



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 11:17 am BST

PDB ID : 4FAN
Title : Crystal Structure of WT MauG in Complex with Pre-Methylamine Dehydrogenase Aged 40 Days
Authors : Yukl, E.T.; Wilmot, C.M.
Deposited on : 2012-05-22
Resolution : 2.08 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

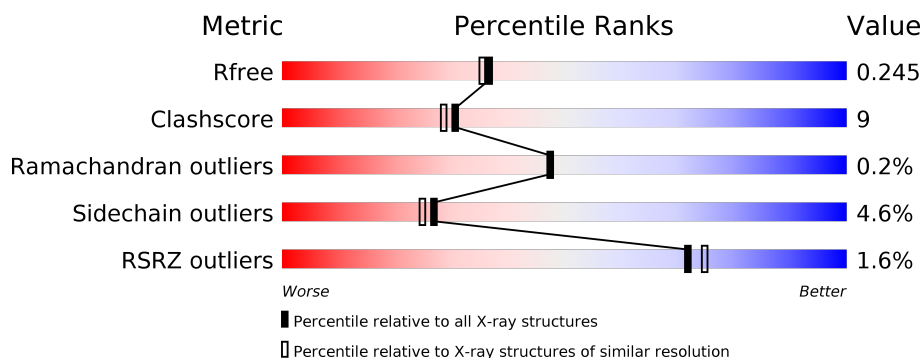
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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 ≥ 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>70%</div> <div>23%</div> <div>5%</div> </div> </div>
1	B	373	<div> <div>%</div> <div> <div>82%</div> <div>13%</div> <div>5%</div> </div> </div>
2	C	137	<div> <div>4%</div> <div> <div>64%</div> <div>28%</div> <div>6%</div> </div> </div>
2	E	137	<div> <div>%</div> <div> <div>63%</div> <div>25%</div> <div>9%</div> </div> </div>
3	D	385	<div> <div>3%</div> <div> <div>72%</div> <div>24%</div> <div>4%</div> </div> </div>
3	F	385	<div> <div>82%</div> <div>16%</div> <div>2%</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14569 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	5	0
			2777	1731	498	537	11			
1	B	357	Total	C	N	O	S	0	1	0
			2768	1726	497	533	12			

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
2	C	129	Total	C	N	O	S	0	3	0
			1009	622	175	197	15			
2	E	125	Total	C	N	O	S	0	4	0
			972	601	162	193	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

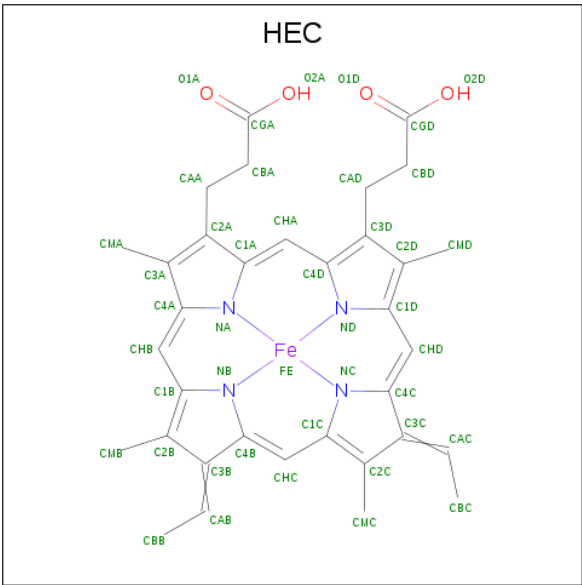
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	2	0
			2934	1859	503	563	9			
3	F	376	Total	C	N	O	S	0	4	0
			2954	1870	509	566	9			

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

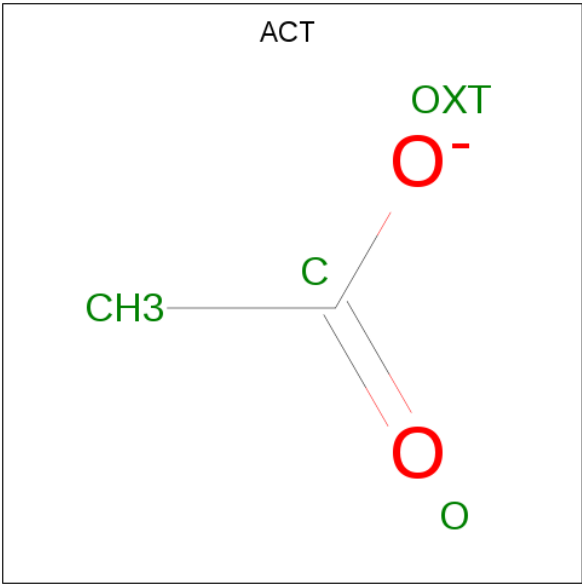
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

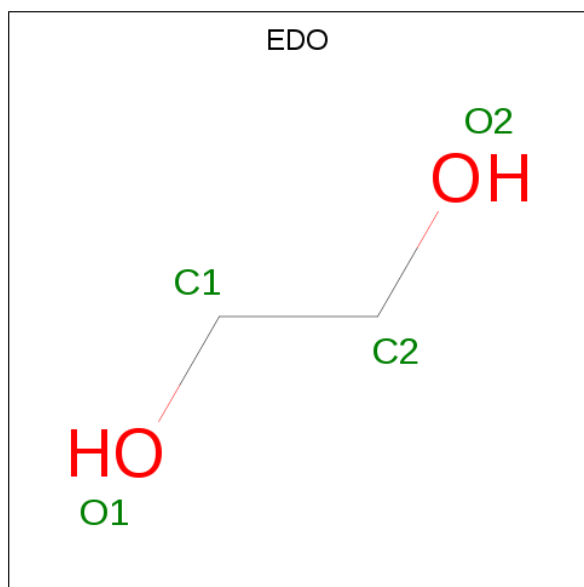


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

- 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		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



