



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 01:36 PM EDT

PDB ID : 6NSZ
Title : X-ray reduced Catalase 3 from N.Crassa (0.526 MGy)
Authors : Zarate-Romero, A.; Rudino-Pinera, E.; Stojanoff, V.
Deposited on : 2019-01-27
Resolution : 2.20 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)
Xtrriage (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 2.20 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.

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 23961 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 Catalase-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	682	Total	C	N	O	S	0	9	0
			5420	3426	960	1028	6			
1	B	677	Total	C	N	O	S	0	9	0
			5372	3400	953	1013	6			
1	C	679	Total	C	N	O	S	0	11	0
			5411	3420	962	1023	6			
1	D	678	Total	C	N	O	S	0	9	0
			5385	3408	956	1015	6			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



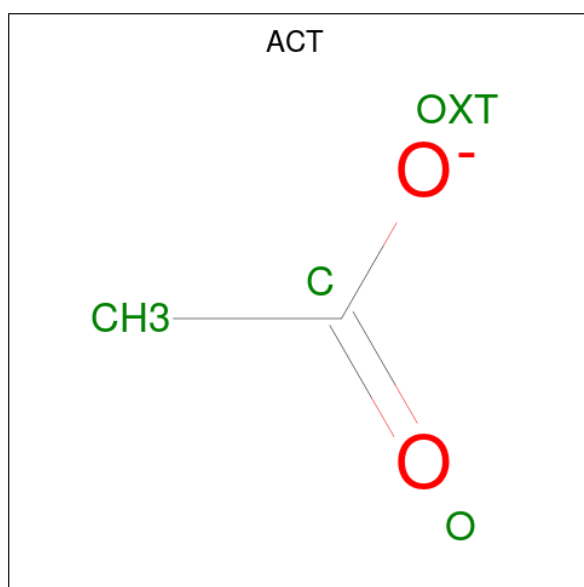
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



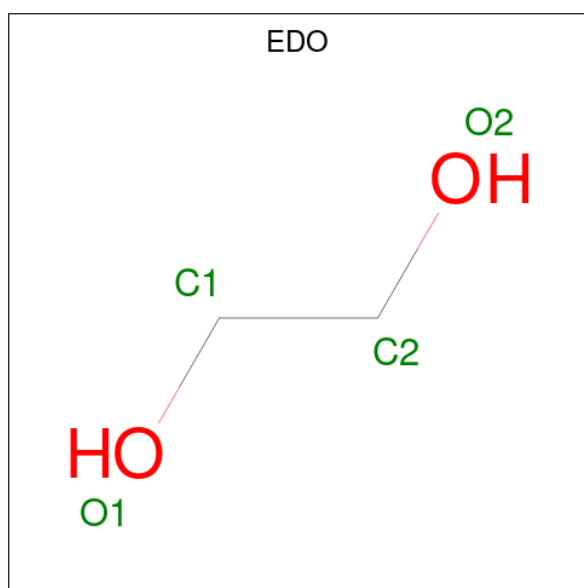
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



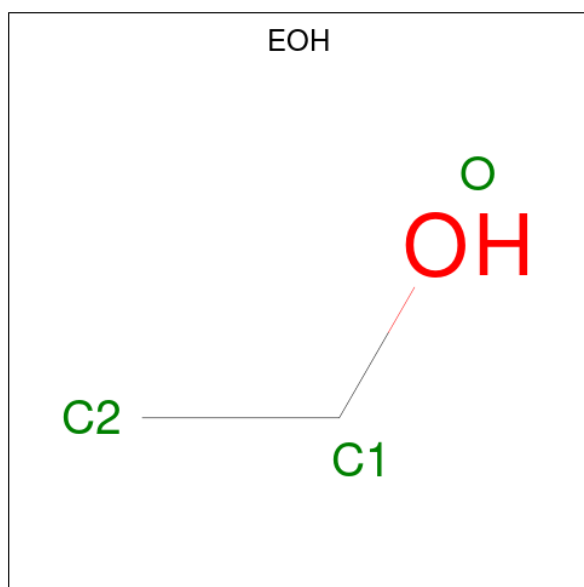
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0

