



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 13, 2021 – 09:08 pm GMT

PDB ID : 7OUA  
Title : Crystal structure of dimeric chlorite dismutase variant R127K (CCld R127K) from *Cyanothece* sp. PCC7425  
Authors : Schmidt, D.; Mlynek, G.; Djinovic-Carugo, K.; Obinger, C.  
Deposited on : 2021-06-11  
Resolution : 2.09 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.24  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.24

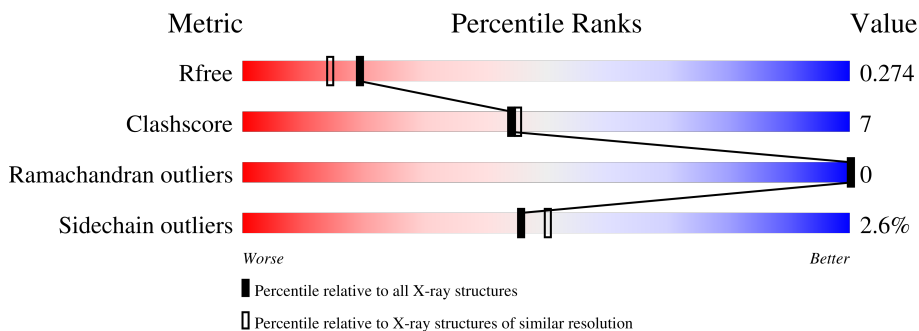
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	188	
1	B	188	

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6275 atoms, of which 3105 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 Chlorite dismutase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	181	2972	955	1482	267	264	4	0	0	0
1	B	181	2972	955	1482	267	264	4	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP B8HNS6
A	-4	PRO	-	expression tag	UNP B8HNS6
A	-3	GLY	-	expression tag	UNP B8HNS6
A	-2	TYR	-	expression tag	UNP B8HNS6
A	-1	GLN	-	expression tag	UNP B8HNS6
A	0	ASP	-	expression tag	UNP B8HNS6
A	1	PRO	-	expression tag	UNP B8HNS6
A	127	LYS	ARG	engineered mutation	UNP B8HNS6
B	-5	GLY	-	expression tag	UNP B8HNS6
B	-4	PRO	-	expression tag	UNP B8HNS6
B	-3	GLY	-	expression tag	UNP B8HNS6
B	-2	TYR	-	expression tag	UNP B8HNS6
B	-1	GLN	-	expression tag	UNP B8HNS6
B	0	ASP	-	expression tag	UNP B8HNS6
B	1	PRO	-	expression tag	UNP B8HNS6
B	127	LYS	ARG	engineered mutation	UNP B8HNS6

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Fe	H	N			O
2	A	1	73	34	1	30	4	4	0	0
2	B	1	73	34	1	30	4	4	0	0

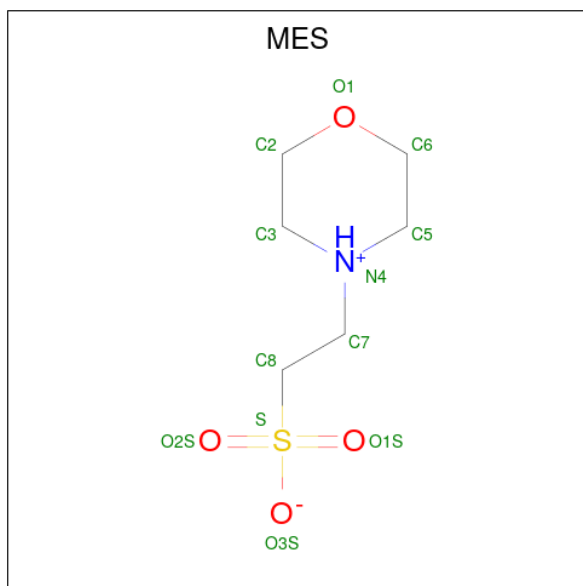
- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	H			O
3	A	1	9	3	3	3	0	0

