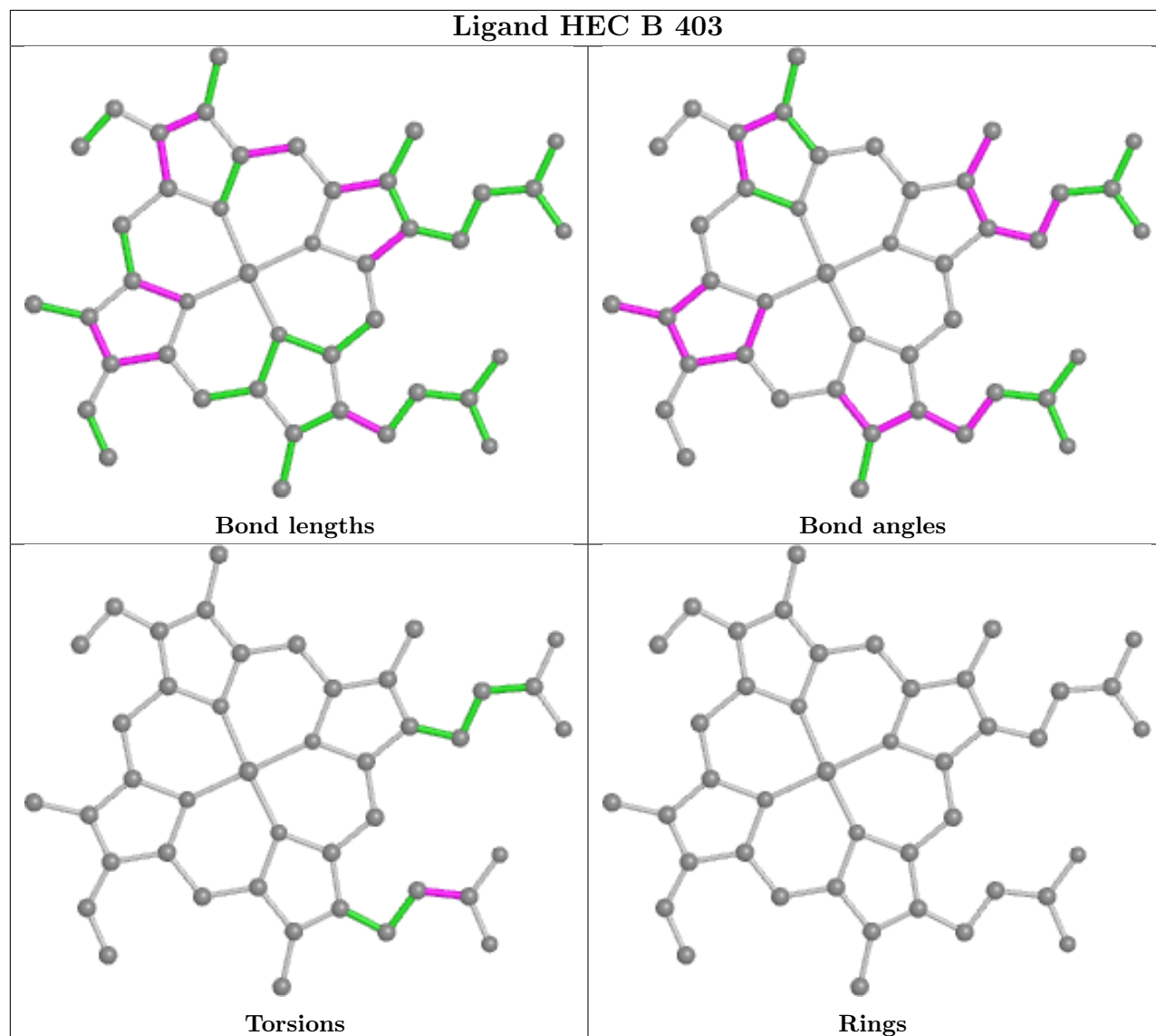
There are no ring outliers.

