



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 08:35 AM EDT

PDB ID : 6VDS
Title : Crystal Structure of Dehaloperoxidase B in Complex with cofactor Iron(III) Deuteroporphyrin IX and Substrate 4-bromo-ortho-cresol
Authors : Ghiladi, R.A.; de Serrano, V.S.; McGuire, A.; Malewschik, T.
Deposited on : 2019-12-27
Resolution : 1.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FDE	A	201	X	-	-	-
2	FDE	B	201[A]	X	-	-	-
2	FDE	B	201[B]	X	-	-	-

2 Entry composition i

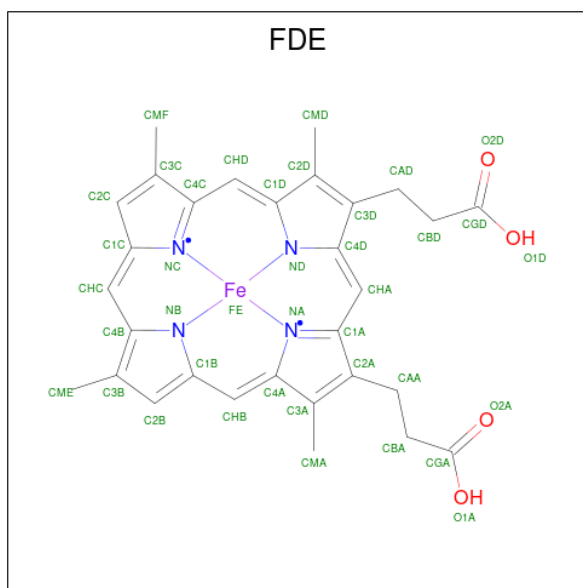
There are 6 unique types of molecules in this entry. The entry contains 2725 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dehaloperoxidase B.

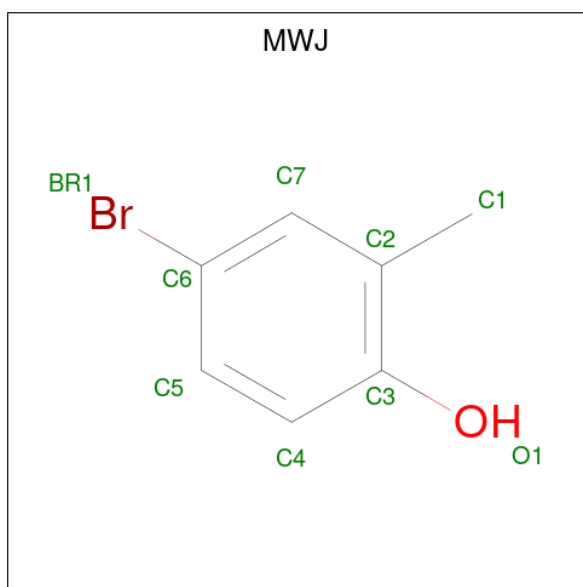
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	137	1245	778	219	240	8	0	26	0
1	B	137	1227	772	210	236	9	0	23	0

- Molecule 2 is FE(III) DEUTEROPORPHYRIN IX (three-letter code: FDE) (formula: $C_{30}H_{28}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	39	30	1	4	4	0	0
2	B	1	78	60	2	8	8	0	1

- Molecule 3 is 4-bromo-2-methylphenol (three-letter code: MWJ) (formula: C_7H_7BrO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	O		
3	A	1	9	1	7	1	0	0
3	B	1	9	1	7	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



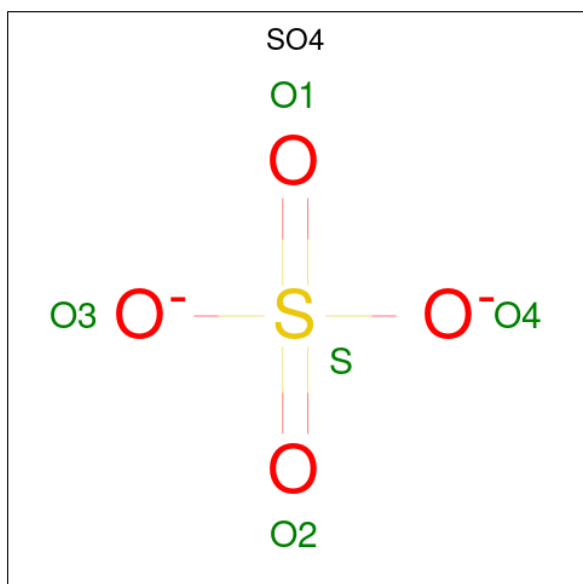
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
4	A	1	4	2	2	0	0

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	44	Total O 44 44	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	32	Total	O	0	0
			32	32		