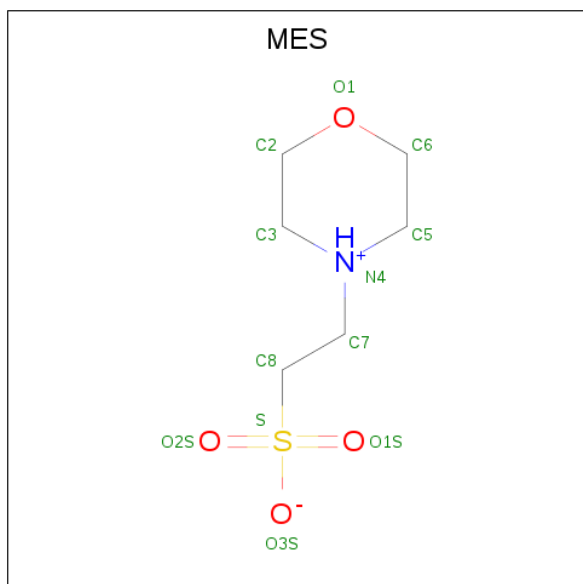
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	133	Total 135	O 135	0	2
11	B	243	Total 246	O 246	0	3
11	C	53	Total 54	O 54	0	1
11	D	149	Total 152	O 152	0	3
11	E	79	Total 80	O 80	0	1
11	F	268	Total 270	O 270	0	2

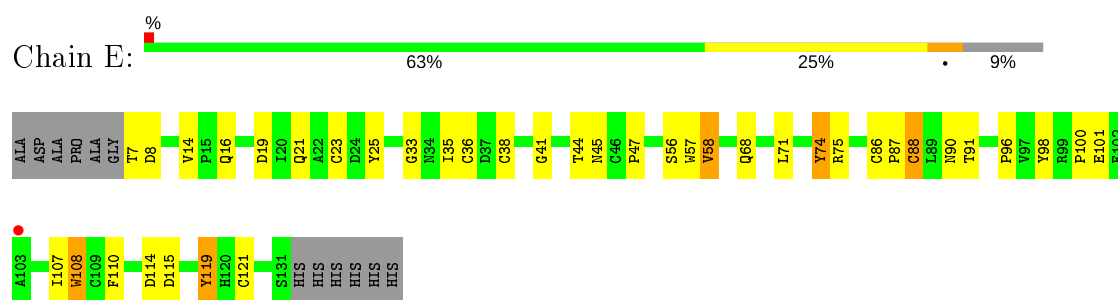
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

- Chain A:
-
- 70% 23% 5%
- GLU GLN ALA ARG PRG A6 D7 G14 P21 A22 L23 S24 R25 N26 A27 H35 A40 F41 K48 L51 Q60 S61 H62 R65 P68 T69 L70 G71 L75 N84 Q91 F92 H93 D94 G95 R96 D99 P107 V112 E113 M114 A115 F136 P137 F140 G141 K142 G143 V144 D147 R150 A158 Q163 G166 E167 F168 S169 P170 F171 D172 S173 K174 Y175 D176 R177 V178 K184 E189 V195 F196 T197 L198 V199 R202 K206 Q207 R208 K209 Q210 E214 R215 E216 T217 F218 T219 N220 F221 E222 Y223 W231

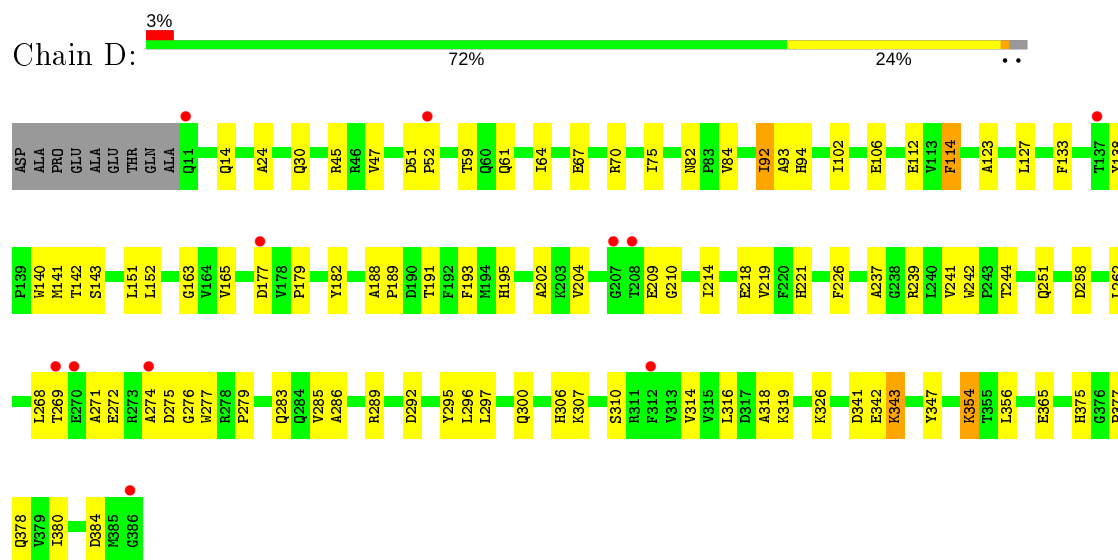
- [illegible]

- Chain C:
-
- | Amino Acid | Color | Percentage | Present (Red Dot) |
|------------|--------|------------|-------------------|
| ALA | Grey | 4% | Yes |
| ASP | Red | | Yes |
| ALA | Red | | Yes |
| PRO | Red | | Yes |
| ALA | Yellow | 28% | No |
| GLY | Yellow | | No |
| T7 | Green | | Yes |
| K12 | Yellow | | No |
| W13 | Yellow | 64% | No |
| Q16 | Yellow | | No |
| D17 | Green | | Yes |
| M18 | Green | | Yes |
| D19 | Yellow | 6% | No |
| I20 | Yellow | | No |
| Q21 | Yellow | | No |
| D24 | Yellow | | No |
| Y25 | Yellow | 6% | No |
| W26 | Yellow | | No |
| R27 | Yellow | | No |
| H28 | Yellow | | No |
| D32 | Yellow | 6% | No |
| G33 | Green | | Yes |
| I34 | Green | | Yes |
| I35 | Yellow | | No |
| C36 | Yellow | 6% | No |
| T44 | Yellow | | No |
| M45 | Green | | Yes |
| C46 | Orange | | No |
| P47 | Yellow | 6% | No |
| T50 | Yellow | | No |
| A53 | Yellow | | No |
| W57 | Yellow | | No |
| V58 | Yellow | 6% | No |
| A59 | Yellow | | No |
| Y62 | Yellow | | No |
| N63 | Yellow | | No |
| P64 | Yellow | 6% | No |
| G67 | Yellow | | No |
| L71 | Red | | Yes |
| V82 | Green | | Yes |
| C86 | Yellow | 6% | No |
| P87 | Yellow | | No |
| C88 | Yellow | | No |
| T91 | Yellow | | No |
| T106 | Yellow | 6% | Yes |
| I107 | Yellow | | No |
| W108 | Yellow | | No |
| C109 | Yellow | | No |
| D115 | Yellow | 6% | No |
| Y119 | Yellow | | No |
| K129 | Yellow | | No |
| A130 | Yellow | | No |
| S131 | Orange | 6% | Yes |
| H135 | Green | | Yes |
| HIS | Green | | Yes |
| HIS | Grey | | No |