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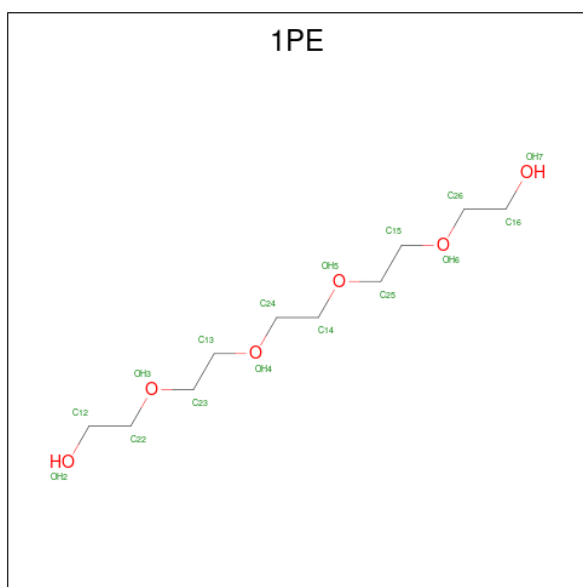
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is ETHANOL (three-letter code: EOH) (formula: C₂H₆O).



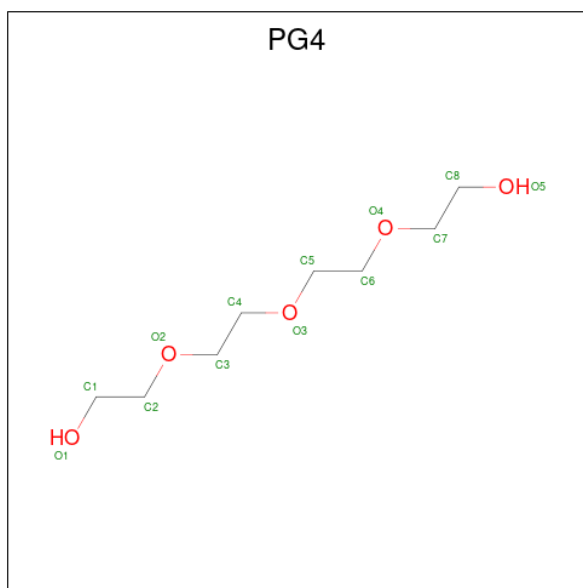
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			3	2	1		
7	B	1	Total	C	O	0	0
			3	2	1		
7	B	1	Total	C	O	0	0
			3	2	1		
7	D	1	Total	C	O	0	0
			3	2	1		
7	D	1	Total	C	O	0	0
			3	2	1		
7	D	1	Total	C	O	0	0
			3	2	1		

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	492	Total 492	O 492	0	0
10	B	494	Total 494	O 494	0	0
10	C	522	Total 522	O 522	0	0
10	D	506	Total 506	O 506	0	0

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

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	131.10Å 154.50Å 160.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 2.20	Depositor
% Data completeness (in resolution range)	96.9 (29.60-2.20)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.157 , 0.204	Depositor
Wilson B-factor (Å ²)	15.1	Xtrriage
Anisotropy	0.025	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.017 for -h,l,k	Xtrriage
Total number of atoms	23961	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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](#)

