W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Sep 3, 2023 – 09:02 AM EDT

PDB ID	:	3SXT
Title	:	Crystal Structure of the Quinol Form of Methylamine Dehydrogenase in Complex with the Diferrous Form of MauG
Authors	:	Jensen, L.M.R.; Wilmot, C.M.
Deposited on	:	2011-07-15
Resolution	:	1.81 Å(reported)

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

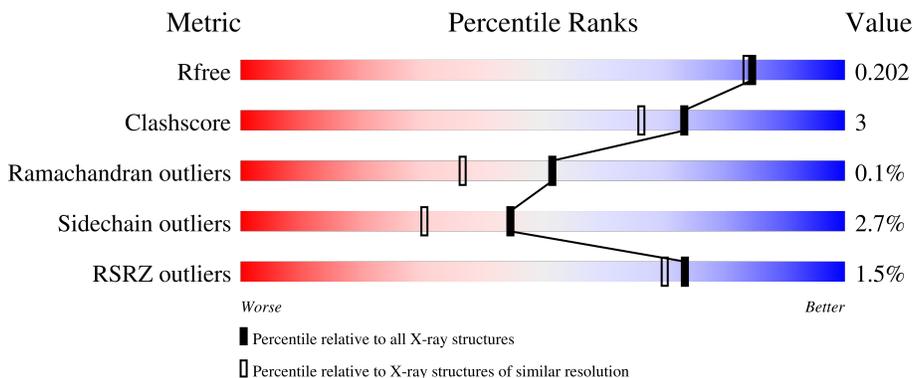|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	Percentile Ranks	Value
Rfree		0.202
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		2.7%
RSRZ outliers		1.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	2% / 88% / 7% / 5%
1	B	373	.% / 86% / 9% / · ·
2	C	137	.% / 81% / 7% / · / 9%
2	E	137	.% / 81% / 8% / · / 9%
3	D	386	.% / 87% / 10% / ·

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Mol	Chain	Length	Quality of chain
3	F	386	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	EDO	D	401	-	-	X	-

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 15339 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	0	0
			2734	1707	490	526	11			
1	B	357	Total	C	N	O	S	0	4	0
			2789	1740	505	532	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	125	Total	C	N	O	S	0	1	0
			961	594	161	193	13			
2	E	125	Total	C	N	O	S	0	1	0
			958	592	161	191	14			

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	375	Total 2943	C 1868	N 509	O 558	S 8	0	4	0
3	F	376	Total 2932	C 1861	N 502	O 561	S 8	0	2	0

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

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

• Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

• Molecule 6 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

HEC

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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	340	Total 340	O 340	0	0
8	B	358	Total 358	O 358	0	0
8	C	123	Total 123	O 123	0	0
8	D	452	Total 452	O 452	0	0
8	E	138	Total 138	O 138	0	0
8	F	413	Total 413	O 413	0	0

3 Residue-property plots ⓘ

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

• Molecule 3: Methylamine dehydrogenase heavy chain

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.64Å 135.66Å 111.56Å 90.00° 97.37° 90.00°	Depositor
Resolution (Å)	35.01 – 1.81	Depositor
	35.01 – 1.81	EDS
% Data completeness (in resolution range)	97.9 (35.01-1.81)	Depositor
	97.9 (35.01-1.81)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.145 , 0.187	Depositor
	0.162 , 0.202	DCC
R_{free} test set	8245 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.2	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15339	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, TOQ, NA, HEC, CA

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	1.13	1/2798 (0.0%)	0.94	2/3797 (0.1%)
1	B	1.22	6/2865 (0.2%)	1.03	13/3883 (0.3%)
2	C	1.28	5/972 (0.5%)	0.98	1/1327 (0.1%)
2	E	1.35	2/969 (0.2%)	1.04	2/1323 (0.2%)
3	D	1.23	6/3032 (0.2%)	1.05	5/4129 (0.1%)
3	F	1.19	4/3015 (0.1%)	1.01	12/4109 (0.3%)
All	All	1.21	24/13651 (0.2%)	1.01	35/18568 (0.2%)

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	303	GLU	CD-OE1	8.33	1.34	1.25
2	C	80	TYR	CD1-CE1	6.52	1.49	1.39
3	F	347	TYR	CD2-CE2	6.14	1.48	1.39
1	B	199	TRP	CB-CG	5.91	1.60	1.50
3	F	282	TRP	CB-CG	5.80	1.60	1.50

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	132	ARG	NE-CZ-NH1	8.71	124.65	120.30
3	D	305	ARG	NE-CZ-NH2	-7.81	116.39	120.30
3	D	197	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	180	ARG	NE-CZ-NH2	7.05	123.83	120.30
2	C	99	ARG	NE-CZ-NH1	-6.97	116.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2734	0	2607	20	0
1	B	2789	0	2679	12	0
2	C	961	0	864	10	0
2	E	958	0	864	10	0
3	D	2943	0	2850	18	0
3	F	2932	0	2826	20	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	86	0	60	1	0
6	B	86	0	60	2	0
7	A	8	0	12	2	0
7	B	4	0	6	0	0
7	D	4	0	6	4	0
7	F	4	0	6	3	0
8	A	340	0	0	5	0
8	B	358	0	0	2	0
8	C	123	0	0	1	0
8	D	452	0	0	9	0
8	E	138	0	0	0	0
8	F	413	0	0	6	0
All	All	15339	0	12840	88	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 3.