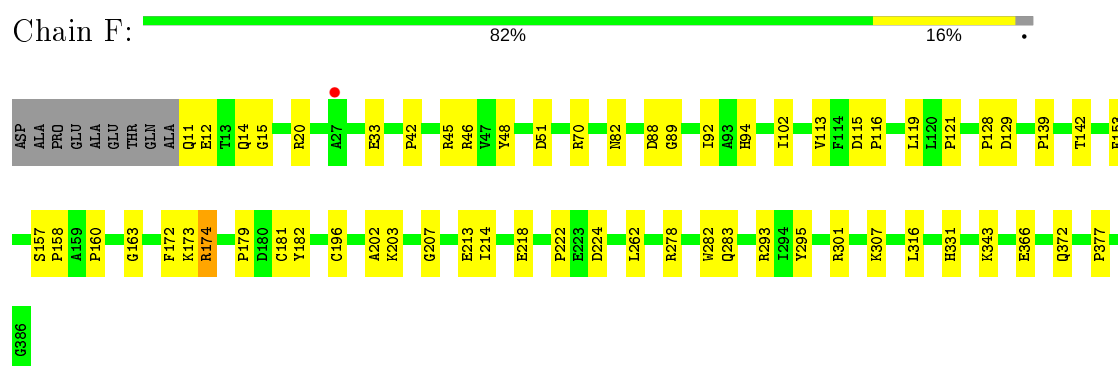
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- Molecule 3: Methylamine dehydrogenase heavy chain



- Molecule 3: Methylamine dehydrogenase heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.53Å 83.52Å 107.78Å 109.94° 91.54° 105.78°	Depositor
Resolution (Å)	44.49 – 2.08 44.49 – 2.08	Depositor EDS
% Data completeness (in resolution range)	97.1 (44.49-2.08) 97.1 (44.49-2.08)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.170 , 0.234 0.186 , 0.245	Depositor DCC
R_{free} test set	5095 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14569	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, 0AF, NA, CA, HEC, EDO, MES, 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	0.91	1/2844 (0.0%)	0.88	1/3859 (0.0%)
1	B	1.12	2/2832 (0.1%)	0.94	1/3841 (0.0%)
2	C	1.00	2/1025 (0.2%)	0.93	2/1399 (0.1%)
2	E	1.27	5/990 (0.5%)	1.05	0/1352
3	D	0.91	3/3015 (0.1%)	0.89	2/4108 (0.0%)
3	F	1.10	1/3034 (0.0%)	0.98	1/4133 (0.0%)
All	All	1.03	14/13740 (0.1%)	0.93	7/18692 (0.0%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	283	VAL	CB-CG2	5.87	1.65	1.52
2	E	74	TYR	CB-CG	5.80	1.60	1.51
2	C	108	TRP	NE1-CE2	-5.55	1.30	1.37
2	C	46	CYS	CB-SG	-5.41	1.73	1.81
3	D	24	ALA	CA-CB	5.38	1.63	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	71	LEU	CA-CB-CG	5.93	128.93	115.30
3	F	70	ARG	NE-CZ-NH2	-5.54	117.53	120.30
3	D	70	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	99	ASP	CB-CG-OD2	5.50	123.25	118.30
3	D	384	ASP	CB-CG-OD1	5.42	123.18	118.30

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	2777	0	2642	61	0
1	B	2768	0	2639	39	0
2	C	1009	0	898	34	0
2	E	972	0	878	35	0
3	D	2934	0	2814	57	0
3	F	2954	0	2835	36	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	86	0	60	7	0
5	B	86	0	60	6	0
6	A	4	0	3	0	0
7	B	2	0	0	0	0
8	B	4	0	6	0	0
9	B	10	0	14	1	0
10	D	12	0	12	0	0
10	F	12	0	12	0	0
11	A	135	0	0	3	0
11	B	246	0	0	2	0
11	C	54	0	0	2	0
11	D	152	0	0	4	0
11	E	80	0	0	3	0
11	F	270	0	0	3	0
All	All	14569	0	12873	245	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 9.

The worst 5 of 245 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:THR:HG22	1:B:286:ASP:OD1	1.52	1.08
3:F:174[A]:ARG:HG3	3:F:174[A]:ARG:HH21	0.86	1.01
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.24	1.00
3:F:174[A]:ARG:CG	3:F:174[A]:ARG:HH21	1.76	0.98
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.27	0.97

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	357/373 (96%)	343 (96%)	13 (4%)	1 (0%)	41	39
1	B	356/373 (95%)	347 (98%)	9 (2%)	0	100	100
2	C	129/137 (94%)	121 (94%)	6 (5%)	2 (2%)	9	4
2	E	126/137 (92%)	124 (98%)	2 (2%)	0	100	100
3	D	376/385 (98%)	358 (95%)	17 (4%)	1 (0%)	41	39
3	F	378/385 (98%)	364 (96%)	13 (3%)	1 (0%)	41	39
All	All	1722/1790 (96%)	1657 (96%)	60 (4%)	5 (0%)	47	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	131[A]	SER
2	C	131[B]	SER
3	D	102	ILE
1	A	166	GLY
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	281/292 (96%)	259 (92%)	22 (8%)	12	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	280/292 (96%)	269 (96%)	11 (4%)	32	32
2	C	111/112 (99%)	107 (96%)	4 (4%)	35	35
2	E	108/112 (96%)	104 (96%)	4 (4%)	34	34
3	D	306/310 (99%)	296 (97%)	10 (3%)	38	39
3	F	308/310 (99%)	295 (96%)	13 (4%)	30	29
All	All	1394/1428 (98%)	1330 (95%)	64 (5%)	27	25

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	321	ARG
2	C	115	ASP
3	F	218	GLU
1	B	323	LEU
1	B	361	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	210	GLN
2	C	68	GLN
3	F	14	GLN
1	B	91	GLN
1	B	163	GLN