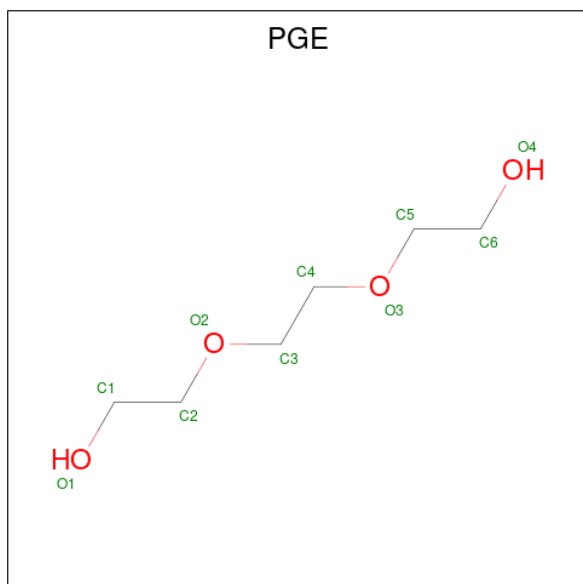
- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES)

(formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
			Total	C	H	N	O			S	
4	A	1	Total	25	6	13	1	4	1	0	0
4	B	1	Total	25	6	13	1	4	1	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



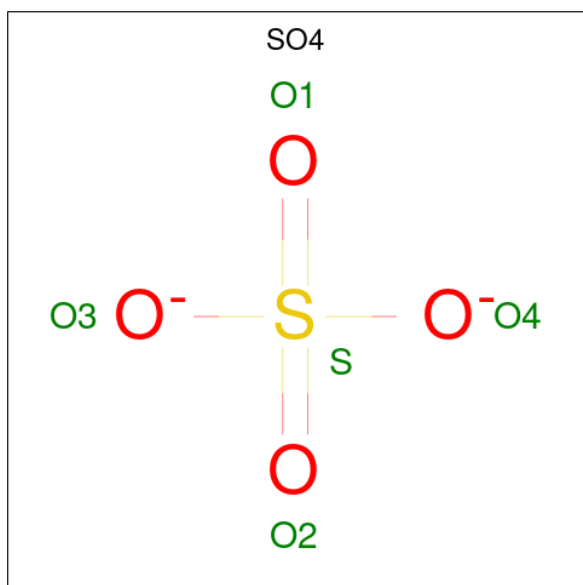
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	O			
5	A	1	Total	24	6	14	4	0	0

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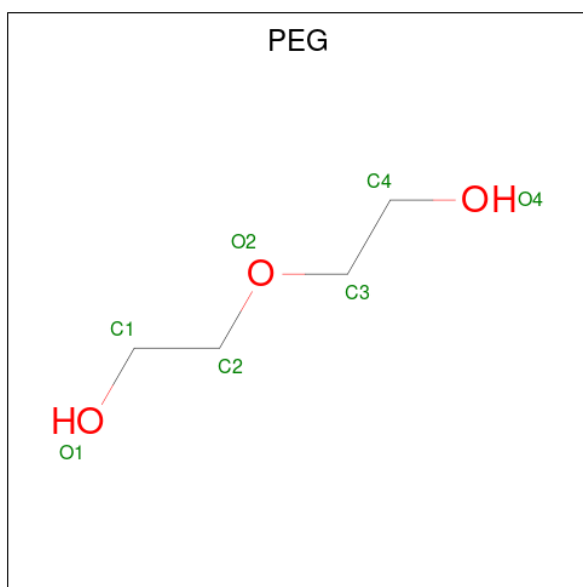
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			24	6	14	4		
5	B	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			17	4	10	3		


- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	13	Total	O	0	0
			13	13		
8	B	19	Total	O	0	0
			19	19		

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


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. 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. 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: Chlorite dismutase

Chain A:  81% 14% ..



- Molecule 1: Chlorite dismutase

Chain B:  79% 17% ..