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3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.56Å 67.49Å 67.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.88 – 1.97	Depositor
% Data completeness (in resolution range)	96.4 (47.88-1.97)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.215 , 0.256	Depositor
Wilson B-factor (Å ²)	32.5	Xtrriage
Anisotropy	0.192	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.327 for -h,l,k	Xtrriage
Reported twinning fraction	0.695 for H, K, L 0.305 for -H, L, K	Depositor
Outliers	0 of 19240 reflections	Xtrriage
Total number of atoms	2725	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.55% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

15 ligands 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
4	EDO	A	206	-	3,3,3	0.09	0	2,2,2	0.06	0
3	MWJ	B	202	-	9,9,9	0.14	0	12,12,12	0.53	0
2	FDE	B	201[B]	1	44,46,46	2.65	19 (43%)	52,76,76	2.90	23 (44%)
3	MWJ	A	202	-	9,9,9	0.26	0	12,12,12	0.53	0
5	SO4	A	208	-	4,4,4	0.37	0	6,6,6	0.10	0
4	EDO	A	205	-	3,3,3	0.20	0	2,2,2	0.30	0
2	FDE	B	201[A]	1	44,46,46	2.66	19 (43%)	52,76,76	3.02	18 (34%)
4	EDO	B	205	-	3,3,3	0.05	0	2,2,2	0.30	0
5	SO4	A	207	-	4,4,4	0.37	0	6,6,6	0.10	0
4	EDO	B	206	-	3,3,3	0.09	0	2,2,2	0.12	0
4	EDO	A	204	-	3,3,3	0.07	0	2,2,2	0.20	0
4	EDO	A	203	-	3,3,3	0.11	0	2,2,2	0.11	0
4	EDO	B	203	-	3,3,3	0.17	0	2,2,2	0.03	0
4	EDO	B	204	-	3,3,3	0.20	0	2,2,2	0.14	0
2	FDE	A	201	1	44,46,46	2.61	19 (43%)	52,76,76	2.90	17 (32%)

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
4	EDO	A	206	-	-	1/1/1/1	-
3	MWJ	B	202	-	-	-	0/1/1/1
2	FDE	B	201[B]	1	1/1/3/7	9/10/50/50	-
3	MWJ	A	202	-	-	-	0/1/1/1
4	EDO	A	205	-	-	0/1/1/1	-
2	FDE	B	201[A]	1	1/1/3/7	6/10/50/50	-
4	EDO	B	205	-	-	1/1/1/1	-
4	EDO	B	206	-	-	0/1/1/1	-
4	EDO	A	204	-	-	1/1/1/1	-
4	EDO	A	203	-	-	1/1/1/1	-
4	EDO	B	203	-	-	0/1/1/1	-
4	EDO	B	204	-	-	1/1/1/1	-
2	FDE	A	201	1	1/1/3/7	3/10/50/50	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201[B]	FDE	C2A-C3A	6.15	1.49	1.36
2	B	201[A]	FDE	C2A-C3A	6.03	1.49	1.36
2	A	201	FDE	C2A-C3A	5.78	1.49	1.36
2	B	201[B]	FDE	C3D-C2D	5.34	1.48	1.36
2	B	201[A]	FDE	CHD-C1D	5.34	1.48	1.38
2	B	201[A]	FDE	C3D-C2D	5.22	1.47	1.36
2	B	201[B]	FDE	CHB-C4A	5.20	1.48	1.35
2	A	201	FDE	CHB-C4A	5.14	1.48	1.35
2	A	201	FDE	C3D-C2D	5.09	1.47	1.36
2	B	201[A]	FDE	CHB-C4A	5.01	1.47	1.35
2	A	201	FDE	CHD-C1D	4.93	1.48	1.38
2	B	201[B]	FDE	CHD-C1D	4.93	1.48	1.38
2	B	201[A]	FDE	CHA-C4D	4.72	1.47	1.38
2	B	201[B]	FDE	CHA-C4D	4.58	1.47	1.38
2	A	201	FDE	CHA-C4D	4.51	1.47	1.38
2	A	201	FDE	C4A-NA	4.49	1.48	1.40
2	B	201[A]	FDE	C4A-NA	4.46	1.48	1.40
2	B	201[B]	FDE	FE-ND	4.41	2.12	1.95
2	B	201[A]	FDE	C1A-NA	4.30	1.47	1.38
2	B	201[B]	FDE	C1A-NA	4.29	1.47	1.38
2	B	201[B]	FDE	C4A-NA	4.09	1.47	1.40
2	B	201[A]	FDE	FE-ND	4.03	2.11	1.95
2	B	201[A]	FDE	CHD-C4C	3.97	1.48	1.39
2	A	201	FDE	FE-ND	3.96	2.11	1.95
2	A	201	FDE	CHD-C4C	3.81	1.47	1.39
2	B	201[B]	FDE	CHD-C4C	3.66	1.47	1.39
2	B	201[B]	FDE	CHC-C1C	3.63	1.48	1.39
2	B	201[A]	FDE	CHA-C1A	3.62	1.47	1.39
2	A	201	FDE	C1A-NA	3.44	1.45	1.38
2	B	201[B]	FDE	CHA-C1A	3.35	1.46	1.39
2	B	201[A]	FDE	CHC-C1C	3.25	1.47	1.39
2	A	201	FDE	C4A-C3A	3.22	1.50	1.44
2	B	201[A]	FDE	C4C-C3C	3.19	1.48	1.42
2	A	201	FDE	CHC-C1C	3.14	1.47	1.39
2	B	201[B]	FDE	C4C-C3C	3.12	1.48	1.42
2	A	201	FDE	CHA-C1A	3.12	1.46	1.39
2	A	201	FDE	C1A-C2A	3.00	1.50	1.45
2	B	201[B]	FDE	C4A-C3A	2.95	1.50	1.44
2	A	201	FDE	C4C-C3C	2.88	1.47	1.42
2	B	201[A]	FDE	C4A-C3A	2.69	1.49	1.44
2	A	201	FDE	C1C-NC	-2.66	1.34	1.40
2	B	201[A]	FDE	C1A-C2A	2.60	1.49	1.45
2	B	201[B]	FDE	C1C-NC	-2.59	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201[B]	FDE	C4D-C3D	2.58	1.49	1.45
2	B	201[B]	FDE	C4B-CHC	2.54	1.48	1.41
2	A	201	FDE	C4C-NC	-2.46	1.33	1.38
2	B	201[A]	FDE	FE-NC	2.44	2.10	1.97
2	B	201[A]	FDE	C4B-CHC	2.42	1.47	1.41
2	A	201	FDE	C4B-CHC	2.39	1.47	1.41
2	B	201[A]	FDE	C1C-NC	-2.36	1.35	1.40
2	A	201	FDE	C1B-CHB	2.32	1.48	1.43
2	B	201[B]	FDE	FE-NC	2.29	2.09	1.97
2	A	201	FDE	C4D-ND	-2.28	1.35	1.39
2	B	201[B]	FDE	C4C-NC	-2.27	1.34	1.38
2	B	201[B]	FDE	C1B-CHB	2.22	1.48	1.43
2	B	201[A]	FDE	C4D-ND	-2.17	1.35	1.39
2	B	201[A]	FDE	C1D-C2D	2.02	1.49	1.45

