



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 03:11 pm BST

PDB ID : 4L1Q  
Title : Crystal Structure of the E113Q-MauG/pre-Methylamine Dehydrogenase Complex  
Authors : Yukl, E.Y.; Wilmot, C.M.  
Deposited on : 2013-06-03  
Resolution : 1.92 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.

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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)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

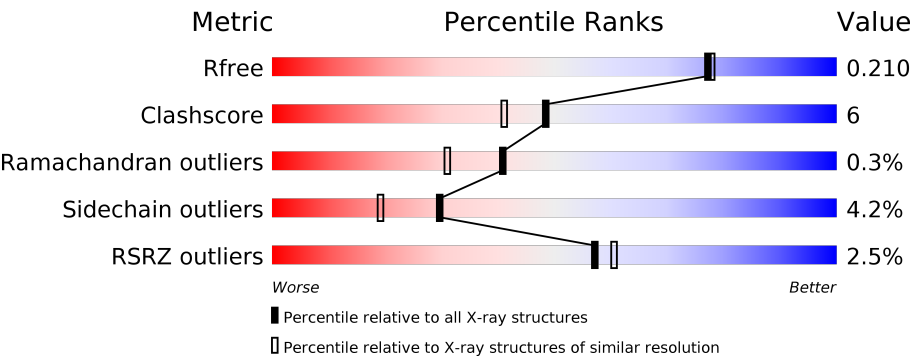
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 on 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	<div><div>2%</div><div><div></div><div>84%</div><div>10%</div><div>5%</div></div></div>
1	B	373	<div><div>%</div><div><div></div><div>84%</div><div>10%</div><div>..</div></div></div>
2	C	137	<div><div>5%</div><div><div></div><div>77%</div><div>15%</div><div>..</div></div></div>
2	E	137	<div><div>%</div><div><div></div><div>73%</div><div>17%</div><div>9%</div></div></div>
3	D	385	<div><div>4%</div><div><div></div><div>82%</div><div>15%</div><div>..</div></div></div>
3	F	385	<div><div>2%</div><div><div></div><div>86%</div><div>11%</div><div>..</div></div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15249 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
1	A	354	Total	C	N	O	S	0	6	0
			2795	1742	509	533	11			
1	B	357	Total	C	N	O	S	0	4	0
			2801	1745	510	535	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
2	C	131	Total	C	N	O	S	0	1	0
			1017	628	179	196	14			
2	E	125	Total	C	N	O	S	0	4	0
			976	604	163	194	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

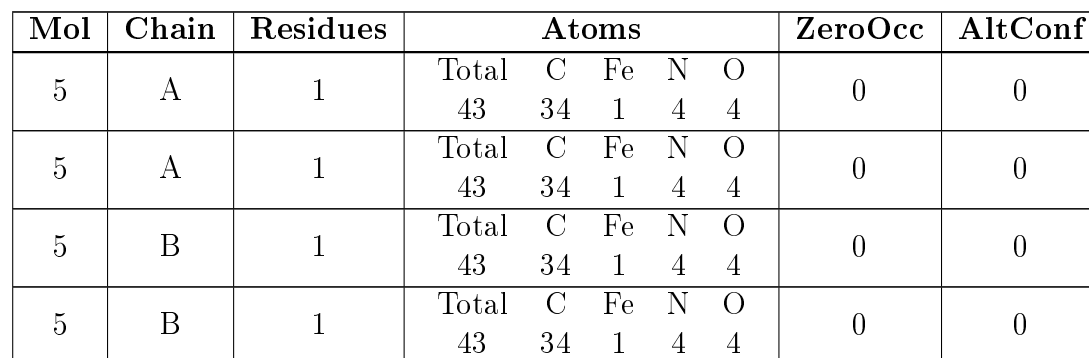
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	2	0
			2943	1864	507	564	8			
3	F	376	Total	C	N	O	S	0	5	0
			2963	1875	511	568	9			

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

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



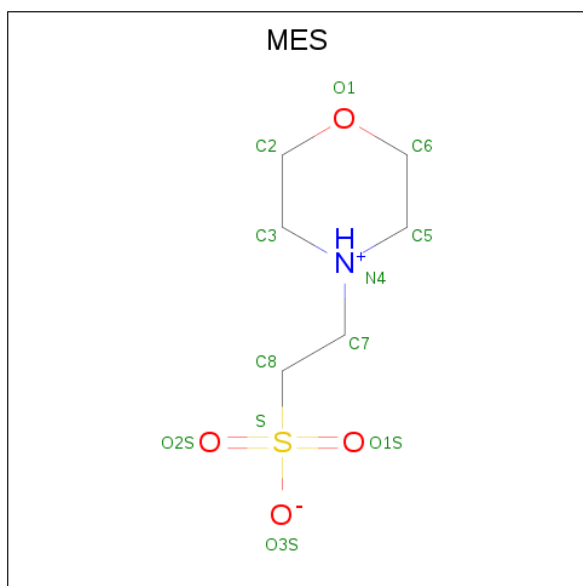
- 
- EDO
- Chemical structure of EDO (Ethane-1,2-diol) showing the zigzag conformation. The structure consists of two carbon atoms, C1 and C2, connected by a single bond. Each carbon is bonded to a hydroxyl group (OH). The oxygen atoms are labeled O1 and O2. The hydroxyl groups are shown in red, and the carbon atoms are labeled in green.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Na	0	0
			2	2		
7	A	1	Total	Na	0	0
			1	1		