The worst 5 of 88 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:HH12	7:A:406:EDO:H12	1.09	1.15
7:D:401:EDO:H22	8:D:555:HOH:O	1.50	1.12
2:E:130:ALA:O	2:E:131:SER:HB2	1.48	1.06
3:F:126:GLU:H	7:F:401:EDO:H21	1.29	0.97
1:B:48:LYS:H	1:B:62:HIS:HE1	1.15	0.94

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	352/373 (94%)	345 (98%)	7 (2%)	0	100	100
1	B	359/373 (96%)	349 (97%)	10 (3%)	0	100	100
2	C	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
2	E	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
3	D	377/386 (98%)	367 (97%)	8 (2%)	2 (0%)	29	15
3	F	376/386 (97%)	363 (96%)	12 (3%)	1 (0%)	41	27
All	All	1710/1792 (95%)	1666 (97%)	41 (2%)	3 (0%)	51	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	102[A]	ILE
3	D	102[B]	ILE
3	F	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	276/292 (94%)	269 (98%)	7 (2%)	47	33
1	B	283/292 (97%)	274 (97%)	9 (3%)	39	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	105/112 (94%)	102 (97%)	3 (3%)	42	28
2	E	105/112 (94%)	102 (97%)	3 (3%)	42	28
3	D	307/311 (99%)	299 (97%)	8 (3%)	46	32
3	F	306/311 (98%)	298 (97%)	8 (3%)	46	32
All	All	1382/1430 (97%)	1344 (97%)	38 (3%)	44	30

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	129	LYS
3	F	262	LEU
2	E	131	SER
3	F	209	GLU
3	F	365	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	235	GLN
3	D	378	GLN
3	F	378	GLN
3	F	30	GLN
3	F	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	TOQ	C	57	2	14,17,18	1.22	1 (7%)	13,24,26	1.96	3 (23%)
2	TOQ	E	57	2	14,17,18	1.48	4 (28%)	13,24,26	2.64	5 (38%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	TOQ	CZ2-CE2	-3.30	1.37	1.42
2	E	57	TOQ	CD1-NE1	-2.73	1.31	1.36
2	E	57	TOQ	CZ2-CE2	-2.21	1.39	1.42
2	E	57	TOQ	CD1-CG	2.10	1.43	1.37
2	E	57	TOQ	CE3-CZ3	2.03	1.40	1.36

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	TOQ	CB-CG-CD1	-6.57	119.85	127.97
2	E	57	TOQ	CB-CG-CD2	4.74	133.63	126.25
2	C	57	TOQ	CB-CG-CD1	-4.63	122.24	127.97
2	C	57	TOQ	CB-CG-CD2	4.17	132.74	126.25
2	E	57	TOQ	CE3-CZ3-CH2	-2.70	117.65	120.32

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	C	57	TOQ	1	0
2	E	57	TOQ	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	#$|Z| > 2$
7	EDO	A	406	-	3,3,3	0.31	0	2,2,2	0.60	0
7	EDO	A	407	-	3,3,3	0.40	0	2,2,2	0.92	0
7	EDO	D	401	-	3,3,3	0.73	0	2,2,2	0.50	0
7	EDO	F	401	-	3,3,3	0.58	0	2,2,2	0.36	0
6	HEC	B	405	1	32,50,50	1.23	2 (6%)	24,82,82	3.22	11 (45%)
6	HEC	A	404	8,1	32,50,50	1.40	5 (15%)	24,82,82	2.67	11 (45%)
6	HEC	A	405	1	32,50,50	1.25	3 (9%)	24,82,82	3.35	12 (50%)
6	HEC	B	404	1	32,50,50	1.58	7 (21%)	24,82,82	2.30	8 (33%)
7	EDO	B	406	-	3,3,3	0.58	0	2,2,2	0.38	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
7	EDO	A	406	-	-	1/1/1/1	-
7	EDO	A	407	-	-	0/1/1/1	-
7	EDO	D	401	-	-	1/1/1/1	-
7	EDO	F	401	-	-	1/1/1/1	-
6	HEC	B	405	1	-	2/10/54/54	-
6	HEC	A	404	8,1	-	2/10/54/54	-
6	HEC	A	405	1	-	2/10/54/54	-
6	HEC	B	404	1	-	4/10/54/54	-
7	EDO	B	406	-	-	0/1/1/1	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	404	HEC	C1B-CHB	3.40	1.50	1.41
6	A	404	HEC	C1B-CHB	3.13	1.49	1.41
6	B	405	HEC	C3C-C4C	3.00	1.48	1.43
6	B	404	HEC	C1D-CHD	2.91	1.49	1.41
6	B	404	HEC	O2D-CGD	-2.72	1.21	1.30

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	405	HEC	CBD-CAD-C3D	-10.33	94.99	112.62
6	B	405	HEC	CBD-CAD-C3D	-9.41	96.57	112.62
6	B	405	HEC	C1D-C2D-C3D	-7.61	101.70	107.00
6	A	404	HEC	CBD-CAD-C3D	-7.29	100.18	112.62
6	B	404	HEC	CBD-CAD-C3D	-6.01	102.37	112.62