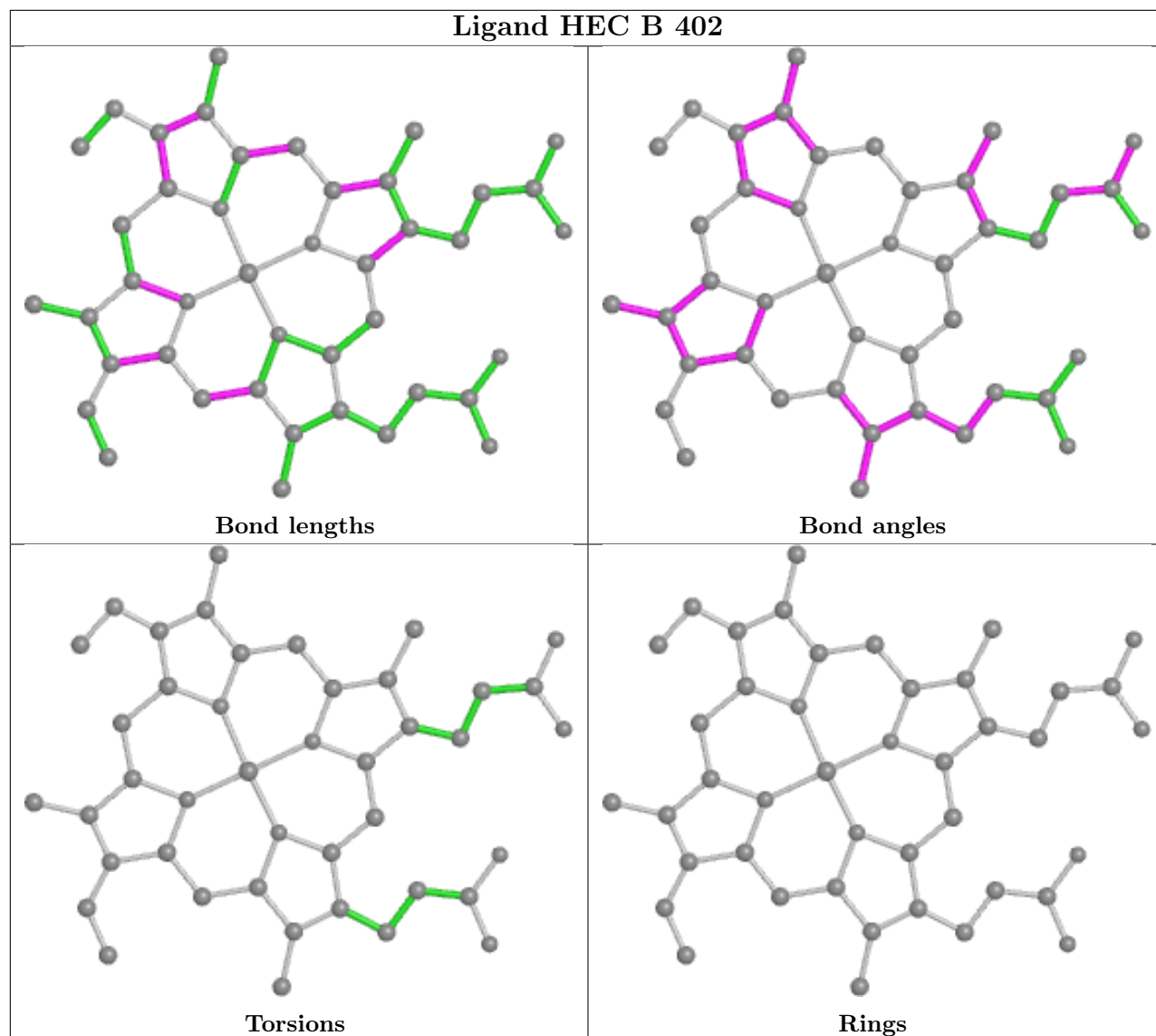
3 monomers are involved in 5 short contacts:

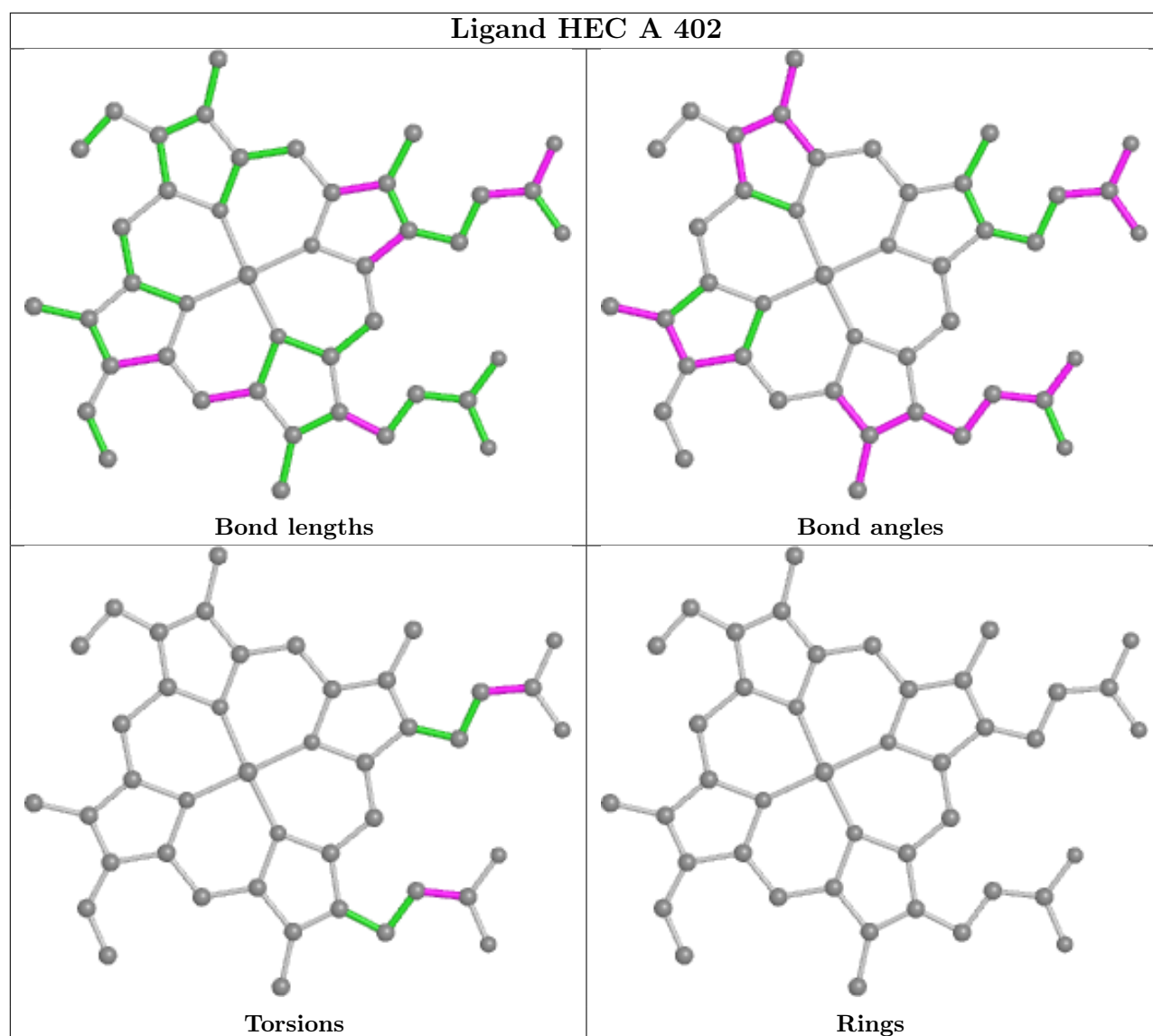
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	403	HEC	1	0
7	B	405	EDO	2	0
5	B	402	HEC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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%)	-0.69	2 (0%) 89 88	17, 25, 42, 75	0
1	B	357/373 (95%)	-0.50	7 (1%) 65 63	21, 33, 52, 112	0
2	C	124/137 (90%)	-0.55	0 100 100	18, 21, 29, 48	0
2	E	124/137 (90%)	-0.41	1 (0%) 86 85	21, 27, 40, 56	0
3	D	376/385 (97%)	-0.70	1 (0%) 94 93	17, 23, 37, 71	0
3	F	376/385 (97%)	-0.60	2 (0%) 91 90	20, 29, 44, 68	0
All	All	1711/1790 (95%)	-0.60	13 (0%) 86 85	17, 27, 44, 112	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361	SER	5.8
1	B	6	ALA	5.4
1	B	7	ASP	4.2
1	A	6	ALA	3.7
1	B	362	ARG	3.2