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	1.76	4 (30%)	11,22,24	1.52	3 (27%)
2	0AF	C	57	2	13,16,17	1.62	4 (30%)	11,22,24	2.57	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	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 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CB-CA	4.31	1.63	1.53
2	C	57	0AF	CZ2-CE2	-3.09	1.37	1.42
2	C	57	0AF	CD1-NE1	-2.96	1.30	1.36
2	E	57	0AF	CZ2-CE2	-2.96	1.38	1.42
2	C	57	0AF	CE2-NE1	-2.49	1.30	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	57	0AF	CB-CA-C	5.96	122.64	111.47
2	C	57	0AF	CB-CG-CD1	-4.77	122.07	127.97
2	E	57	0AF	CB-CG-CD1	-3.29	123.91	127.97
2	C	57	0AF	CB-CG-CD2	3.03	130.96	126.25
2	E	57	0AF	CB-CA-C	2.39	115.95	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	57	0AF	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	57	0AF	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 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
8	EDO	B	405	-	3,3,3	0.49	0	2,2,2	0.40	0
9	PGE	B	406	-	9,9,9	0.72	0	8,8,8	0.85	0
10	MES	D	401	-	12,12,12	1.82	1 (8%)	14,16,16	2.76	9 (64%)
10	MES	F	401	-	12,12,12	1.99	1 (8%)	14,16,16	3.27	9 (64%)
5	HEC	A	402	1,11	26,50,50	1.70	8 (30%)	18,82,82	2.97	12 (66%)
5	HEC	B	402	1	26,50,50	1.48	8 (30%)	18,82,82	3.08	10 (55%)
6	ACT	A	404	-	1,3,3	1.84	0	0,3,3	0.00	-
5	HEC	A	403	1	26,50,50	1.67	8 (30%)	18,82,82	3.61	9 (50%)
5	HEC	B	403	1	26,50,50	1.50	6 (23%)	18,82,82	3.22	9 (50%)

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
8	EDO	B	405	-	-	1/1/1/1	-
9	PGE	B	406	-	-	4/7/7/7	-
10	MES	D	401	-	-	5/6/14/14	0/1/1/1
10	MES	F	401	-	-	2/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	A	402	1,11	-	0/6/54/54	-
5	HEC	B	402	1	-	0/6/54/54	-
5	HEC	A	403	1	-	0/6/54/54	-
5	HEC	B	403	1	-	0/6/54/54	-

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	401	MES	C8-S	-6.43	1.68	1.77
10	D	401	MES	C8-S	-5.77	1.69	1.77
5	A	402	HEC	C3C-C4C	4.05	1.50	1.43
5	B	403	HEC	C3C-C4C	3.54	1.49	1.43
5	A	403	HEC	C4A-C3A	3.25	1.49	1.42

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	403	HEC	CBD-CAD-C3D	-7.55	98.56	112.49
5	A	403	HEC	CAD-CBD-CGD	-6.39	101.95	112.67
5	B	403	HEC	CBD-CAD-C3D	-6.21	101.04	112.49
5	B	402	HEC	CMC-C2C-C3C	6.16	133.07	125.82
5	A	403	HEC	C1D-C2D-C3D	-6.14	102.72	107.00

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	401	MES	C7-C8-S-O1S
10	D	401	MES	C7-C8-S-O2S
10	D	401	MES	C7-C8-S-O3S
10	F	401	MES	N4-C7-C8-S
9	B	406	PGE	C4-C3-O2-C2

There are no ring outliers.

5 monomers are involved in 14 short contacts:

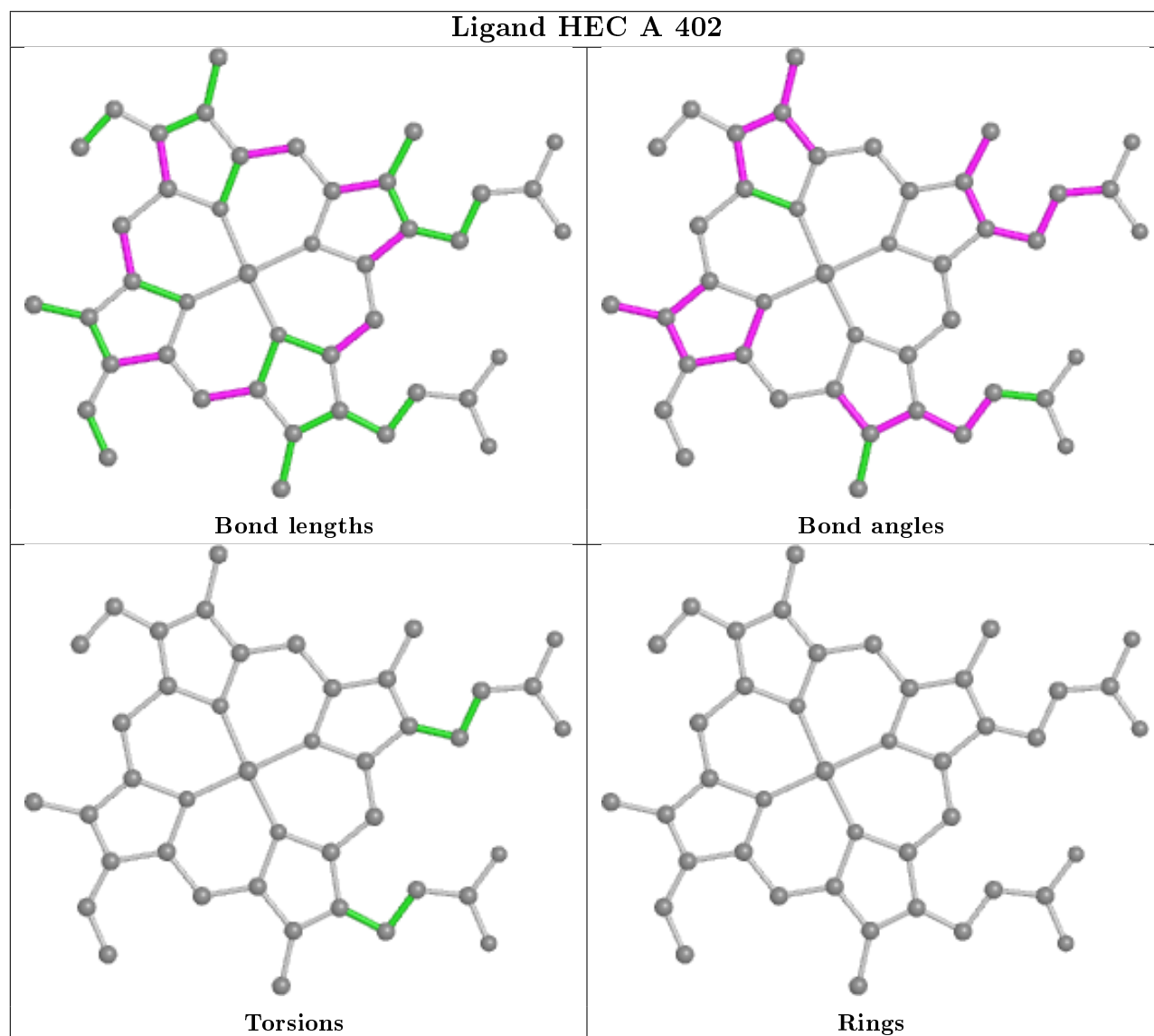
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	406	PGE	1	0
5	A	402	HEC	4	0
5	B	402	HEC	4	0
5	A	403	HEC	3	0