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201[A]	FDE	C2C-C1C-NC	11.05	118.17	109.56
2	A	201	FDE	C2C-C1C-NC	10.43	117.68	109.56
2	B	201[B]	FDE	C2C-C1C-NC	9.93	117.30	109.56
2	B	201[A]	FDE	CMF-C3C-C4C	7.31	136.75	125.51
2	A	201	FDE	CMF-C3C-C4C	7.18	136.54	125.51
2	B	201[A]	FDE	C2B-C1B-NB	6.40	118.36	110.21
2	B	201[B]	FDE	C3D-C4D-ND	6.33	116.49	110.32
2	A	201	FDE	C1C-C2C-C3C	-6.08	102.16	108.89
2	B	201[B]	FDE	C2B-C1B-NB	5.92	117.75	110.21
2	B	201[A]	FDE	C1C-C2C-C3C	-5.89	102.37	108.89
2	B	201[B]	FDE	CMF-C3C-C4C	5.78	134.39	125.51
2	B	201[A]	FDE	C3D-C4D-ND	5.64	115.81	110.32
2	A	201	FDE	C2B-C1B-NB	5.61	117.35	110.21
2	A	201	FDE	C3D-C4D-ND	5.59	115.76	110.32
2	B	201[B]	FDE	C1C-C2C-C3C	-5.52	102.78	108.89
2	B	201[A]	FDE	C1B-C2B-C3B	-4.86	102.50	106.36
2	B	201[A]	FDE	C1B-CHB-C4A	-4.53	122.65	129.64
2	B	201[B]	FDE	C1B-C2B-C3B	-4.40	102.87	106.36
2	B	201[B]	FDE	C1B-CHB-C4A	-4.31	122.99	129.64
2	A	201	FDE	C1B-CHB-C4A	-4.17	123.20	129.64
2	B	201[B]	FDE	C4D-C3D-C2D	-4.16	101.71	107.13
2	A	201	FDE	C1B-C2B-C3B	-4.14	103.08	106.36
2	A	201	FDE	CMF-C3C-C2C	-4.02	116.24	125.63
2	B	201[A]	FDE	CMF-C3C-C2C	-3.93	116.44	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	FDE	CME-C3B-C2B	-3.90	117.79	124.93
2	B	201[A]	FDE	C2C-C1C-CHC	-3.80	116.45	125.72
2	B	201[A]	FDE	CME-C3B-C2B	-3.73	118.10	124.93
2	A	201	FDE	C2C-C1C-CHC	-3.71	116.68	125.72
2	B	201[A]	FDE	C4C-NC-C1C	-3.63	102.13	106.71
2	B	201[A]	FDE	C4D-C3D-C2D	-3.60	102.44	107.13
2	A	201	FDE	C4D-C3D-C2D	-3.54	102.51	107.13
2	B	201[B]	FDE	CME-C3B-C2B	-3.43	118.65	124.93
2	B	201[B]	FDE	C2D-C1D-ND	3.31	115.79	109.69
2	B	201[B]	FDE	CAD-C3D-C4D	3.26	131.04	124.89
2	B	201[B]	FDE	C4C-NC-C1C	-3.21	102.66	106.71
2	B	201[B]	FDE	C2C-C1C-CHC	-3.00	118.39	125.72
2	A	201	FDE	C4C-NC-C1C	-2.88	103.07	106.71
2	A	201	FDE	C2D-C1D-ND	2.84	114.93	109.69
2	A	201	FDE	CMD-C2D-C1D	2.78	129.61	124.71
2	B	201[B]	FDE	C4D-ND-C1D	-2.75	102.65	105.35
2	B	201[A]	FDE	C2D-C1D-ND	2.74	114.75	109.69
2	A	201	FDE	CHA-C4D-C3D	-2.71	120.55	124.94
2	A	201	FDE	C1D-C2D-C3D	-2.68	103.02	106.94
2	B	201[B]	FDE	CHA-C1A-C2A	-2.66	120.93	124.84
2	B	201[A]	FDE	C1D-C2D-C3D	-2.61	103.14	106.94
2	B	201[B]	FDE	CAA-CBA-CGA	-2.58	108.05	113.60
2	B	201[B]	FDE	C2A-C1A-NA	2.58	112.85	110.36
2	A	201	FDE	CMA-C3A-C4A	2.55	128.92	125.04
2	B	201[B]	FDE	CMF-C3C-C2C	-2.52	119.73	125.63
2	B	201[A]	FDE	C2A-C1A-NA	2.51	112.79	110.36
2	B	201[A]	FDE	CHA-C4D-C3D	-2.50	120.89	124.94
2	B	201[A]	FDE	C4A-NA-C1A	-2.45	102.54	105.07
2	B	201[B]	FDE	C1D-C2D-C3D	-2.45	103.36	106.94
2	B	201[B]	FDE	CHA-C4D-ND	-2.38	121.86	124.44
2	B	201[B]	FDE	CHD-C1D-C2D	-2.38	120.49	125.48
2	B	201[A]	FDE	C3A-C4A-NA	2.10	112.33	109.84
2	B	201[B]	FDE	CHA-C4D-C3D	-2.04	121.64	124.94
2	B	201[B]	FDE	CMD-C2D-C1D	2.02	128.28	124.71