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	406	EDO	O1-C1-C2-O2
7	D	401	EDO	O1-C1-C2-O2
7	F	401	EDO	O1-C1-C2-O2
6	B	404	HEC	CAD-CBD-CGD-O2D
6	A	404	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.
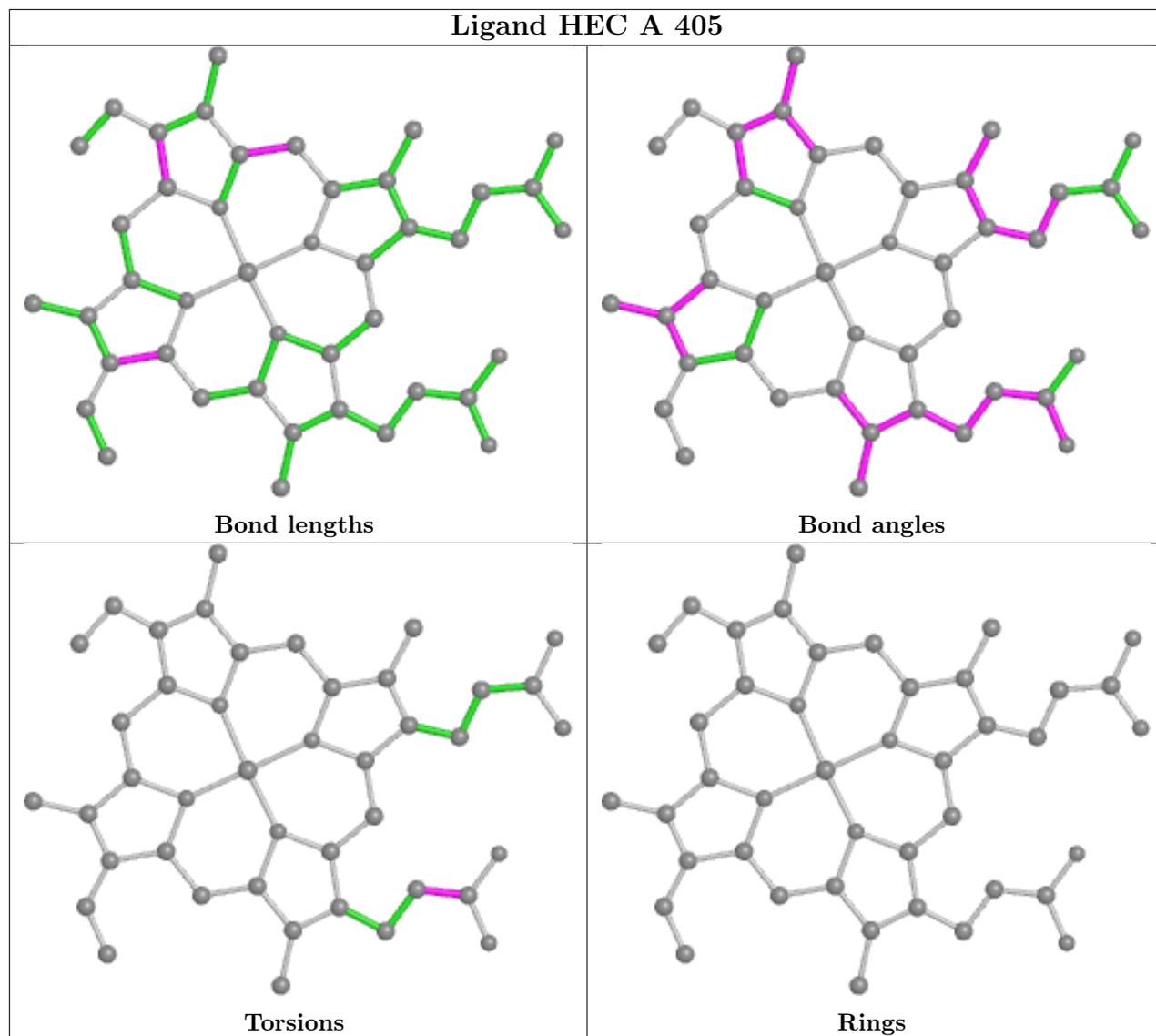
6 monomers are involved in 12 short contacts:

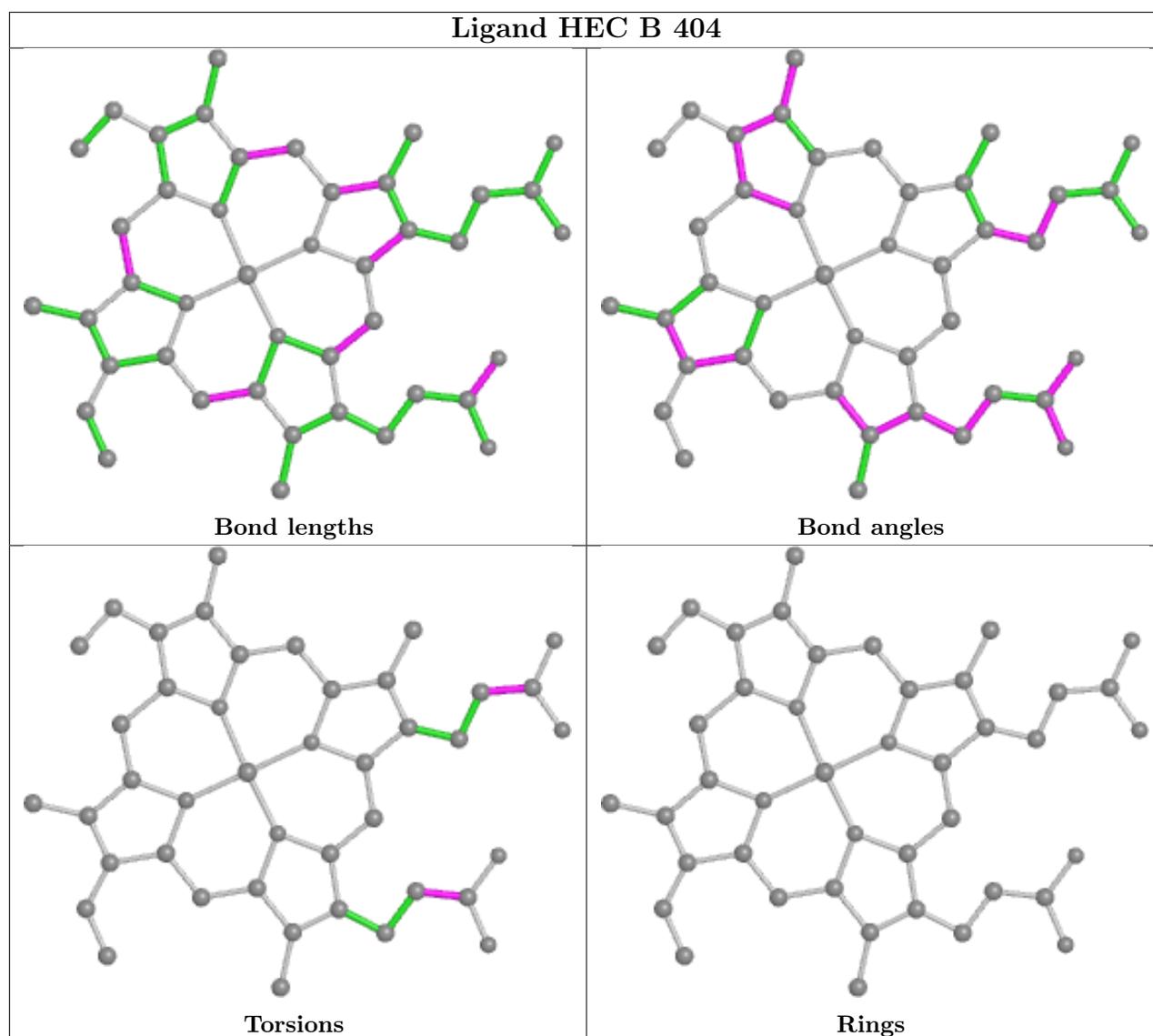| Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	406	EDO	2	0
7	D	401	EDO	4	0
7	F	401	EDO	3	0
6	B	405	HEC	1	0
6	A	405	HEC	1	0
6	B	404	HEC	1	0

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 then 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 B 405