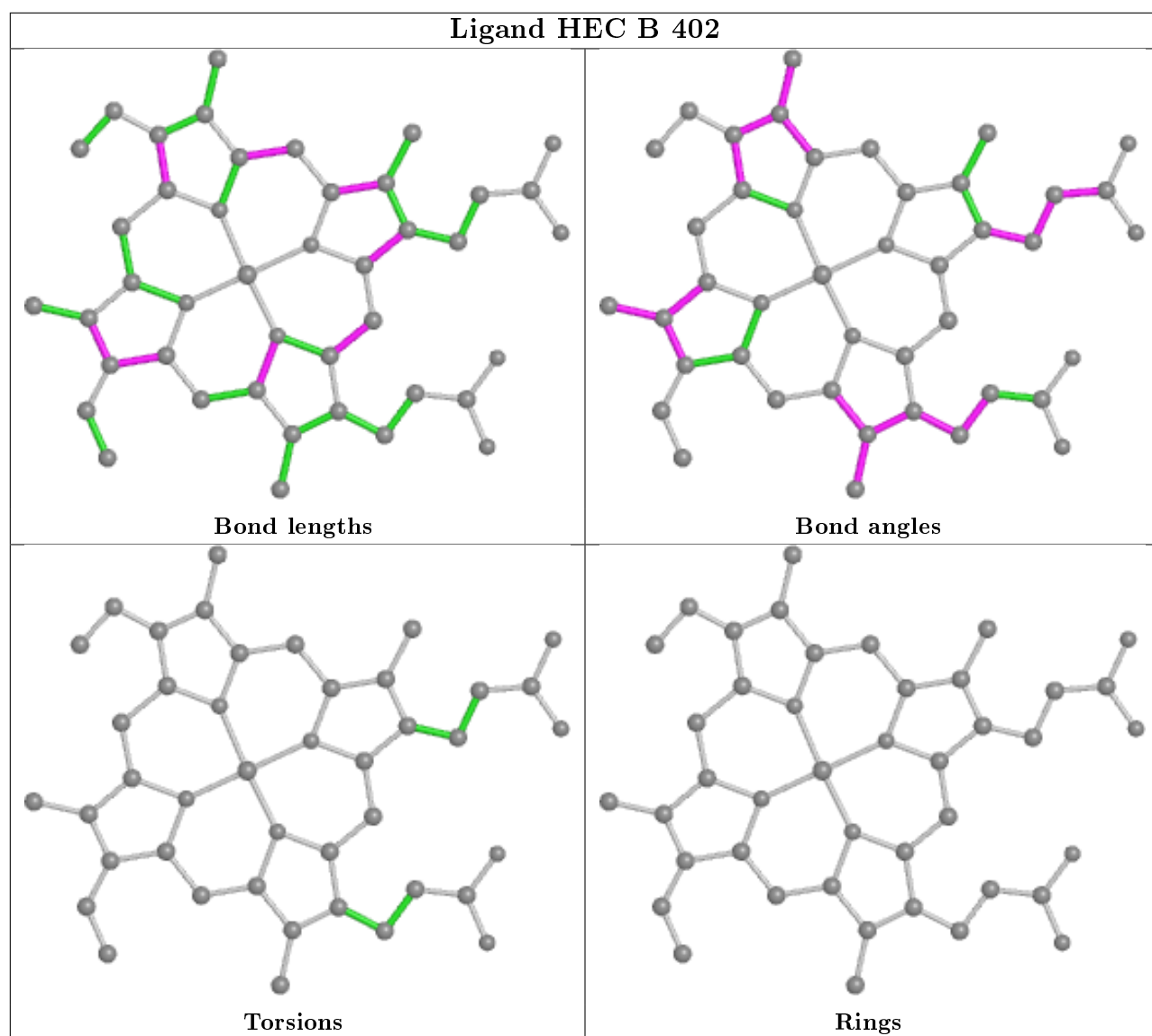
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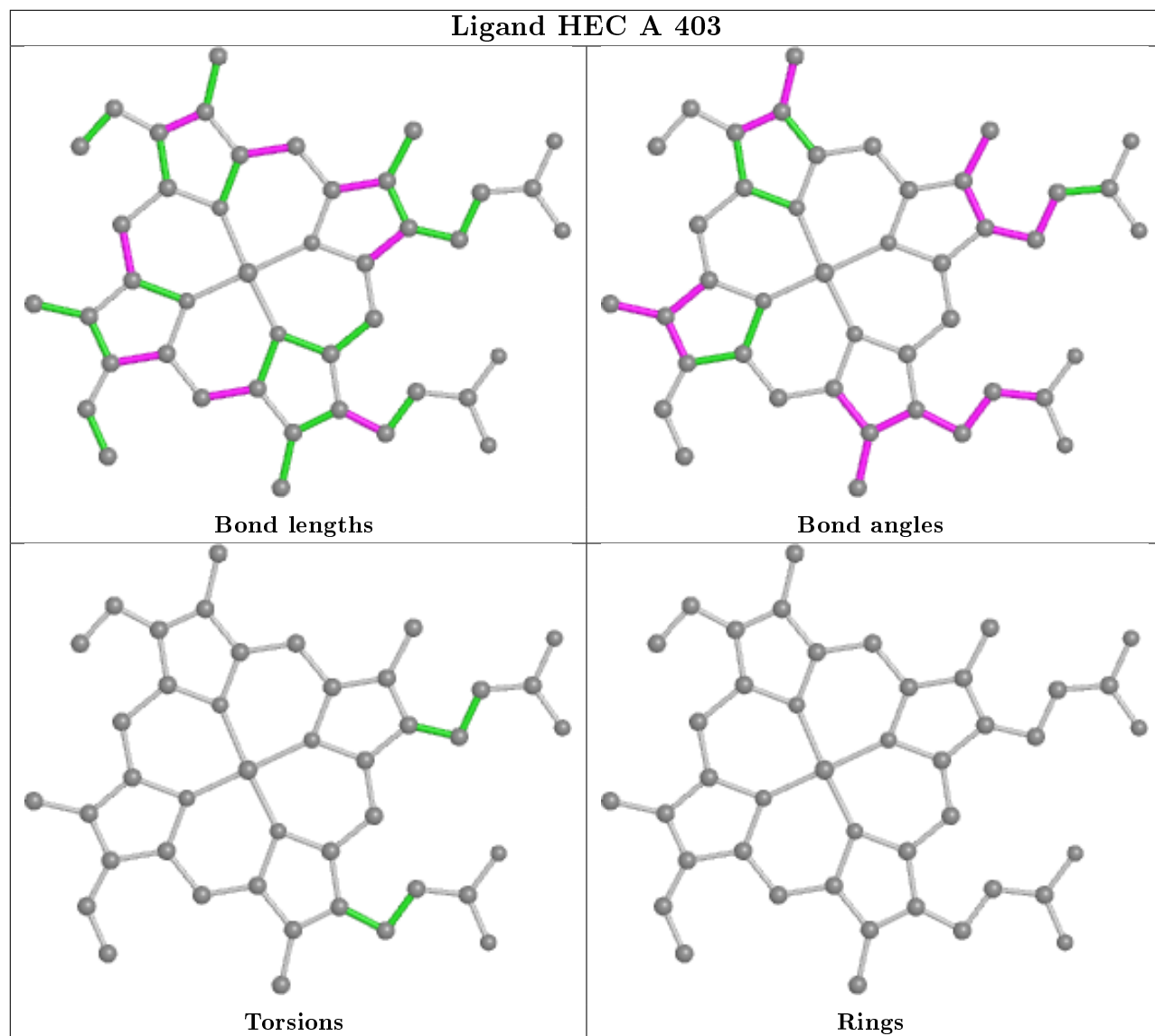
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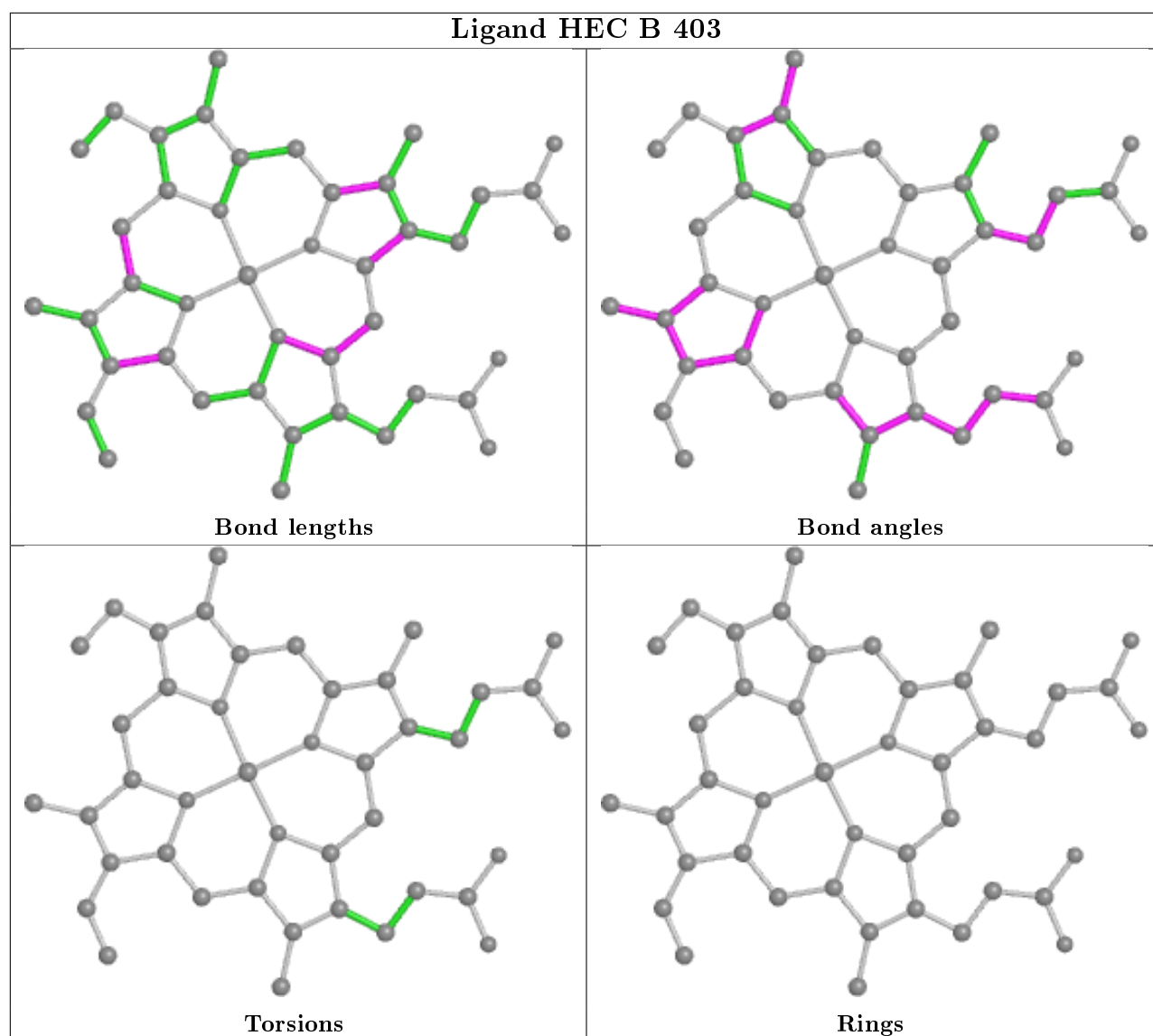
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	403	HEC	2	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	354/373 (94%)	-0.16	6 (1%) 70 73	32, 46, 67, 77	0
1	B	357/373 (95%)	-0.32	3 (0%) 86 87	19, 36, 57, 79	0
2	C	128/137 (93%)	0.32	5 (3%) 39 44	27, 42, 69, 92	0
2	E	124/137 (90%)	0.18	1 (0%) 86 87	24, 31, 44, 67	0
3	D	376/385 (97%)	0.15	11 (2%) 51 56	28, 50, 80, 88	0
3	F	376/385 (97%)	-0.15	1 (0%) 94 94	23, 33, 52, 70	0
All	All	1715/1790 (95%)	-0.06	27 (1%) 72 75	19, 40, 70, 92	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	5.7
3	D	208	THR	5.7
2	C	131[A]	SER	5.0
1	B	6	ALA	4.5
3	D	274	ALA	4.4