- 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		

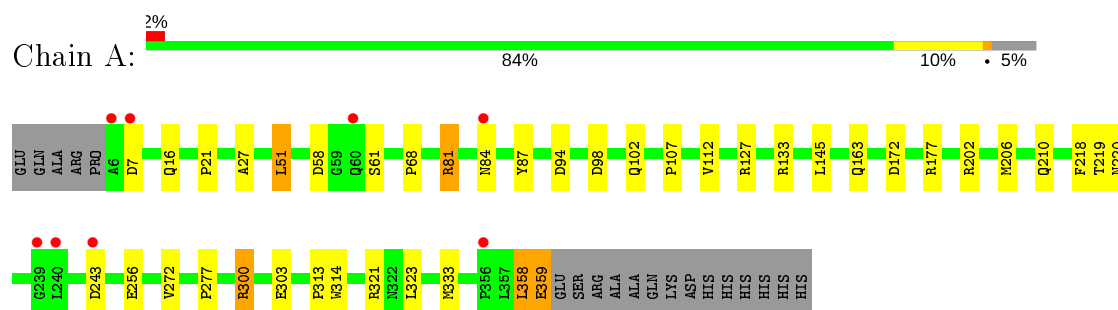
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	270	Total 274	O 274	0	4
9	B	384	Total 390	O 390	0	6
9	C	81	Total 81	O 81	0	0
9	D	272	Total 277	O 277	0	5
9	E	125	Total 125	O 125	0	0
9	F	389	Total 394	O 394	0	5

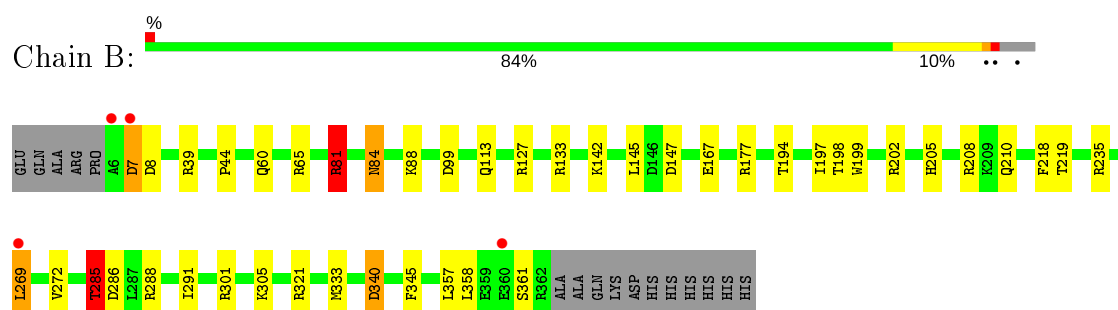
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

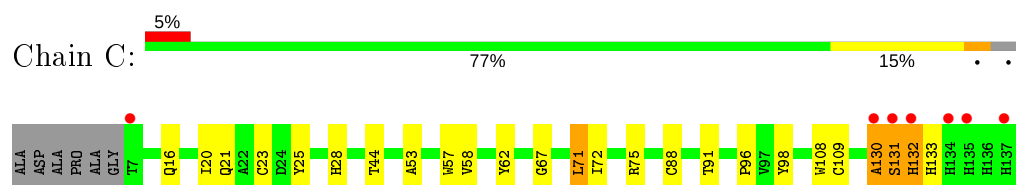
- Molecule 1: Methylamine utilization protein MauG



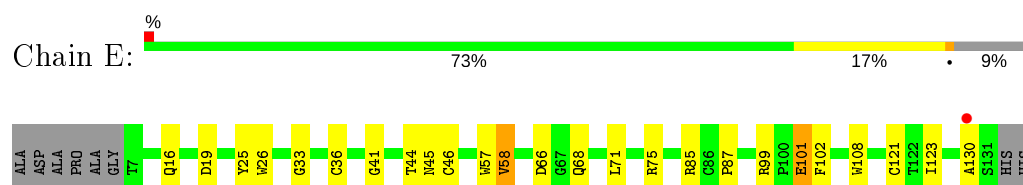
- Molecule 1: Methylamine utilization protein MauG



- Molecule 2: Methylamine dehydrogenase light chain

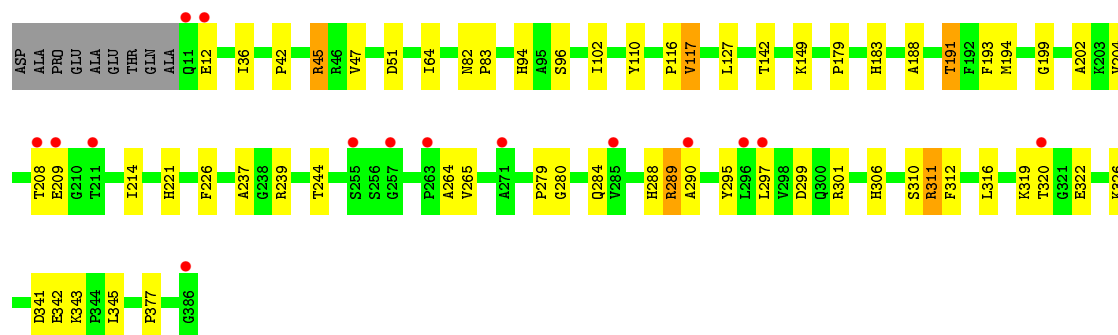
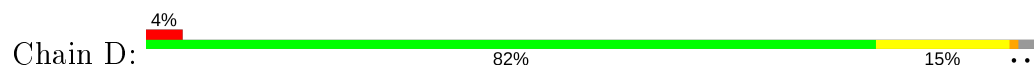