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC A 404

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC A 405

Bond lengths

Bond angles

Torsions

Rings

Ligand HEC B 404

Bond lengths

Bond angles

Torsions

Rings
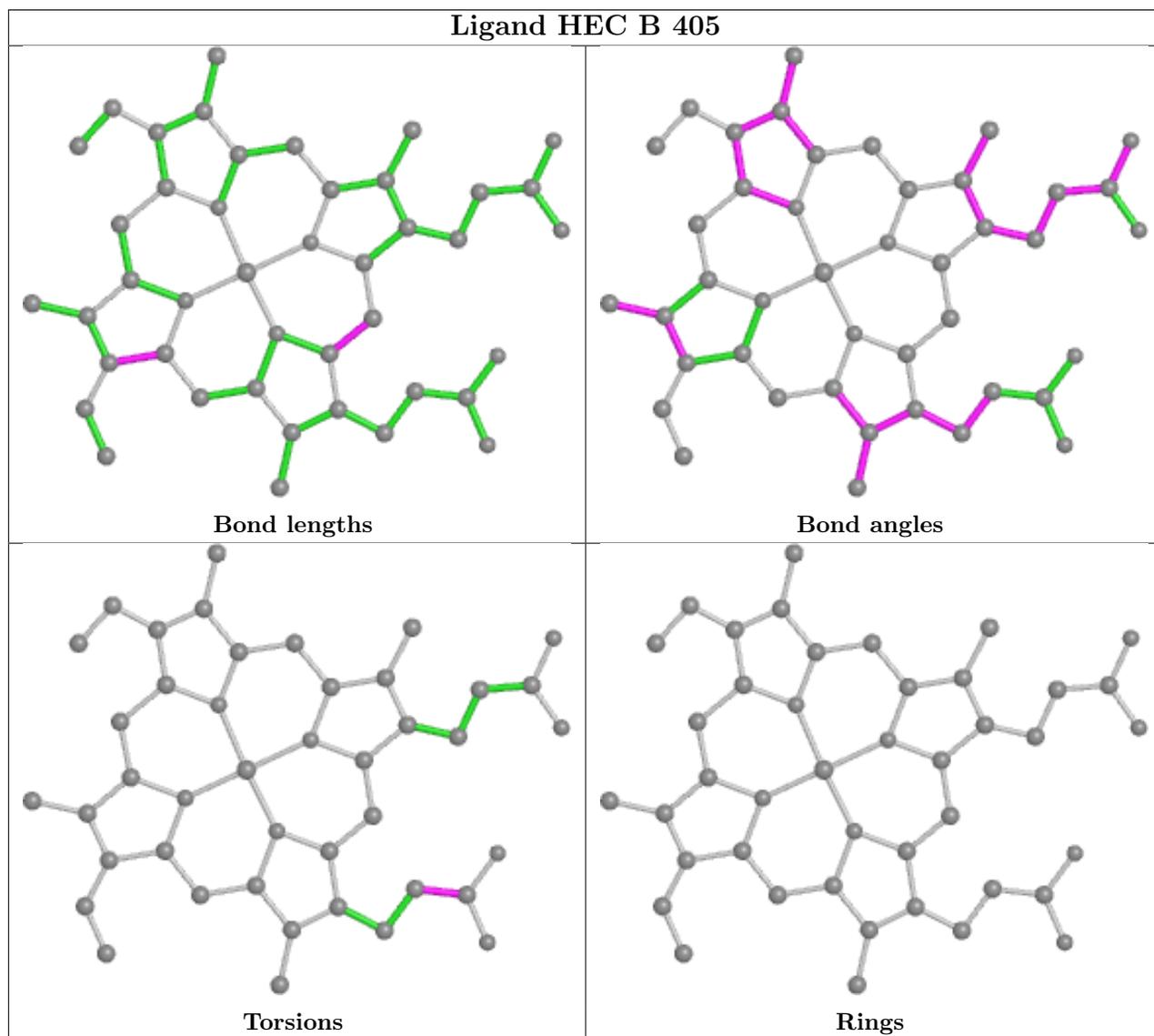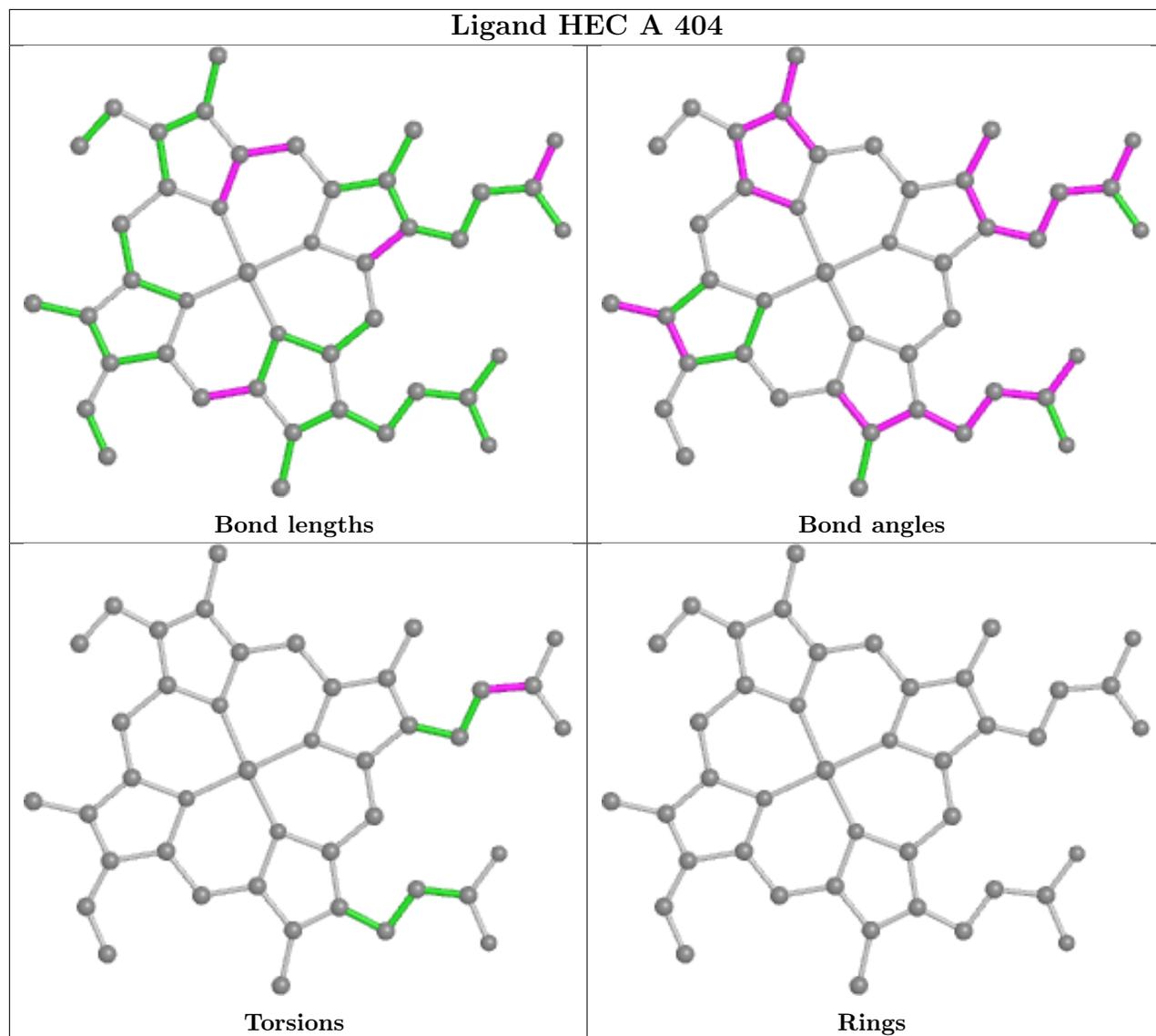
5.7 Other polymers (i)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.19	7 (1%)	65	61	22, 33, 46, 68	0
1	B	357/373 (95%)	-0.16	3 (0%)	86	84	20, 30, 50, 63	0
2	C	124/137 (90%)	-0.22	1 (0%)	86	84	19, 26, 36, 52	0
2	E	124/137 (90%)	-0.30	2 (1%)	72	68	16, 21, 31, 52	0
3	D	375/386 (97%)	-0.34	2 (0%)	91	89	17, 25, 40, 60	0
3	F	376/386 (97%)	-0.15	11 (2%)	51	46	18, 29, 46, 66	0
All	All	1710/1792 (95%)	-0.22	26 (1%)	73	70	16, 28, 45, 68	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ASP	5.4
1	A	7	ASP	5.3
1	A	6	ALA	4.9
3	F	208	THR	4.5
3	F	209	GLU	3.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