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	0AF	E	57	15/16	0.89	0.20	31,35,38,38	0
2	0AF	C	57	15/16	0.92	0.19	44,46,48,48	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

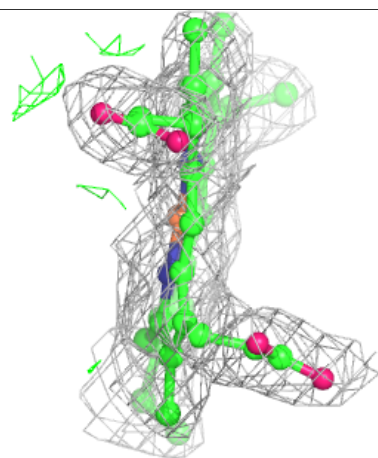
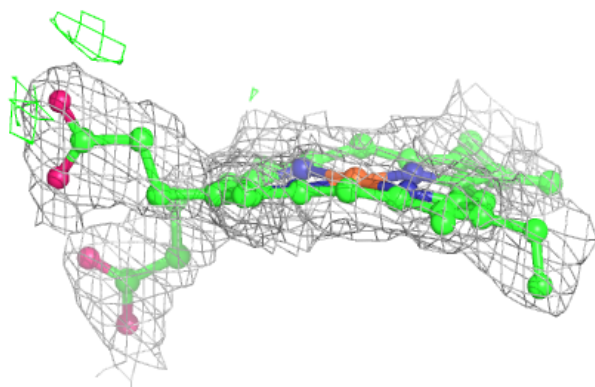
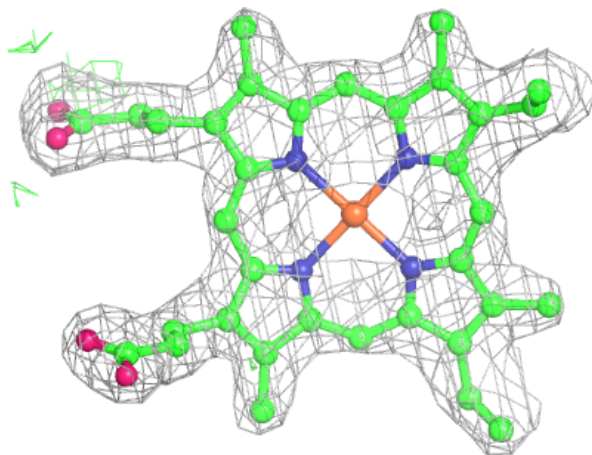
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	PGE	B	406	10/10	0.75	0.19	61,66,69,69	0
7	NA	B	407	1/1	0.84	0.14	46,46,46,46	0
6	ACT	A	404	4/4	0.84	0.12	75,76,76,76	0
10	MES	D	401	12/12	0.89	0.27	80,90,93,93	0
10	MES	F	401	12/12	0.91	0.25	72,80,82,83	0
8	EDO	B	405	4/4	0.94	0.08	53,53,54,57	0
4	CA	A	401	1/1	0.96	0.08	45,45,45,45	0
5	HEC	A	402	43/43	0.97	0.11	31,39,43,44	0
5	HEC	B	402	43/43	0.97	0.11	23,29,33,34	0
7	NA	B	404	1/1	0.98	0.08	39,39,39,39	0
5	HEC	A	403	43/43	0.98	0.11	35,39,42,45	0
5	HEC	B	403	43/43	0.98	0.11	18,22,26,28	0
4	CA	B	401	1/1	1.00	0.12	25,25,25,25	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.

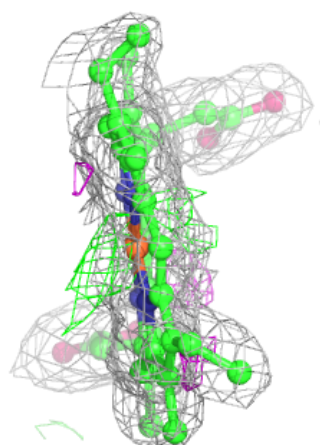
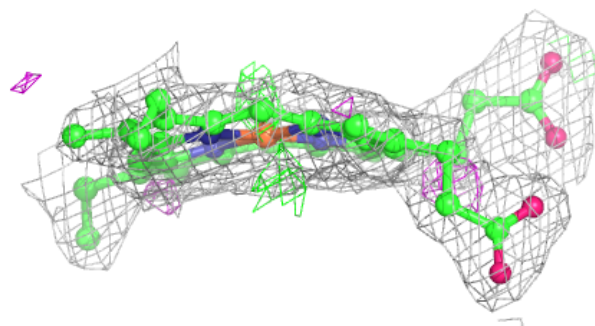
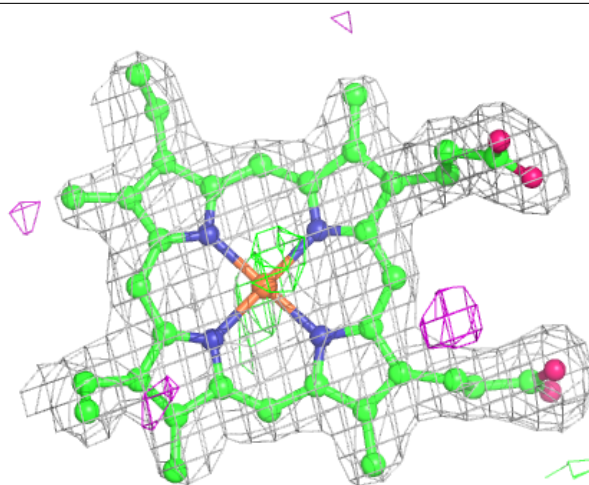
Electron density around HEC A 402:

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



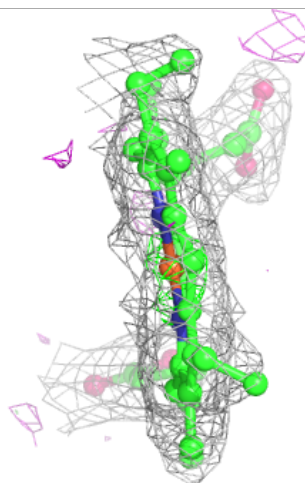
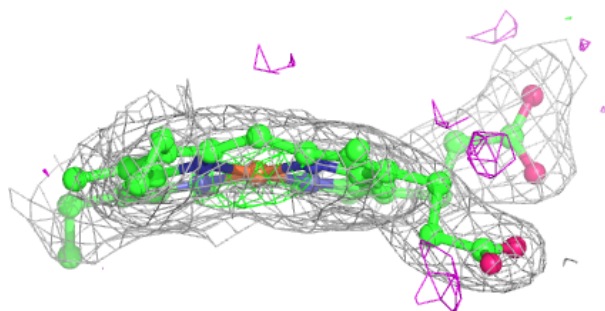
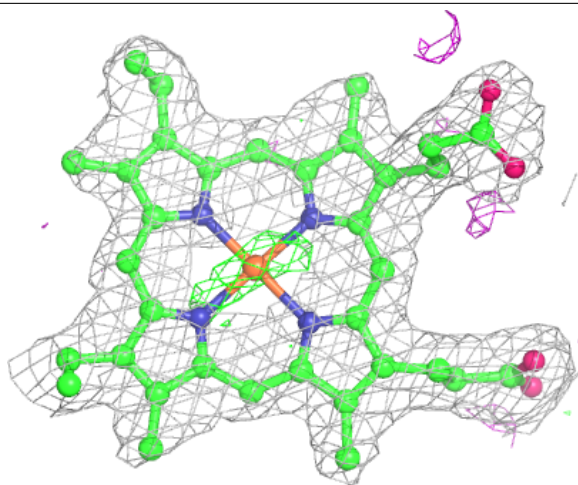
Electron density around HEC B 402:

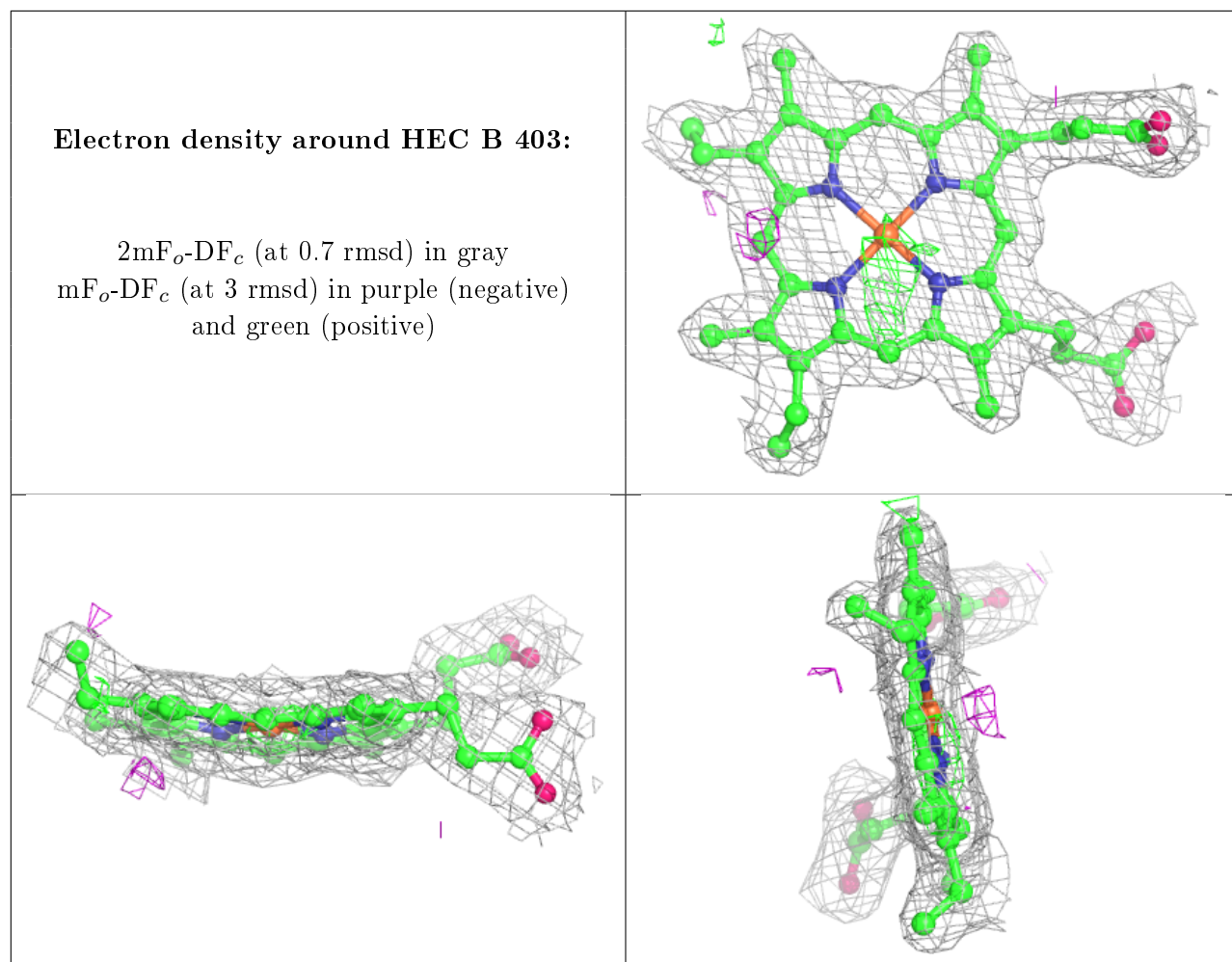
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.