- Molecule 2: Methylamine dehydrogenase light chain

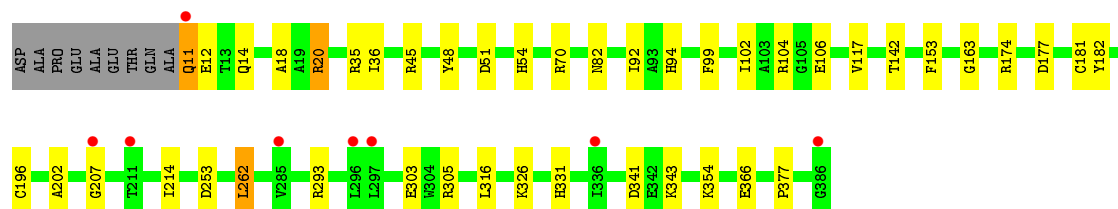
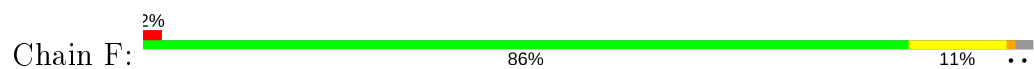


- Molecule 3: Methylamine dehydrogenase heavy chain





• 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)	24.35 – 1.92 24.34 – 1.92	Depositor EDS
% Data completeness (in resolution range)	97.3 (24.35-1.92) 97.4 (24.34-1.92)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.160 , 0.207 0.169 , 0.210	Depositor DCC
$R_{free}$ test set	6447 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 0AF, NA, CA, EDO, MES, 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	0.91	0/2859	0.94	2/3876 (0.1%)
1	B	1.06	1/2865 (0.0%)	1.02	11/3884 (0.3%)
2	C	0.95	0/1035	0.96	2/1413 (0.1%)
2	E	1.20	3/991 (0.3%)	1.06	3/1353 (0.2%)
3	D	0.89	0/3020	0.93	1/4114 (0.0%)
3	F	1.08	1/3043 (0.0%)	1.06	3/4145 (0.1%)
All	All	1.00	5/13813 (0.0%)	0.99	22/18785 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	26	TRP	CB-CG	-5.96	1.39	1.50
2	E	101[A]	GLU	CD-OE1	-5.52	1.19	1.25
2	E	101[B]	GLU	CD-OE1	-5.52	1.19	1.25
1	B	345	PHE	CB-CG	-5.42	1.42	1.51
3	F	303	GLU	CD-OE2	-5.18	1.20	1.25

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	ARG	NE-CZ-NH1	5.97	123.29	120.30
2	C	75	ARG	NE-CZ-NH1	-5.85	117.38	120.30
3	F	35	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	E	85	ARG	NE-CZ-NH1	5.68	123.14	120.30
3	F	305	ARG	NE-CZ-NH2	-5.68	117.46	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2795	0	2673	28	0
1	B	2801	0	2679	34	0
2	C	1017	0	906	31	0
2	E	976	0	883	19	0
3	D	2943	0	2825	36	0
3	F	2963	0	2842	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	4	0	6	0	0
6	B	8	0	12	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
8	D	12	0	13	0	0
8	F	12	0	13	0	0
9	A	274	0	0	5	0
9	B	390	0	0	5	0
9	C	81	0	0	3	0
9	D	277	0	0	3	0
9	E	125	0	0	2	0
9	F	394	0	0	4	0
All	All	15249	0	12972	160	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 160 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)
2:C:131:SER:H	2:C:132:HIS:HA	0.91	1.08
2:C:131:SER:N	2:C:132:HIS:HA	1.55	1.06
2:E:130:ALA:HB3	9:E:293:HOH:O	1.69	0.93
2:C:131:SER:H	2:C:132:HIS:CA	1.81	0.92
1:B:198:THR:HG22	2:E:58[B]:VAL:HG23	1.50	0.91

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	358/373 (96%)	345 (96%)	12 (3%)	1 (0%)	41	31
1	B	359/373 (96%)	350 (98%)	9 (2%)	0	100	100
2	C	129/137 (94%)	119 (92%)	8 (6%)	2 (2%)	9	2
2	E	126/137 (92%)	124 (98%)	2 (2%)	0	100	100
3	D	376/385 (98%)	360 (96%)	15 (4%)	1 (0%)	41	31
3	F	379/385 (98%)	366 (97%)	12 (3%)	1 (0%)	41	31
All	All	1727/1790 (96%)	1664 (96%)	58 (3%)	5 (0%)	41	31

All (5) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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	282/292 (97%)	265 (94%)	17 (6%)	19	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	283/292 (97%)	268 (95%)	15 (5%)	22	12
2	C	111/112 (99%)	109 (98%)	2 (2%)	59	53
2	E	108/112 (96%)	103 (95%)	5 (5%)	27	16
3	D	306/310 (99%)	291 (95%)	15 (5%)	25	14
3	F	309/310 (100%)	300 (97%)	9 (3%)	42	33
All	All	1399/1428 (98%)	1336 (96%)	63 (4%)	30	17

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	285	THR
3	D	45	ARG
3	F	117	VAL
1	B	357	LEU
1	B	361	SER

Some 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	60	GLN
1	B	163	GLN
3	D	331	HIS
1	B	29	GLN
3	D	54	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	0AF	E	57	2	13,16,17	1.50	4 (30%)	11,22,24	1.40	1 (9%)
2	0AF	C	57	2	13,16,17	1.50	2 (15%)	11,22,24	1.37	1 (9%)