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	201	FDE	ND
2	B	201[A]	FDE	ND
2	B	201[B]	FDE	ND

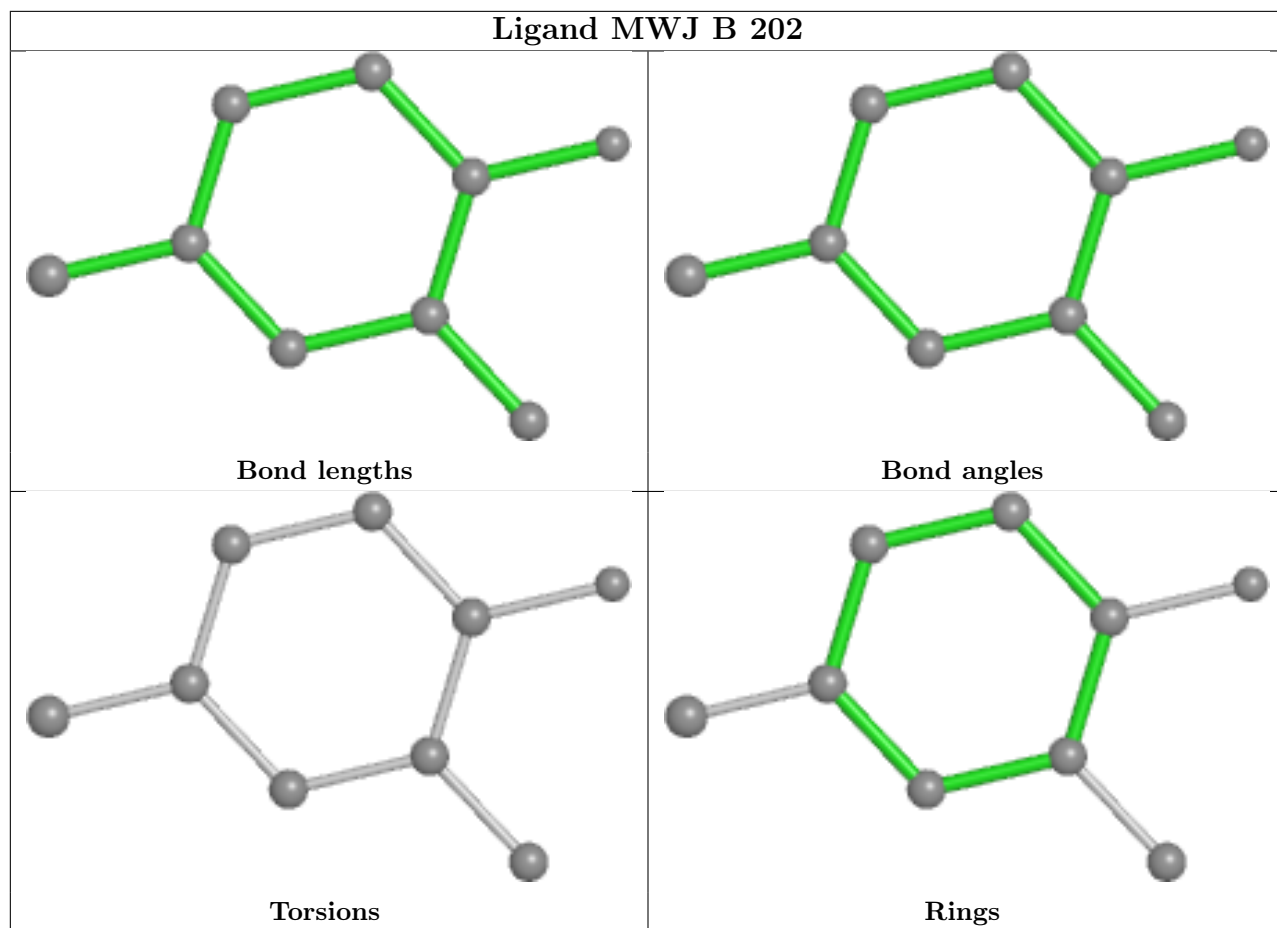
All (23) torsion outliers are listed below:

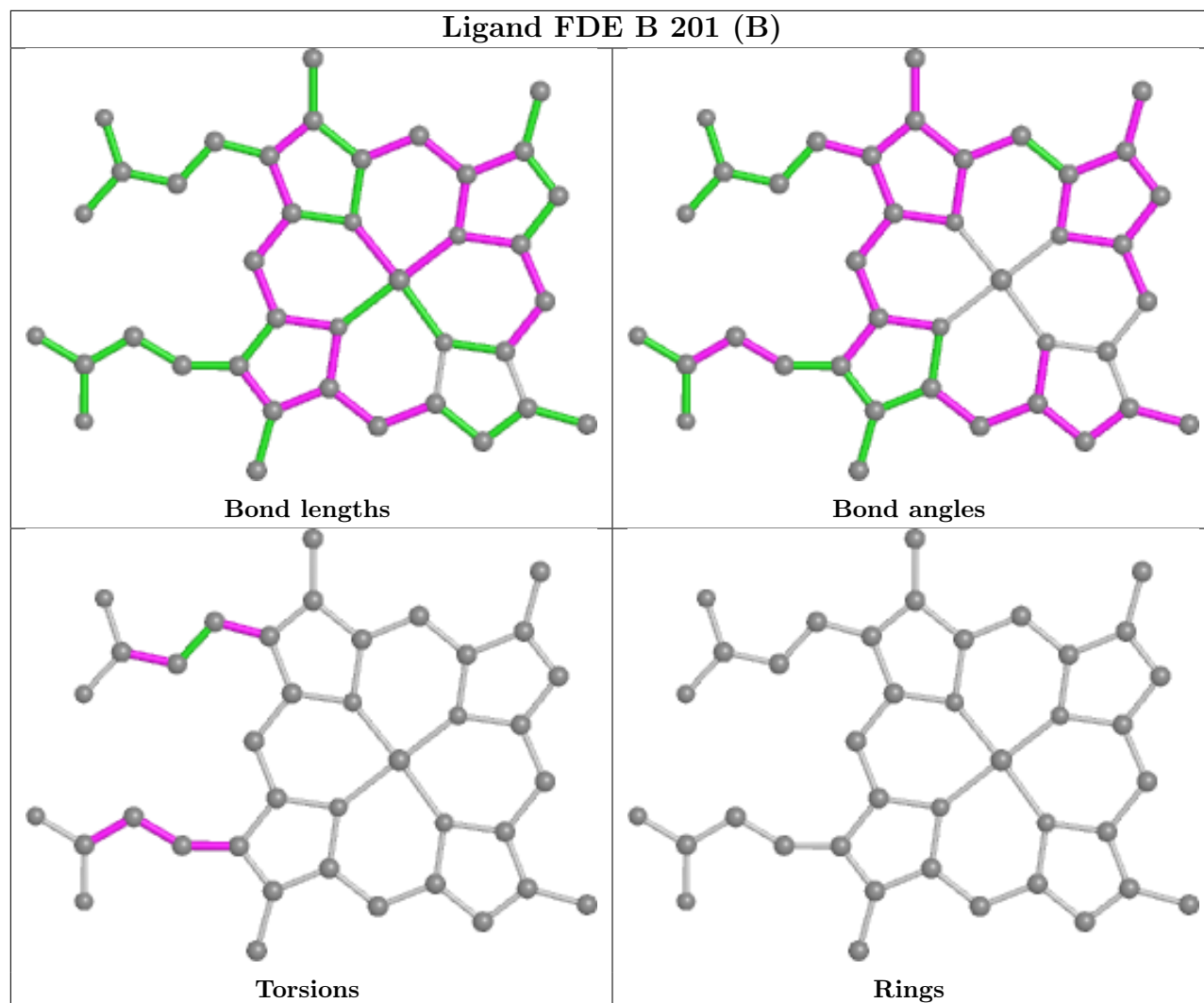
Mol	Chain	Res	Type	Atoms
2	B	201[B]	FDE	C3A-C2A-CAA-CBA
2	B	201[A]	FDE	C3A-C2A-CAA-CBA
2	B	201[B]	FDE	C1A-C2A-CAA-CBA
2	B	201[A]	FDE	C1A-C2A-CAA-CBA
2	B	201[A]	FDE	C2A-CAA-CBA-CGA
4	A	206	EDO	O1-C1-C2-O2
4	B	205	EDO	O1-C1-C2-O2
2	A	201	FDE	C2A-CAA-CBA-CGA
2	B	201[B]	FDE	C4D-C3D-CAD-CBD
2	B	201[A]	FDE	C3D-CAD-CBD-CGD
2	B	201[B]	FDE	C2D-C3D-CAD-CBD
4	A	204	EDO	O1-C1-C2-O2
2	A	201	FDE	CAA-CBA-CGA-O2A
2	B	201[B]	FDE	CAA-CBA-CGA-O2A
2	B	201[B]	FDE	CAA-CBA-CGA-O1A
2	B	201[B]	FDE	C2A-CAA-CBA-CGA
4	A	203	EDO	O1-C1-C2-O2
2	B	201[B]	FDE	CAD-CBD-CGD-O1D
2	B	201[B]	FDE	CAD-CBD-CGD-O2D
2	A	201	FDE	CAA-CBA-CGA-O1A
2	B	201[A]	FDE	CAD-CBD-CGD-O1D
2	B	201[A]	FDE	CAD-CBD-CGD-O2D
4	B	204	EDO	O1-C1-C2-O2