38 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
6	EDO	B	807	-	3,3,3	0.44	0	2,2,2	0.26	0
5	PEG	C	806	-	6,6,6	0.48	0	5,5,5	0.44	0
2	HEM	B	801	1	41,50,50	1.47	4 (9%)	45,82,82	1.37	5 (11%)
7	EOH	B	810	-	2,2,2	0.47	0	1,1,1	0.20	0
6	EDO	C	809	-	3,3,3	0.46	0	2,2,2	0.38	0
6	EDO	B	808	-	3,3,3	0.48	0	2,2,2	0.34	0
4	PGE	D	804	-	9,9,9	0.36	0	8,8,8	0.22	0
5	PEG	A	806	-	6,6,6	0.44	0	5,5,5	0.53	0
7	EOH	D	809	-	2,2,2	0.46	0	1,1,1	0.15	0
7	EOH	D	810	-	2,2,2	0.43	0	1,1,1	0.16	0
2	HEM	C	801	1,10	41,50,50	1.45	5 (12%)	45,82,82	1.41	6 (13%)
8	1PE	B	804	-	15,15,15	0.53	0	14,14,14	0.41	0
2	HEM	A	801	1,10	41,50,50	1.46	4 (9%)	45,82,82	1.38	5 (11%)
5	PEG	C	807	-	6,6,6	0.49	0	5,5,5	0.48	0
3	ACT	C	802	-	3,3,3	1.36	0	3,3,3	1.38	0
6	EDO	A	807	-	3,3,3	0.47	0	2,2,2	0.27	0
3	ACT	D	802	-	3,3,3	1.16	0	3,3,3	1.54	0
7	EOH	B	809	-	2,2,2	0.44	0	1,1,1	0.19	0
3	ACT	A	802	-	3,3,3	1.35	0	3,3,3	1.44	0
5	PEG	C	805	-	6,6,6	0.49	0	5,5,5	0.43	0
6	EDO	D	805	-	3,3,3	0.51	0	2,2,2	0.30	0
6	EDO	C	810	-	3,3,3	0.43	0	2,2,2	0.43	0
6	EDO	D	806	-	3,3,3	0.45	0	2,2,2	0.37	0
5	PEG	B	806	-	6,6,6	0.49	0	5,5,5	0.40	0
6	EDO	D	807	-	3,3,3	0.49	0	2,2,2	0.27	0
7	EOH	D	808	-	2,2,2	0.45	0	1,1,1	0.16	0
7	EOH	A	808	-	2,2,2	0.46	0	1,1,1	0.14	0
3	ACT	C	803	-	3,3,3	1.51	1 (33%)	3,3,3	1.57	1 (33%)
2	HEM	D	801	1,10	41,50,50	1.46	3 (7%)	45,82,82	1.41	6 (13%)
3	ACT	D	803	-	3,3,3	1.59	1 (33%)	3,3,3	1.29	0
3	ACT	A	803	-	3,3,3	1.62	1 (33%)	3,3,3	1.25	0
4	PGE	B	805	-	9,9,9	0.32	0	8,8,8	0.32	0
5	PEG	A	805	-	6,6,6	0.46	0	5,5,5	0.54	0
3	ACT	B	802	-	3,3,3	1.39	0	3,3,3	1.32	0
6	EDO	C	808	-	3,3,3	0.49	0	2,2,2	0.24	0
4	PGE	A	804	-	9,9,9	0.31	0	8,8,8	0.33	0
3	ACT	B	803	-	3,3,3	1.53	1 (33%)	3,3,3	1.16	0
9	PG4	C	804	-	12,12,12	0.51	0	11,11,11	0.44	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
6	EDO	B	807	-	-	0/1/1/1	-
5	PEG	C	806	-	-	0/4/4/4	-
2	HEM	B	801	1	-	4/12/54/54	-
6	EDO	C	809	-	-	1/1/1/1	-
6	EDO	B	808	-	-	0/1/1/1	-
4	PGE	D	804	-	-	4/7/7/7	-
5	PEG	A	806	-	-	1/4/4/4	-
2	HEM	C	801	1,10	-	2/12/54/54	-
8	1PE	B	804	-	-	8/13/13/13	-
2	HEM	A	801	1,10	-	2/12/54/54	-
5	PEG	C	807	-	-	1/4/4/4	-
6	EDO	A	807	-	-	0/1/1/1	-
5	PEG	C	805	-	-	2/4/4/4	-
6	EDO	D	805	-	-	1/1/1/1	-
6	EDO	C	810	-	-	1/1/1/1	-
6	EDO	D	806	-	-	0/1/1/1	-
5	PEG	B	806	-	-	2/4/4/4	-
6	EDO	D	807	-	-	0/1/1/1	-
2	HEM	D	801	1,10	-	2/12/54/54	-
5	PEG	A	805	-	-	2/4/4/4	-
4	PGE	B	805	-	-	5/7/7/7	-
6	EDO	C	808	-	-	0/1/1/1	-
4	PGE	A	804	-	-	3/7/7/7	-
9	PG4	C	804	-	-	7/10/10/10	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3C-C2C	-3.87	1.35	1.40
2	D	801	HEM	C3C-C2C	-3.79	1.35	1.40
2	A	801	HEM	C3C-C2C	-3.77	1.35	1.40
2	D	801	HEM	C3C-CAC	3.75	1.55	1.47
2	C	801	HEM	C3C-CAC	3.70	1.55	1.47
2	B	801	HEM	C3C-CAC	3.70	1.55	1.47
2	A	801	HEM	C3C-CAC	3.70	1.55	1.47
2	C	801	HEM	C3C-C2C	-3.68	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	HEM	CAB-C3B	3.01	1.55	1.47
2	B	801	HEM	CAB-C3B	3.00	1.55	1.47
2	C	801	HEM	CAB-C3B	2.98	1.55	1.47
2	A	801	HEM	CAB-C3B	2.95	1.55	1.47
3	A	803	ACT	CH3-C	2.40	1.59	1.49
3	D	803	ACT	CH3-C	2.36	1.59	1.49
3	B	803	ACT	CH3-C	2.33	1.58	1.49
3	C	803	ACT	CH3-C	2.29	1.58	1.49
2	A	801	HEM	CMB-C2B	2.12	1.55	1.50
2	C	801	HEM	FE-NB	2.09	2.07	1.96
2	C	801	HEM	CMB-C2B	2.07	1.55	1.50
2	B	801	HEM	CMB-C2B	2.07	1.55	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	HEM	C4D-ND-C1D	3.11	108.28	105.07
2	D	801	HEM	C4D-ND-C1D	3.08	108.25	105.07
2	B	801	HEM	C4D-ND-C1D	3.06	108.23	105.07
2	D	801	HEM	C1B-NB-C4B	3.03	108.20	105.07
2	A	801	HEM	C4D-ND-C1D	2.98	108.15	105.07
2	A	801	HEM	C4C-CHD-C1D	2.94	126.44	122.56
2	C	801	HEM	C1B-NB-C4B	2.92	108.09	105.07
2	B	801	HEM	C1B-NB-C4B	2.88	108.05	105.07
2	C	801	HEM	C4C-CHD-C1D	2.88	126.36	122.56
2	A	801	HEM	C1B-NB-C4B	2.85	108.02	105.07
2	D	801	HEM	C4C-CHD-C1D	2.61	126.00	122.56
2	B	801	HEM	CAA-CBA-CGA	-2.60	106.46	113.76
2	C	801	HEM	CAA-CBA-CGA	-2.56	106.58	113.76
2	A	801	HEM	CAA-CBA-CGA	-2.54	106.64	113.76
2	D	801	HEM	CAA-CBA-CGA	-2.53	106.65	113.76
2	B	801	HEM	C4C-CHD-C1D	2.45	125.80	122.56
2	C	801	HEM	C3D-C4D-ND	-2.25	107.66	110.17
2	D	801	HEM	C3D-C4D-ND	-2.19	107.73	110.17
2	B	801	HEM	C3D-C4D-ND	-2.18	107.74	110.17
2	A	801	HEM	C3D-C4D-ND	-2.18	107.74	110.17
2	D	801	HEM	C3B-C2B-C1B	2.14	108.07	106.49
2	C	801	HEM	C3B-C2B-C1B	2.09	108.03	106.49
3	C	803	ACT	O-C-CH3	-2.05	114.35	122.33