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	2	-	0/4/6/8	0/2/2/2
2	0AF	C	57	2	-	0/4/6/8	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	0AF	CZ2-CE2	-3.01	1.37	1.42
2	E	57	0AF	CB-CA	-2.53	1.48	1.53
2	E	57	0AF	CZ2-CE2	-2.50	1.38	1.42
2	C	57	0AF	CA-N	-2.38	1.40	1.48
2	E	57	0AF	CZ3-CE3	2.04	1.41	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	0AF	CG-CB-CA	3.32	119.66	114.53
2	C	57	0AF	CG-CB-CA	3.08	119.29	114.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	57	0AF	1	0
2	C	57	0AF	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 5 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
6	EDO	B	405	-	3,3,3	0.48	0	2,2,2	0.59	0
5	HEC	B	402	1	26,50,50	1.39	3 (11%)	18,82,82	2.39	8 (44%)
6	EDO	A	404	-	3,3,3	0.56	0	2,2,2	0.19	0
8	MES	F	401	-	12,12,12	1.38	1 (8%)	14,16,16	6.75	7 (50%)
8	MES	D	401	-	12,12,12	1.48	2 (16%)	14,16,16	5.92	8 (57%)
5	HEC	A	402	1	26,50,50	1.86	7 (26%)	18,82,82	3.32	9 (50%)
6	EDO	B	404	-	3,3,3	0.45	0	2,2,2	0.11	0
5	HEC	A	403	1	26,50,50	1.56	4 (15%)	18,82,82	3.00	8 (44%)
5	HEC	B	403	1	26,50,50	1.67	8 (30%)	18,82,82	2.50	6 (33%)

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
6	EDO	B	405	-	-	0/1/1/1	-
5	HEC	B	402	1	-	0/6/54/54	-
6	EDO	A	404	-	-	1/1/1/1	-
8	MES	F	401	-	-	3/6/14/14	0/1/1/1
8	MES	D	401	-	-	2/6/14/14	0/1/1/1
5	HEC	A	402	1	-	0/6/54/54	-
6	EDO	B	404	-	-	1/1/1/1	-
5	HEC	A	403	1	-	0/6/54/54	-
5	HEC	B	403	1	-	0/6/54/54	-



The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	402	HEC	C3C-C4C	4.47	1.51	1.43
8	F	401	MES	C8-S	-4.45	1.71	1.77
5	B	403	HEC	C3C-C2C	-4.28	1.36	1.40
5	A	402	HEC	C1A-C2A	3.73	1.51	1.42
5	A	403	HEC	C3C-C2C	-3.70	1.36	1.40

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	401	MES	O3S-S-C8	-14.04	83.06	105.77
8	D	401	MES	O3S-S-O1S	-13.19	79.04	111.27
8	F	401	MES	O1S-S-C8	10.60	119.68	106.92
8	D	401	MES	O3S-S-O2S	-10.60	85.38	111.27
8	F	401	MES	O3S-S-O1S	-10.59	85.39	111.27

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	401	MES	N4-C7-C8-S
8	F	401	MES	C7-C8-S-O3S
8	D	401	MES	C7-C8-S-O1S
6	B	404	EDO	O1-C1-C2-O2
6	A	404	EDO	O1-C1-C2-O2

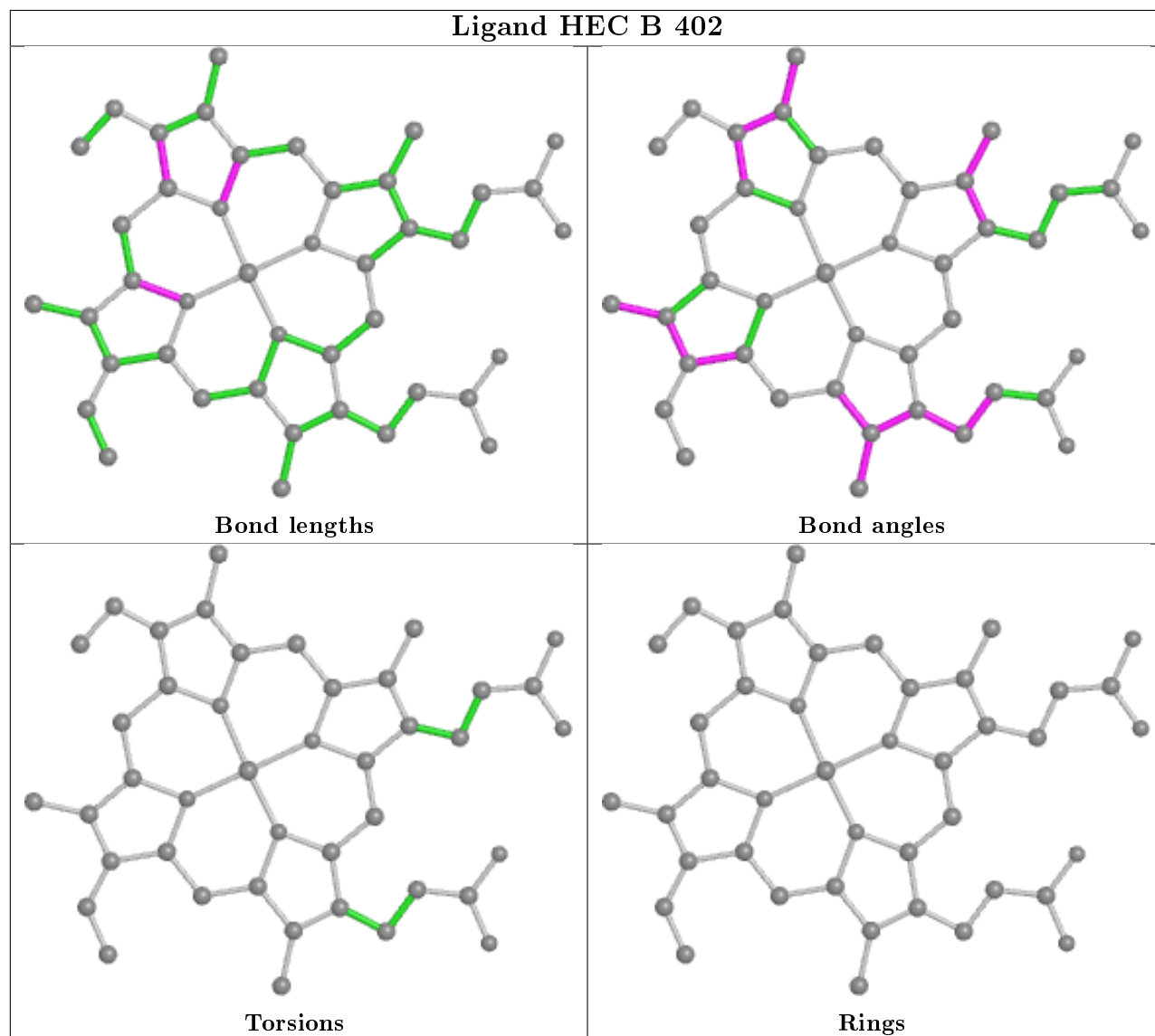
There are no ring outliers.