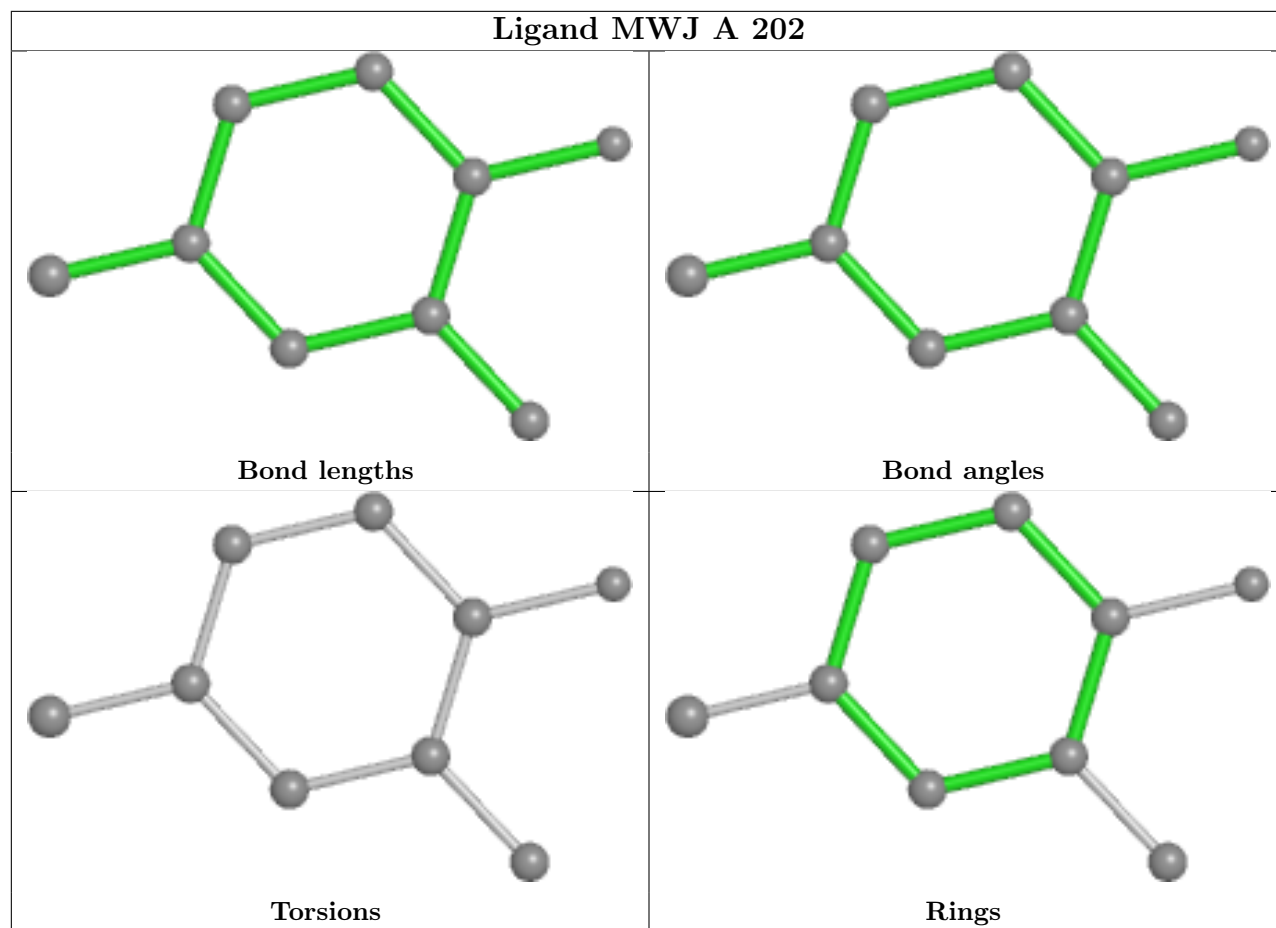
There are no ring outliers.