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	PGE	O2-C3-C4-O3
8	B	804	1PE	OH5-C14-C24-OH4
8	B	804	1PE	OH6-C15-C25-OH5
9	C	804	PG4	O2-C3-C4-O3
8	B	804	1PE	OH4-C13-C23-OH3
4	D	804	PGE	O3-C5-C6-O4
5	C	807	PEG	O1-C1-C2-O2
9	C	804	PG4	C5-C6-O4-C7
4	A	804	PGE	O1-C1-C2-O2
8	B	804	1PE	OH7-C16-C26-OH6
8	B	804	1PE	C23-C13-OH4-C24
4	B	805	PGE	O2-C3-C4-O3
4	D	804	PGE	O1-C1-C2-O2
5	A	806	PEG	O2-C3-C4-O4
8	B	804	1PE	OH2-C12-C22-OH3
9	C	804	PG4	O3-C5-C6-O4
5	C	805	PEG	C4-C3-O2-C2
4	B	805	PGE	C1-C2-O2-C3
5	A	805	PEG	C4-C3-O2-C2
4	B	805	PGE	C4-C3-O2-C2
9	C	804	PG4	C8-C7-O4-C6
6	C	810	EDO	O1-C1-C2-O2
6	D	805	EDO	O1-C1-C2-O2
5	B	806	PEG	C1-C2-O2-C3
5	C	805	PEG	C1-C2-O2-C3
4	B	805	PGE	O3-C5-C6-O4
9	C	804	PG4	C6-C5-O3-C4
5	A	805	PEG	C1-C2-O2-C3
4	B	805	PGE	C6-C5-O3-C4
9	C	804	PG4	C1-C2-O2-C3
9	C	804	PG4	C4-C3-O2-C2
2	B	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAA-CBA-CGA-O1A
4	D	804	PGE	O2-C3-C4-O3
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O2A
5	B	806	PEG	C4-C3-O2-C2
2	D	801	HEM	CAA-CBA-CGA-O1A
8	B	804	1PE	C25-C15-OH6-C26
2	C	801	HEM	CAA-CBA-CGA-O2A
2	C	801	HEM	CAA-CBA-CGA-O1A
2	D	801	HEM	CAA-CBA-CGA-O2A
4	A	804	PGE	O3-C5-C6-O4