4 monomers are involved in 8 short contacts:

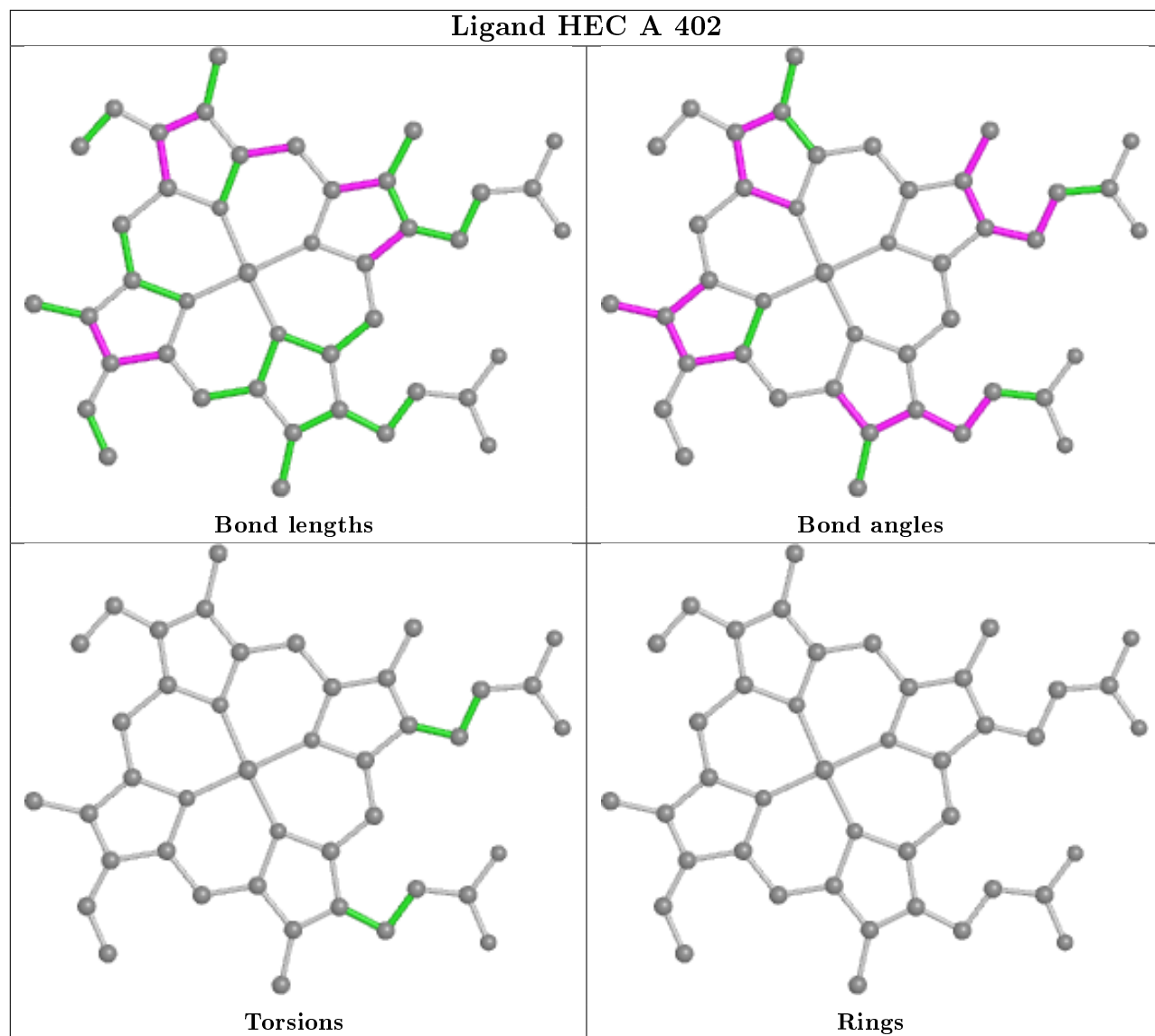
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	402	HEC	1	0
5	A	402	HEC	3	0
5	A	403	HEC	2	0
5	B	403	HEC	2	0