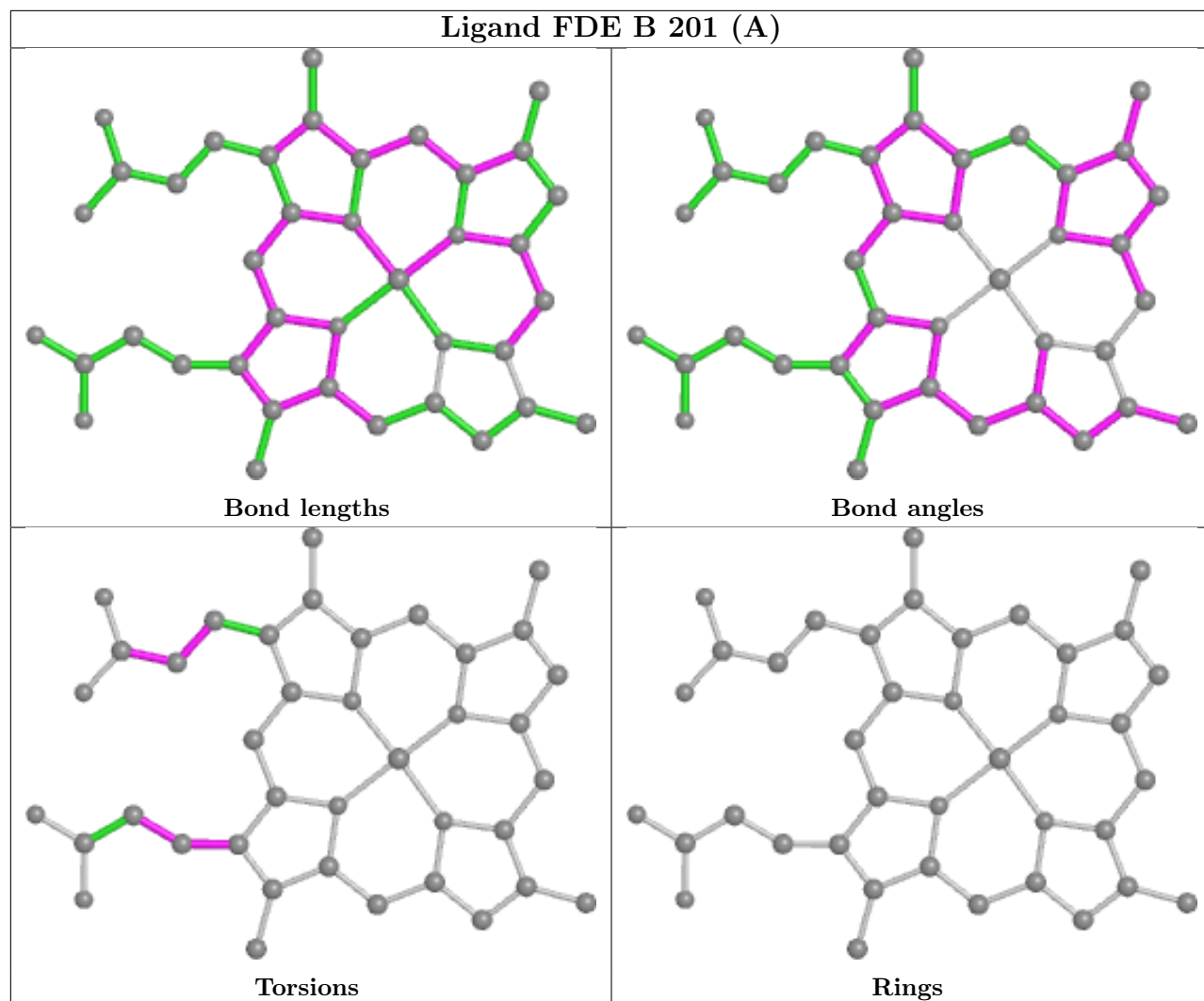
No monomer is involved in short contacts.