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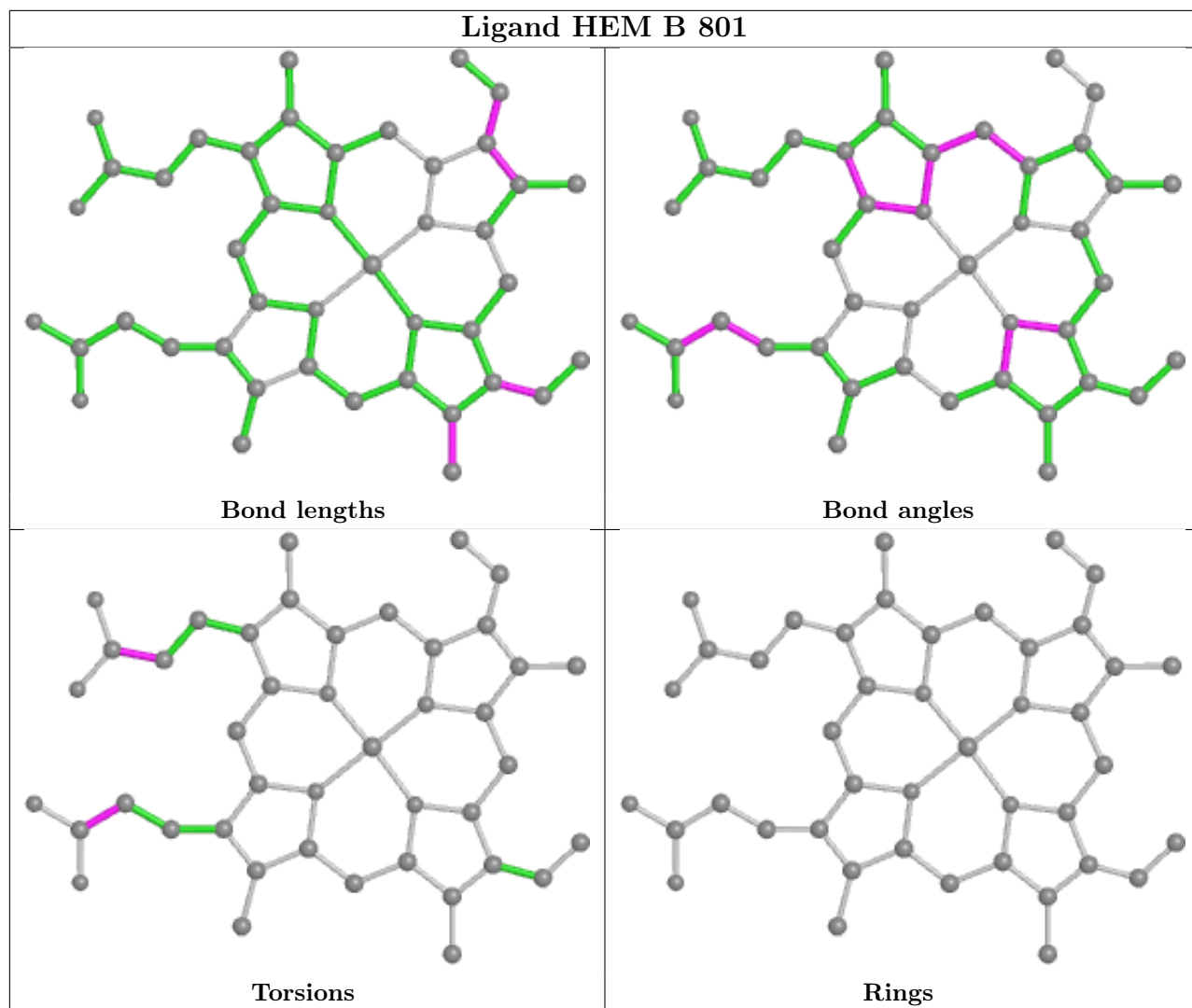
Continued from previous page...