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.71Å 49.61Å 54.58Å 102.48° 104.84° 105.00°	Depositor
Resolution (Å)	44.40 – 2.09 44.40 – 2.09	Depositor EDS
% Data completeness (in resolution range)	82.9 (44.40-2.09) 82.9 (44.40-2.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 2.08Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.222 , 0.270 0.228 , 0.274	Depositor DCC
$R_{free}$ test set	1679 reflections (7.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtrriage
Anisotropy	0.257	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.011 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6275	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, MES, HEM, GOL, PGE, SO4

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	0.26	0/1525	0.56	1/2063 (0.0%)
1	B	0.32	0/1525	0.61	3/2063 (0.1%)
All	All	0.29	0/3050	0.59	4/4126 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	46	LEU	CD1-CG-CD2	7.31	132.43	110.50
1	A	76	MET	CG-SD-CE	6.87	111.18	100.20
1	B	46	LEU	CB-CG-CD1	-6.53	99.91	111.00
1	B	46	LEU	CB-CG-CD2	-5.14	102.27	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	110	ARG	Sidechain
1	B	181	ARG	Sidechain

## 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	1490	1482	1482	16	0
1	B	1490	1482	1482	19	0
2	A	43	30	30	5	0
2	B	43	30	30	5	0
3	A	6	3	8	0	0
4	A	12	13	12	0	0
4	B	12	13	13	0	0
5	A	20	28	28	0	0
5	B	10	14	14	0	0
6	A	5	0	0	0	0
7	B	7	10	10	0	0
8	A	13	0	0	0	0
8	B	19	0	0	1	0
All	All	3170	3105	3109	41	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 7.

The worst 5 of 41 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:67:LEU:HA	1:A:70:LEU:HD12	1.80	0.63
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.83	0.60
2:B:701:HEM:HMB1	2:B:701:HEM:HBB2	1.85	0.57
1:A:73:VAL:HG13	1:A:123:PRO:HG3	1.86	0.57
1:A:21:ARG:NE	1:A:21:ARG:HA	2.20	0.57

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	179/188 (95%)	173 (97%)	6 (3%)	0	100	100
1	B	179/188 (95%)	172 (96%)	7 (4%)	0	100	100
All	All	358/376 (95%)	345 (96%)	13 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	154/159 (97%)	150 (97%)	4 (3%)	46	50
1	B	154/159 (97%)	150 (97%)	4 (3%)	46	50
All	All	308/318 (97%)	300 (97%)	8 (3%)	46	50

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	168	TRP
1	B	152	SER
1	B	6	SER
1	A	168	TRP
1	B	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	B	53	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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
2	HEM	B	701	1	27,50,50	1.85	4 (14%)	17,82,82	1.50	3 (17%)
7	PEG	B	702	-	6,6,6	0.09	0	5,5,5	0.14	0
4	MES	B	704	-	12,12,12	2.28	1 (8%)	14,16,16	1.78	4 (28%)
5	PGE	B	703	-	9,9,9	0.31	0	8,8,8	0.35	0
2	HEM	A	601	1	27,50,50	1.83	4 (14%)	17,82,82	1.49	2 (11%)
5	PGE	A	604	-	9,9,9	0.30	0	8,8,8	0.30	0
5	PGE	A	605	-	9,9,9	0.30	0	8,8,8	0.32	0
4	MES	A	603	-	12,12,12	2.30	1 (8%)	14,16,16	1.85	5 (35%)
3	GOL	A	602	-	5,5,5	0.82	0	5,5,5	1.12	1 (20%)
6	SO4	A	606	-	4,4,4	0.14	0	6,6,6	0.05	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
2	HEM	B	701	1	-	0/6/54/54	-
7	PEG	B	702	-	-	1/4/4/4	-
4	MES	B	704	-	-	1/6/14/14	0/1/1/1
5	PGE	B	703	-	-	2/7/7/7	-
2	HEM	A	601	1	-	0/6/54/54	-
5	PGE	A	604	-	-	3/7/7/7	-
5	PGE	A	605	-	-	5/7/7/7	-
4	MES	A	603	-	-	3/6/14/14	0/1/1/1
3	GOL	A	602	-	-	0/4/4/4	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	MES	C8-S	-7.70	1.66	1.77
4	B	704	MES	C8-S	-7.63	1.66	1.77
2	B	701	HEM	C3C-C2C	-4.09	1.34	1.40
2	B	701	HEM	C3B-C2B	-4.01	1.34	1.40
2	A	601	HEM	C3C-C2C	-3.94	1.34	1.40

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	704	MES	C5-N4-C3	3.67	117.09	108.83
4	A	603	MES	C5-N4-C3	3.47	116.64	108.83
4	B	704	MES	O3S-S-C8	3.04	110.68	105.77
4	A	603	MES	C2-C3-N4	-2.87	105.75	110.10
2	B	701	HEM	CAA-CBA-CGA	-2.71	108.12	112.67