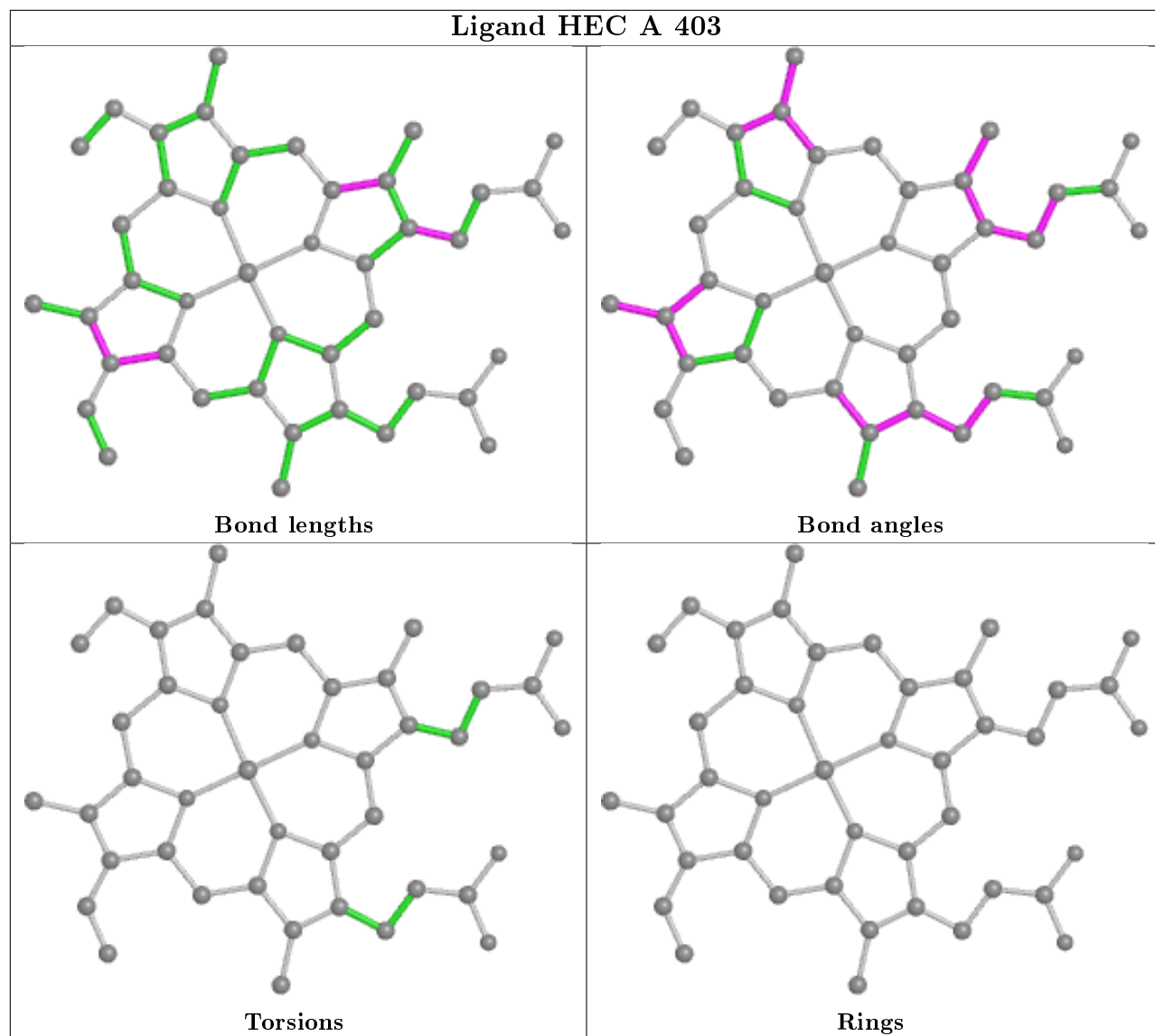
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

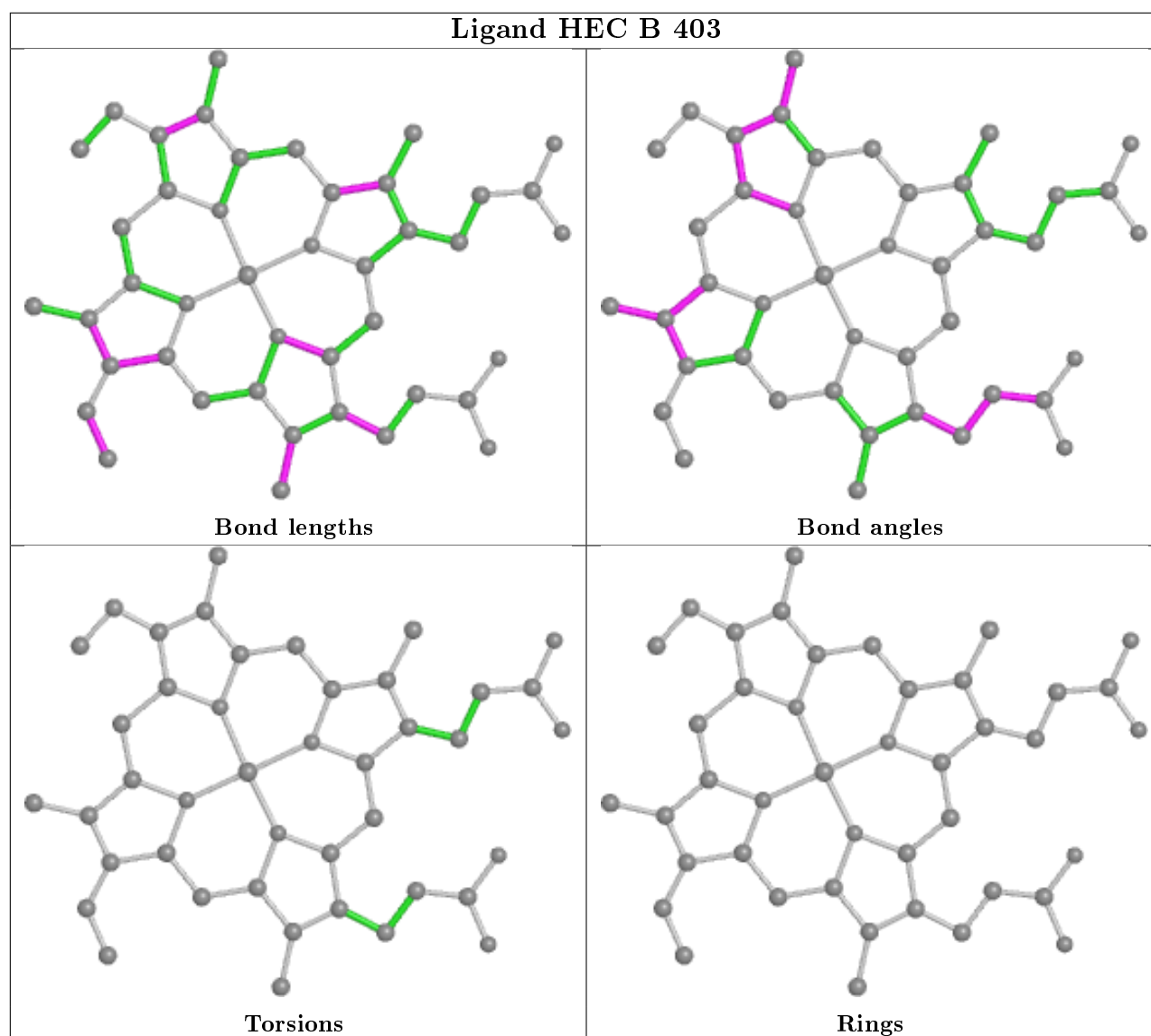
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## Ligand HEC A 402