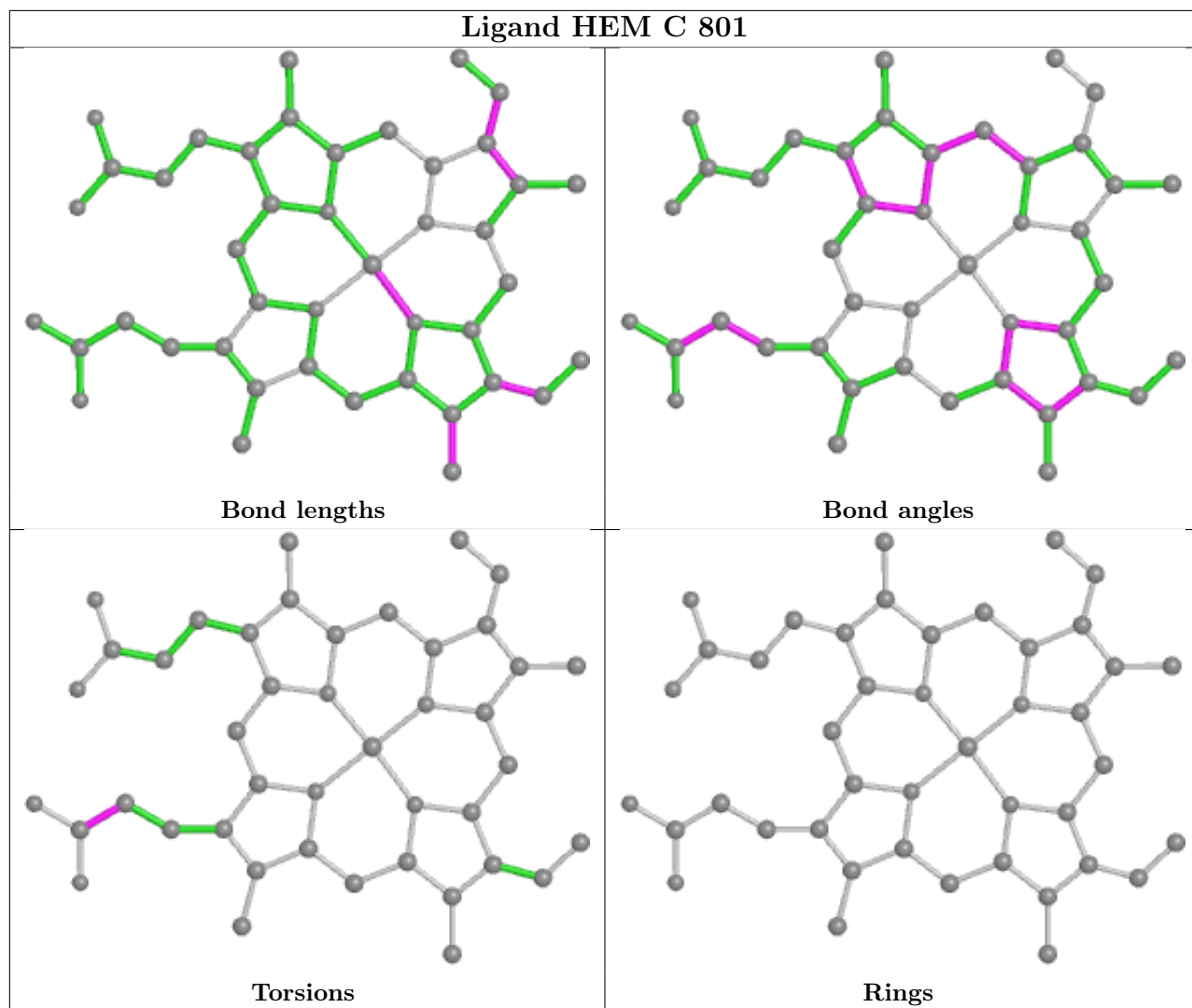
Mol	Chain	Res	Type	Atoms
2	B	801	HEM	CAD-CBD-CGD-O2D
4	D	804	PGE	C6-C5-O3-C4
6	C	809	EDO	O1-C1-C2-O2
2	B	801	HEM	CAD-CBD-CGD-O1D
8	B	804	1PE	C13-C23-OH3-C22