### 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	TOQ	E	57	16/17	0.96	0.16	25,28,32,39	0
2	TOQ	C	57	16/17	0.97	0.16	20,22,29,31	0



### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

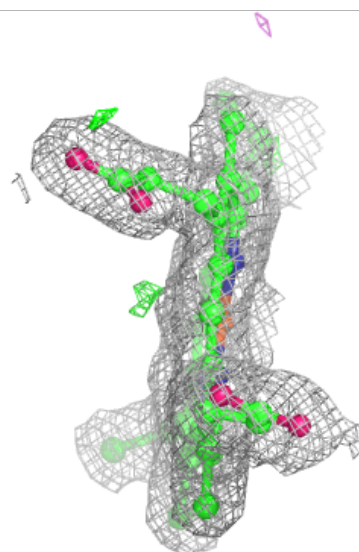
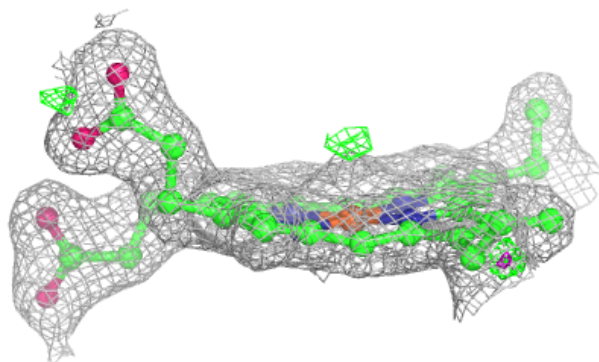
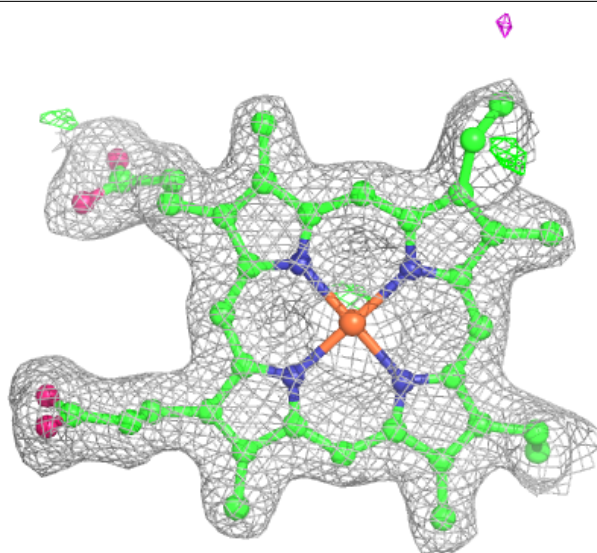
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	EDO	B	405	4/4	0.72	0.16	56,58,58,58	0
7	EDO	A	406	4/4	0.87	0.10	52,52,52,54	0
7	EDO	A	405	4/4	0.90	0.10	54,54,57,63	0
7	EDO	A	408	4/4	0.92	0.13	55,58,60,60	0
8	ACT	D	401	4/4	0.97	0.15	29,37,39,45	0
5	HEC	B	402	43/43	0.98	0.07	23,26,29,32	0
6	NA	A	407	1/1	0.98	0.04	29,29,29,29	0
6	NA	B	404	1/1	0.98	0.09	37,37,37,37	0
5	HEC	A	402	43/43	0.98	0.08	20,22,24,25	0
5	HEC	A	403	43/43	0.99	0.10	17,18,20,22	0
5	HEC	B	403	43/43	0.99	0.09	22,24,27,28	0
6	NA	B	406	1/1	0.99	0.06	32,32,32,32	0
6	NA	A	404	1/1	0.99	0.05	23,23,23,23	0
4	CA	B	401	1/1	1.00	0.03	27,27,27,27	0
4	CA	A	401	1/1	1.00	0.07	19,19,19,19	0