## 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%)	-0.15	8 (2%) 60 63	26, 38, 56, 73	0
1	B	357/373 (95%)	-0.37	4 (1%) 80 82	16, 29, 47, 76	0
2	C	130/137 (94%)	0.11	7 (5%) 25 29	23, 36, 64, 90	2 (1%)
2	E	124/137 (90%)	-0.42	1 (0%) 86 87	20, 26, 38, 71	0
3	D	376/385 (97%)	0.10	15 (3%) 38 41	24, 41, 66, 85	0
3	F	376/385 (97%)	-0.28	8 (2%) 63 66	18, 28, 47, 68	0
All	All	1717/1790 (95%)	-0.17	43 (2%) 57 60	16, 33, 59, 90	2 (0%)

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	131	SER	7.0
1	B	6	ALA	5.4
1	A	6	ALA	5.2
3	D	386	GLY	4.9
3	F	386	GLY	4.5

### 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	15/16	0.96	0.10	37,40,45,46	0
2	0AF	E	57	15/16	0.97	0.11	24,27,32,33	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

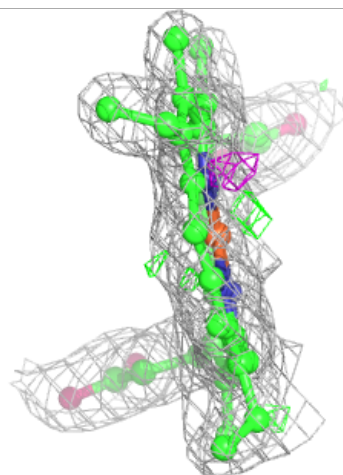
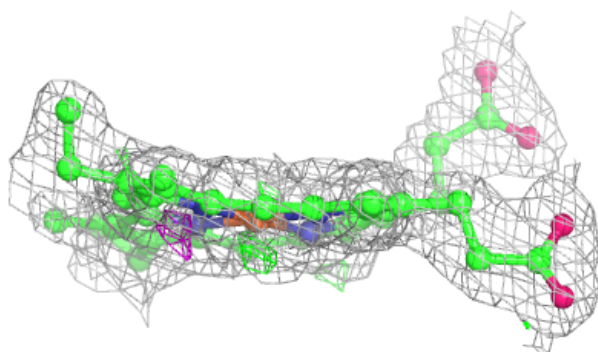
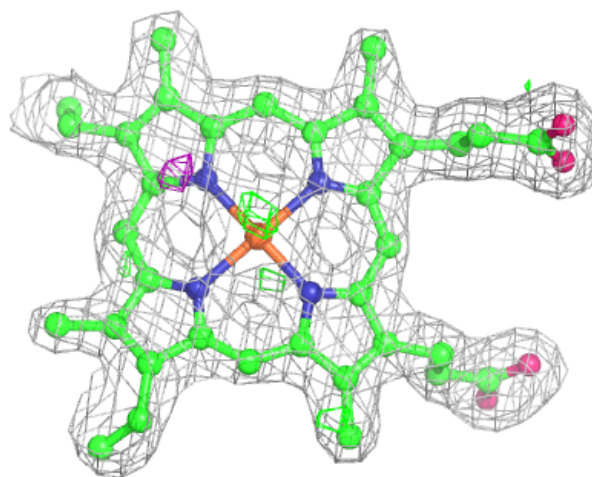
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
6	EDO	A	404	4/4	0.84	0.10	57,57,59,59	0
8	MES	D	401	12/12	0.90	0.21	29,54,60,61	12
6	EDO	B	405	4/4	0.91	0.18	37,50,50,60	0
8	MES	F	401	12/12	0.94	0.18	44,66,68,70	0
6	EDO	B	404	4/4	0.95	0.07	46,47,50,53	0
5	HEC	A	402	43/43	0.97	0.10	28,31,34,36	0
7	NA	A	405	1/1	0.97	0.17	47,47,47,47	0
7	NA	B	407	1/1	0.98	0.15	31,31,31,31	0
5	HEC	B	402	43/43	0.98	0.08	19,23,26,29	0
5	HEC	A	403	43/43	0.98	0.13	26,29,32,32	0
7	NA	B	406	1/1	0.98	0.13	30,30,30,30	0
5	HEC	B	403	43/43	0.99	0.10	15,17,20,21	0
4	CA	A	401	1/1	0.99	0.02	30,30,30,30	0
4	CA	B	401	1/1	1.00	0.06	20,20,20,20	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 402:**