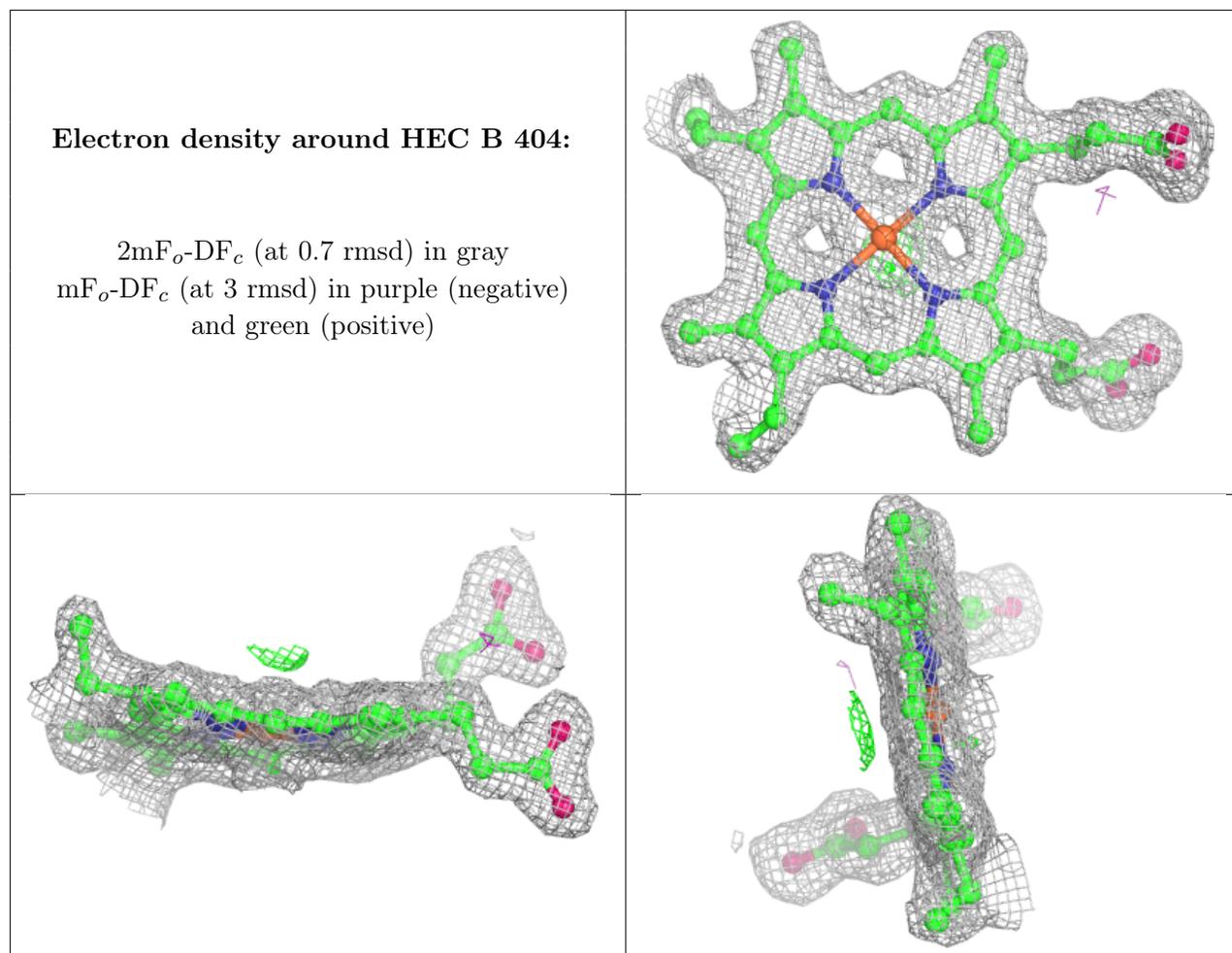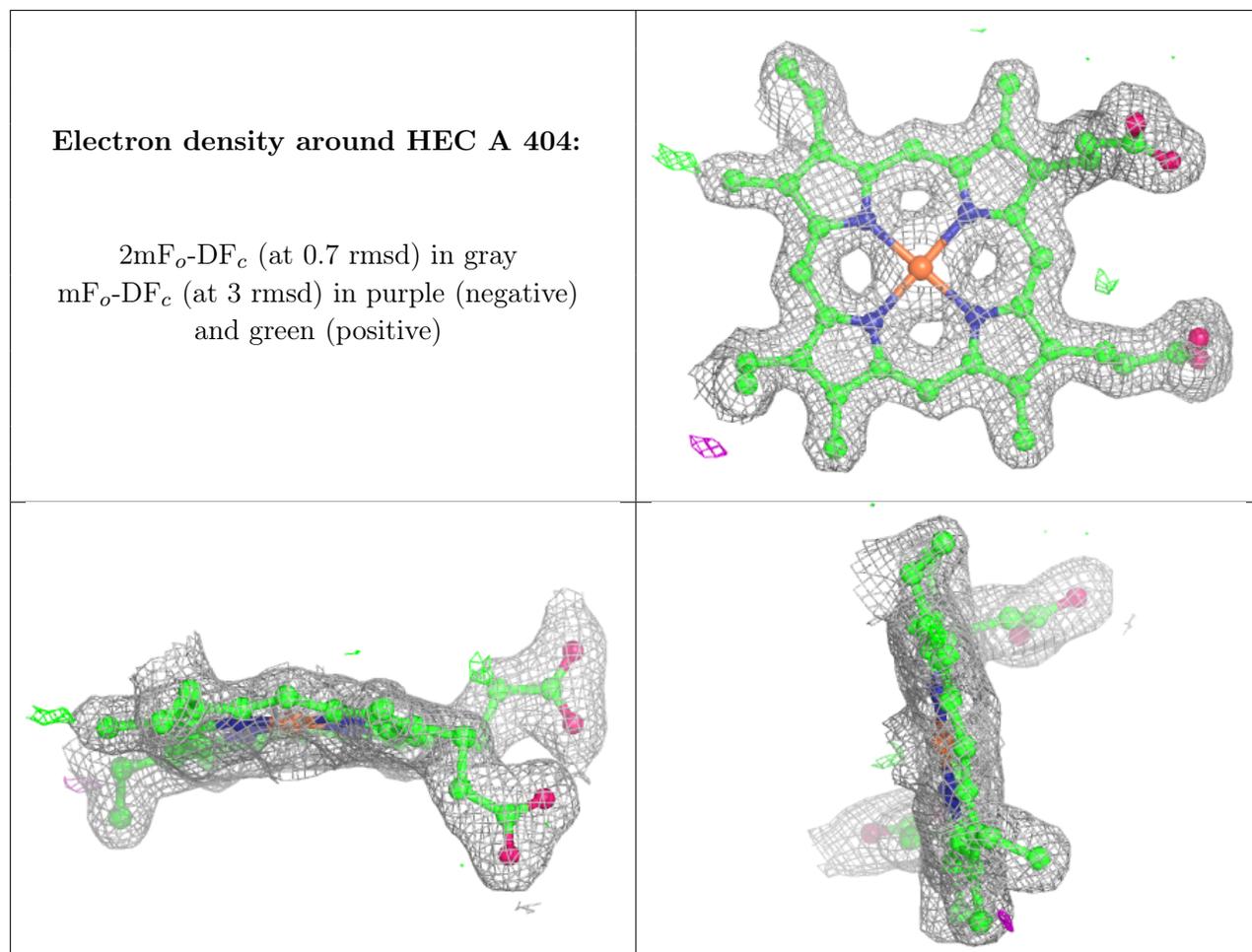| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TOQ	C	57	16/17	0.97	0.11	22,26,29,29	0
2	TOQ	E	57	16/17	0.97	0.12	20,22,28,28	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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.