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

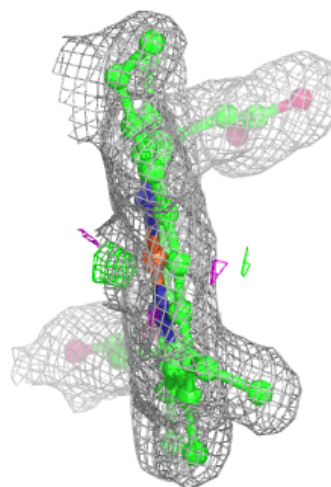
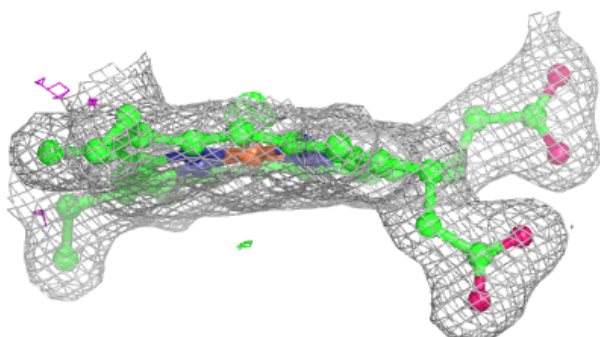
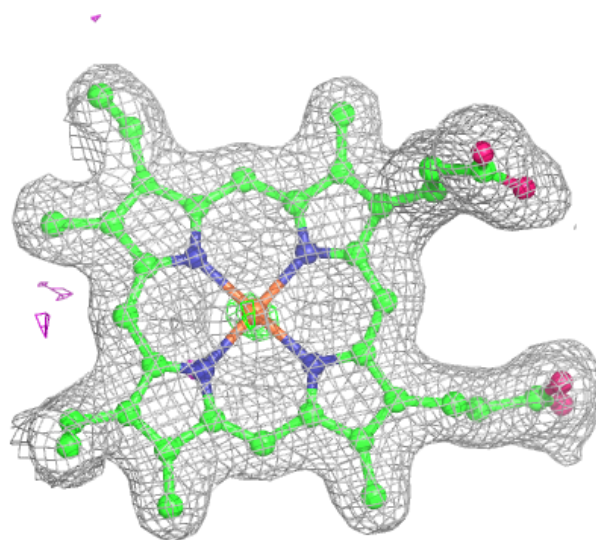
**Electron density around HEC B 402:**

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



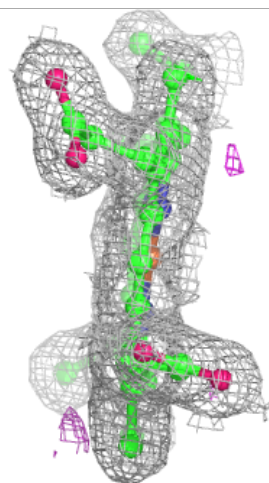
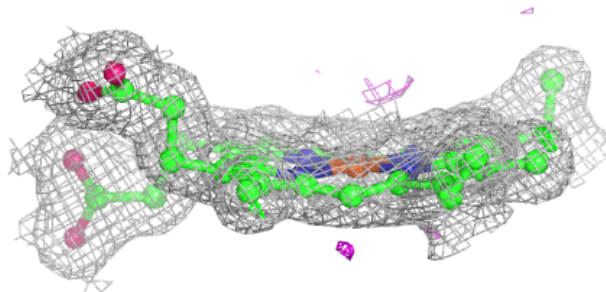
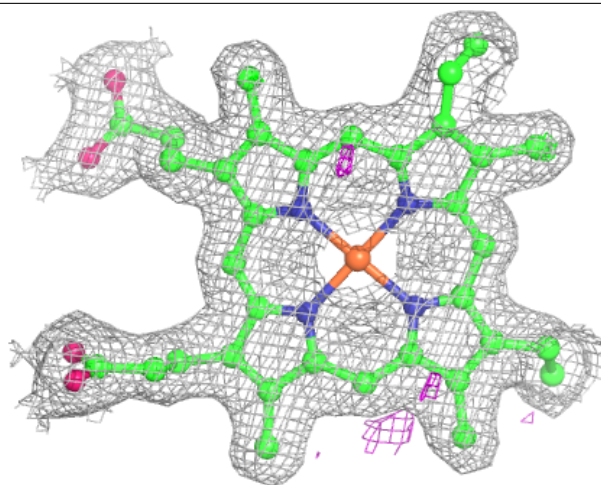
**Electron density around HEC A 402:**