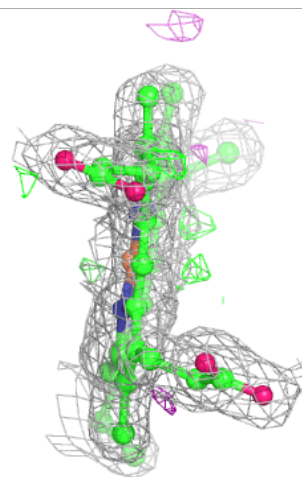
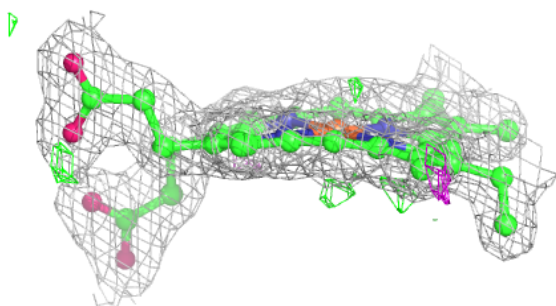
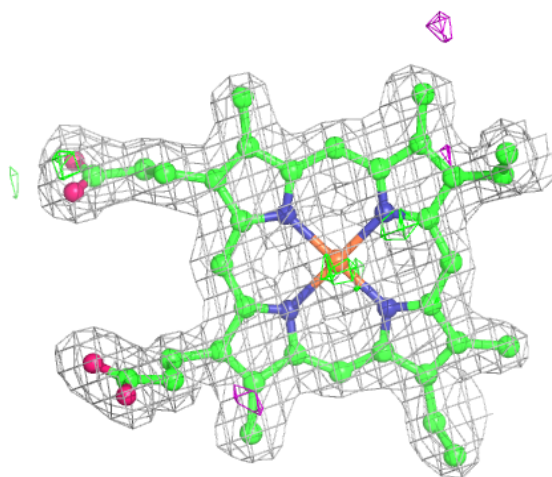
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





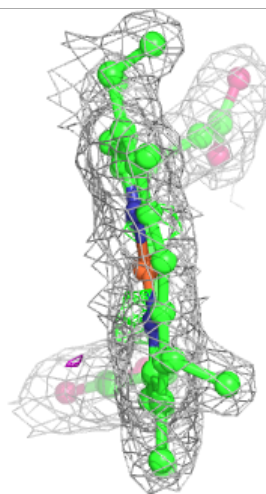
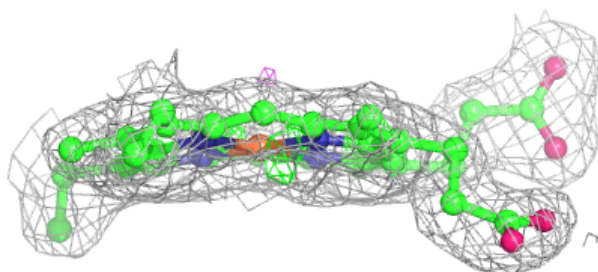
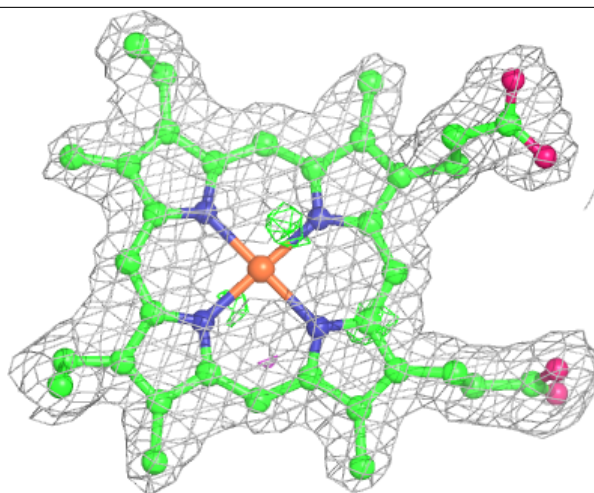
**Electron density around HEC B 402:**

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



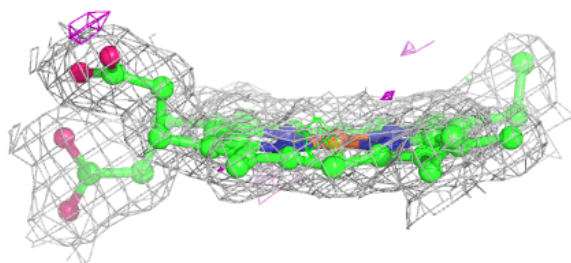
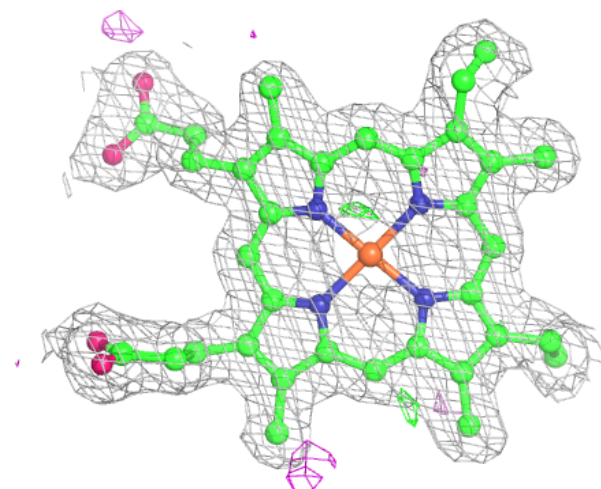
**Electron density around HEC A 403:**

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



**Electron density around HEC B 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.