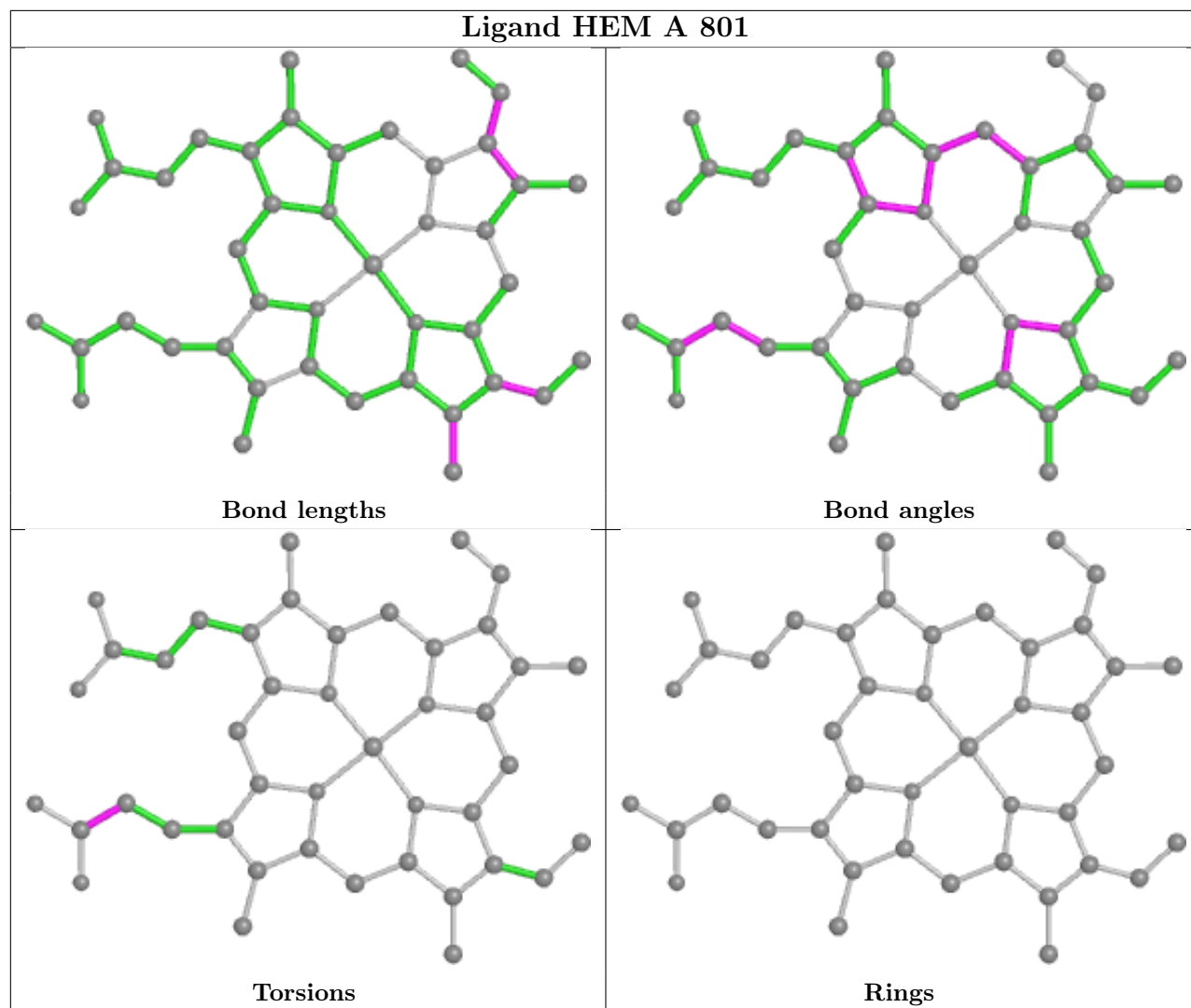
There are no ring outliers.