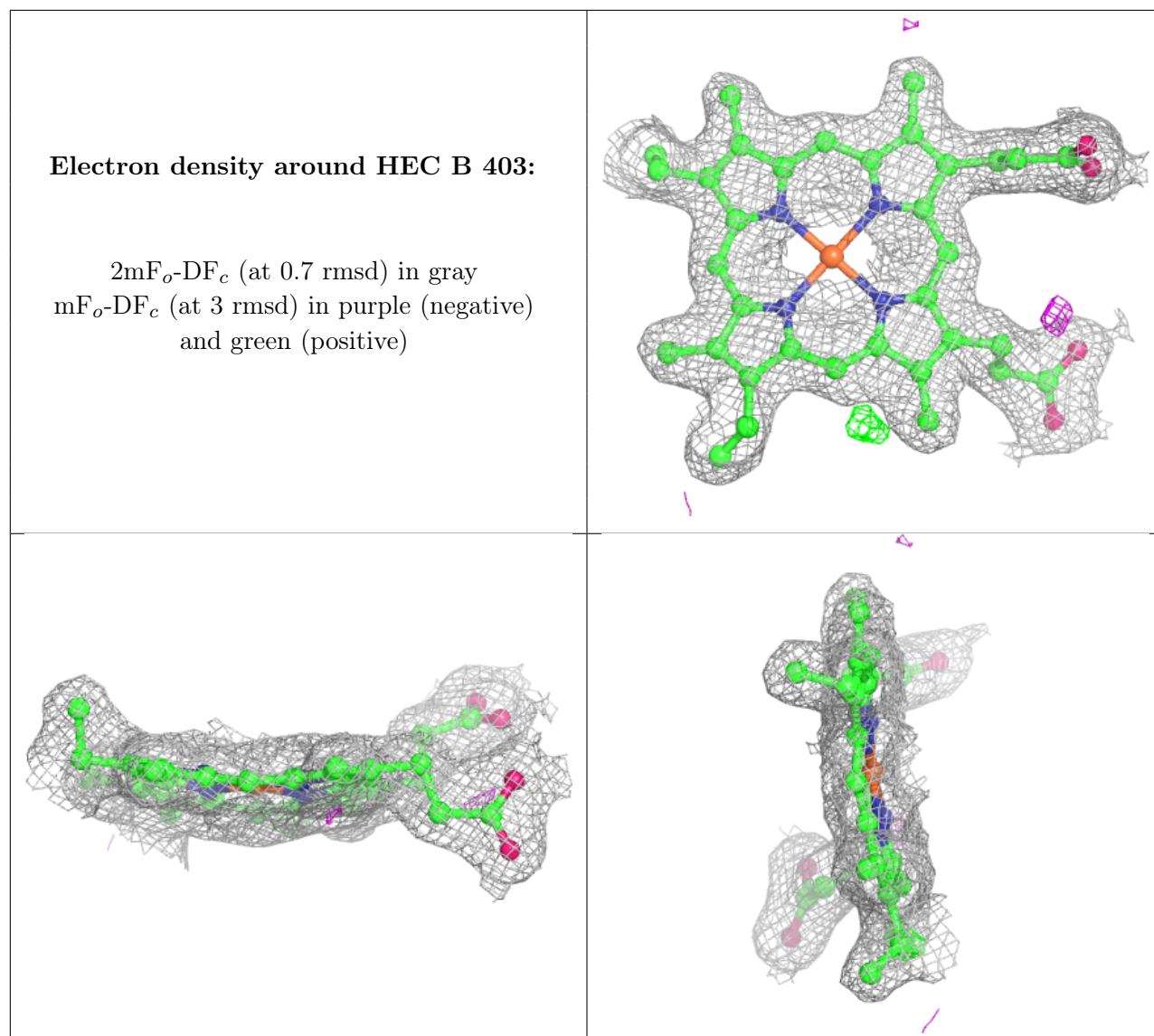
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC A 403:**

$2mF_o-DF_c$  (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.