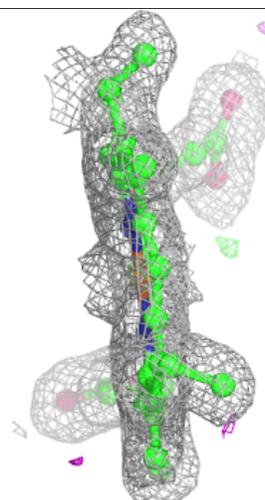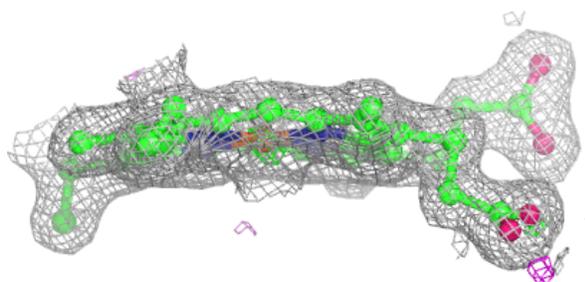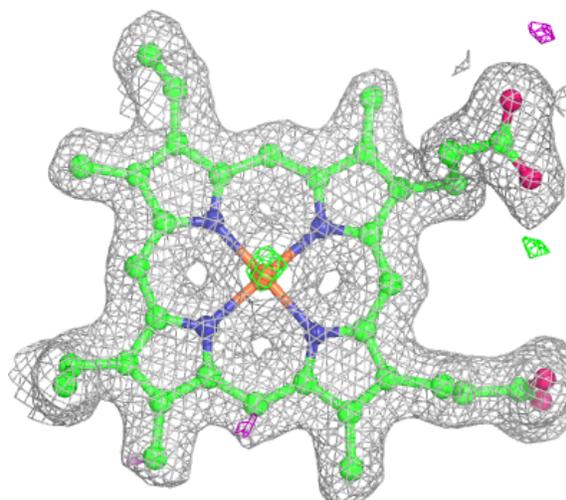| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	A	406	4/4	0.85	0.10	52,53,53,53	0
7	EDO	F	401	4/4	0.86	0.23	42,44,48,49	0
7	EDO	A	407	4/4	0.88	0.16	55,55,55,60	0
7	EDO	D	401	4/4	0.90	0.32	41,46,46,48	0
7	EDO	B	406	4/4	0.91	0.30	40,44,44,45	0
5	NA	B	402	1/1	0.95	0.14	40,40,40,40	0
5	NA	B	403	1/1	0.97	0.09	39,39,39,39	0
5	NA	A	402	1/1	0.97	0.05	34,34,34,34	0
6	HEC	B	404	43/43	0.98	0.11	22,27,30,31	0
5	NA	A	403	1/1	0.98	0.10	40,40,40,40	0
6	HEC	A	404	43/43	0.98	0.10	24,29,31,34	0
6	HEC	A	405	43/43	0.99	0.14	20,22,25,26	0
4	CA	B	401	1/1	0.99	0.10	25,25,25,25	0
6	HEC	B	405	43/43	0.99	0.12	16,20,24,24	0
4	CA	A	401	1/1	0.99	0.08	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.
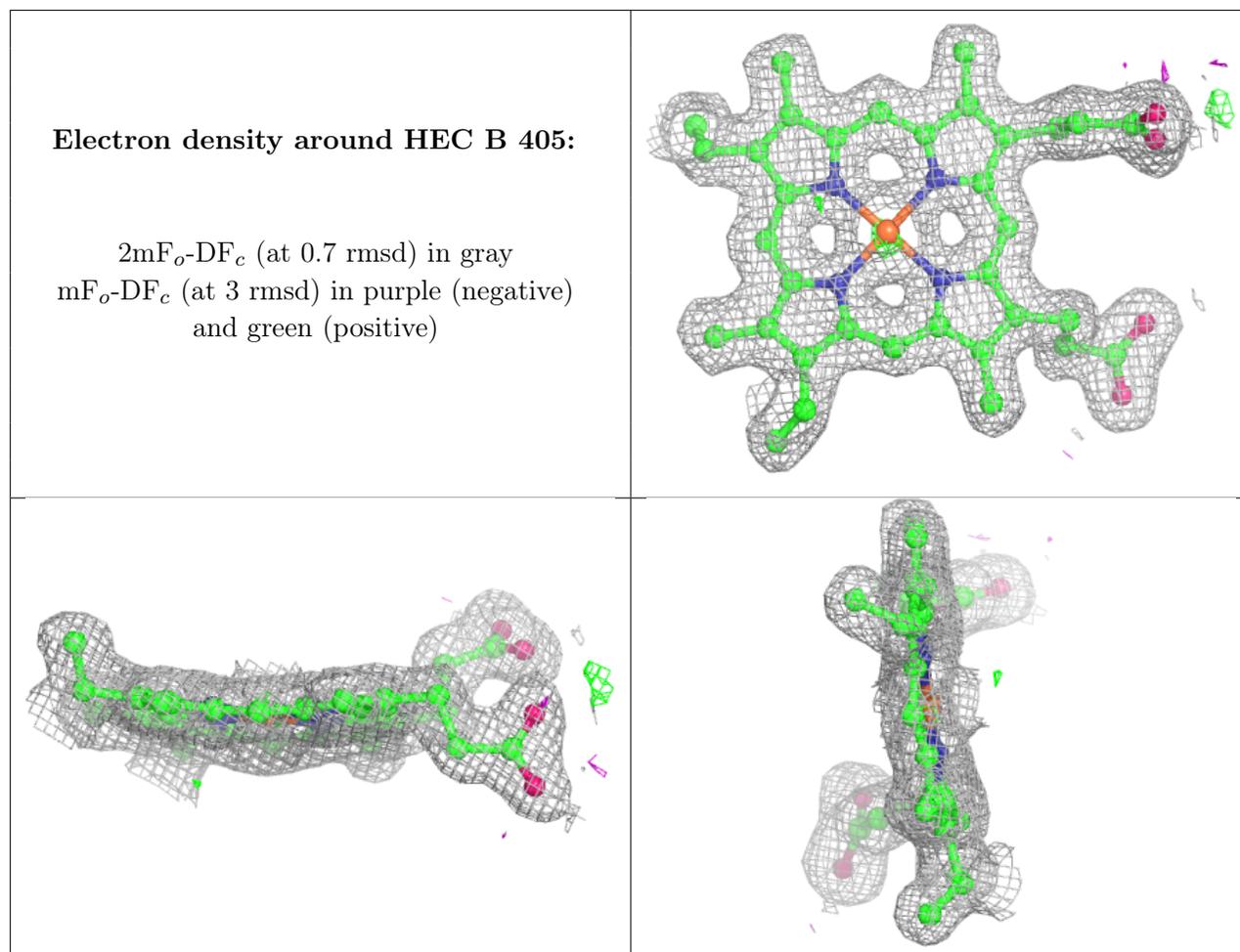
Electron density around HEC B 404:

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 404:

$2mF_o$-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 405:

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

Electron density around HEC B 405:

$2mF_o$-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 ⓘ

There are no such residues in this entry.