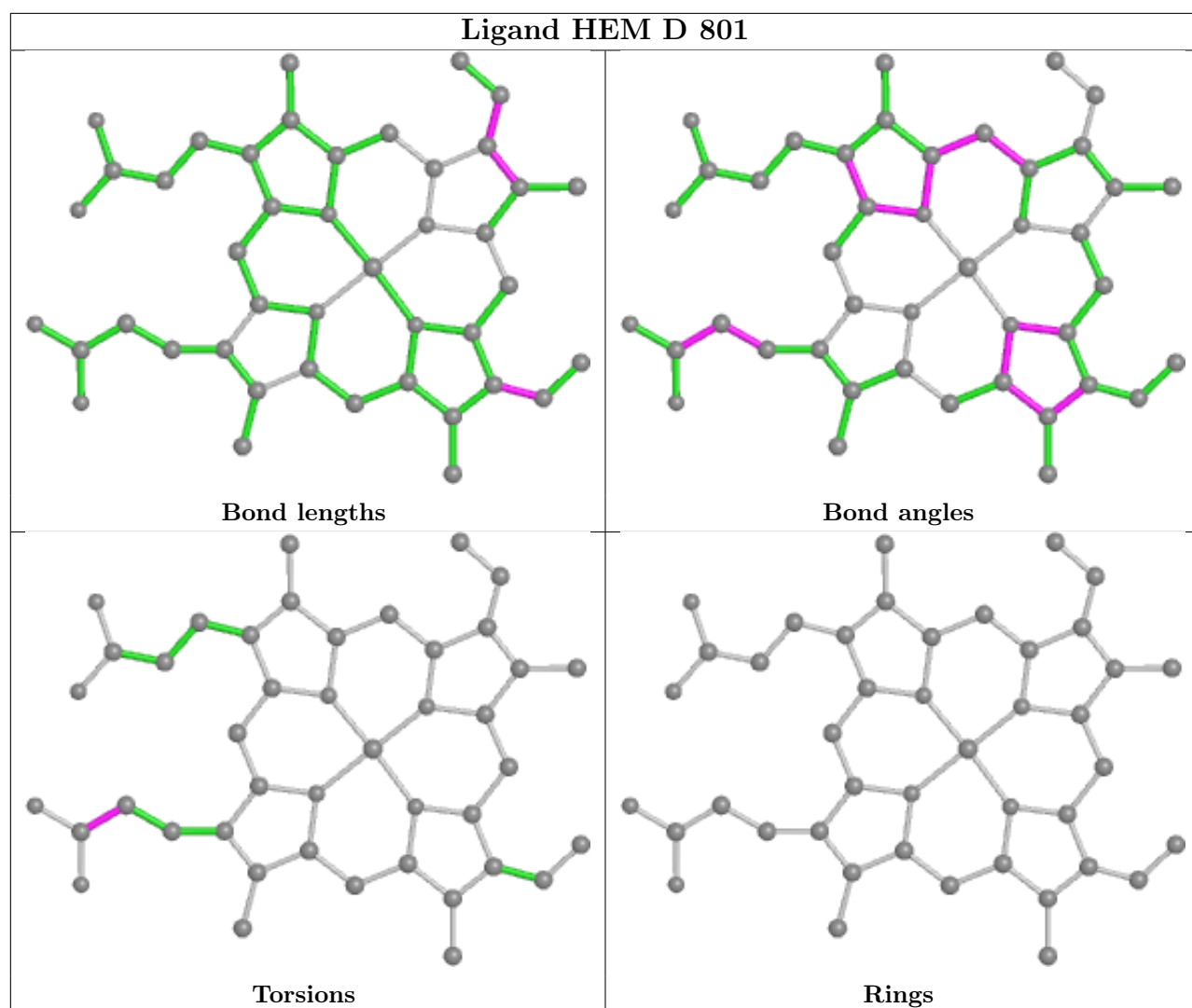
No monomer is involved in short contacts.

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.