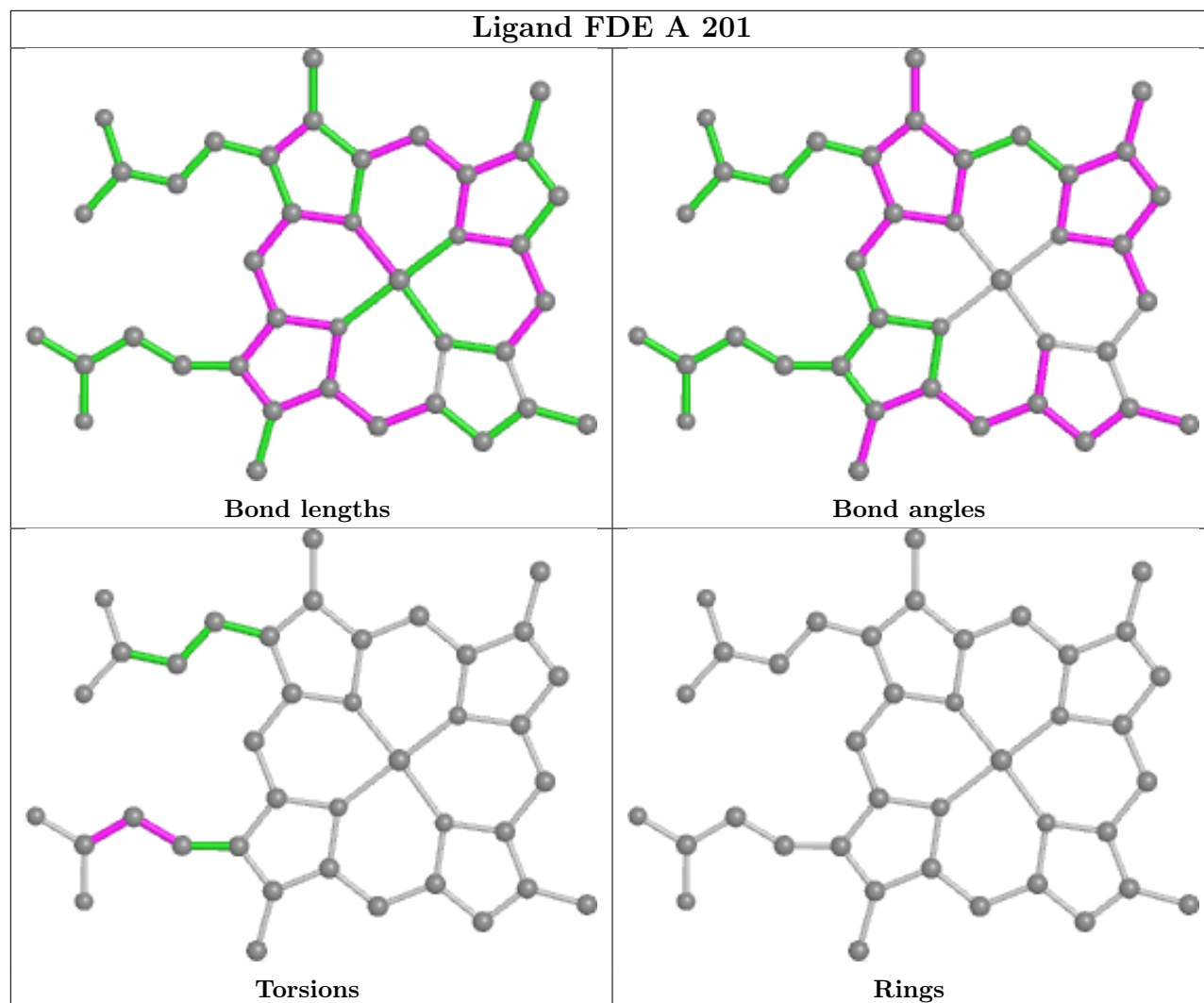
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.