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

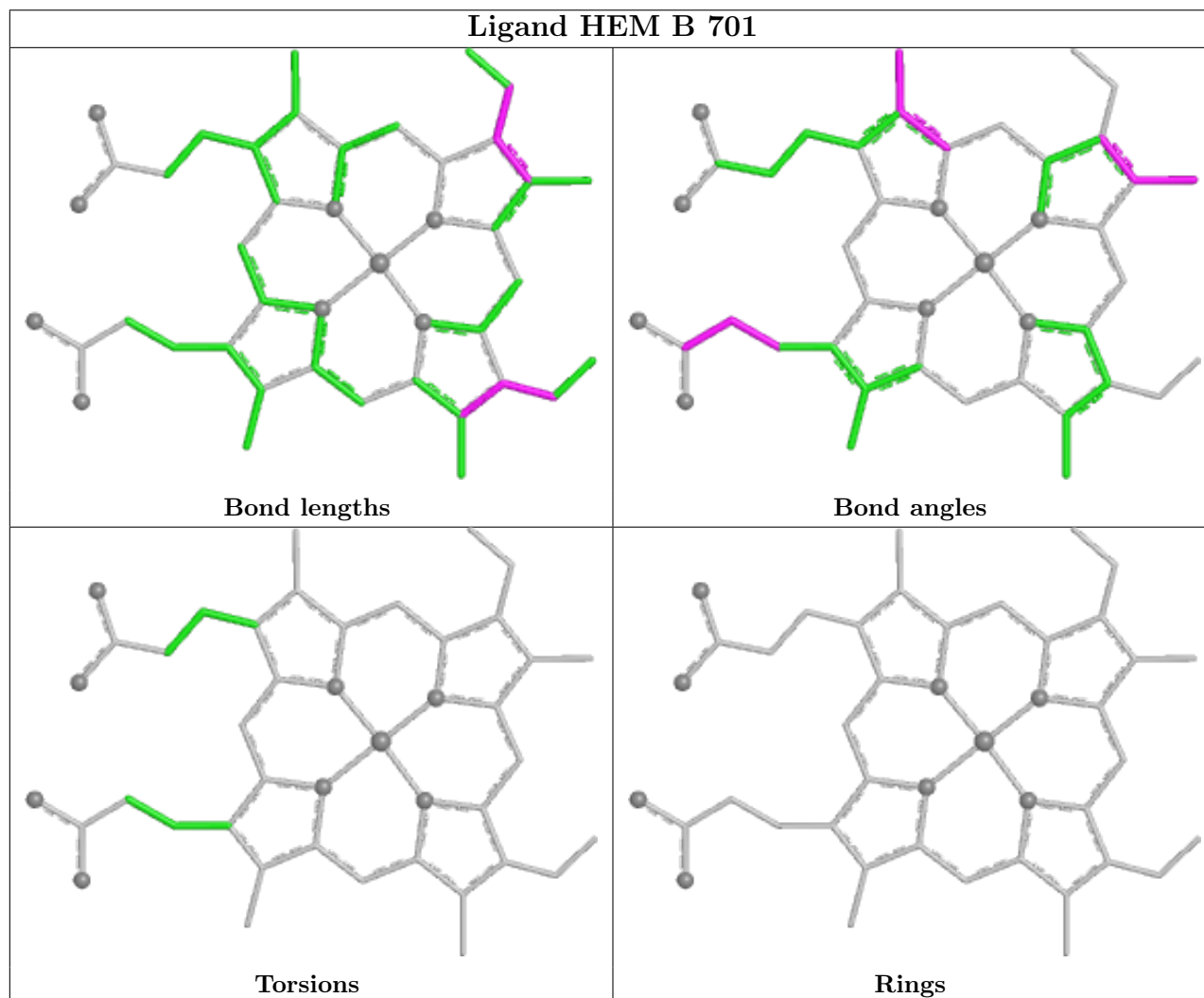
Mol	Chain	Res	Type	Atoms
4	A	603	MES	C7-C8-S-O1S
4	A	603	MES	C7-C8-S-O2S
5	A	604	PGE	O1-C1-C2-O2
5	B	703	PGE	O1-C1-C2-O2
4	A	603	MES	C7-C8-S-O3S

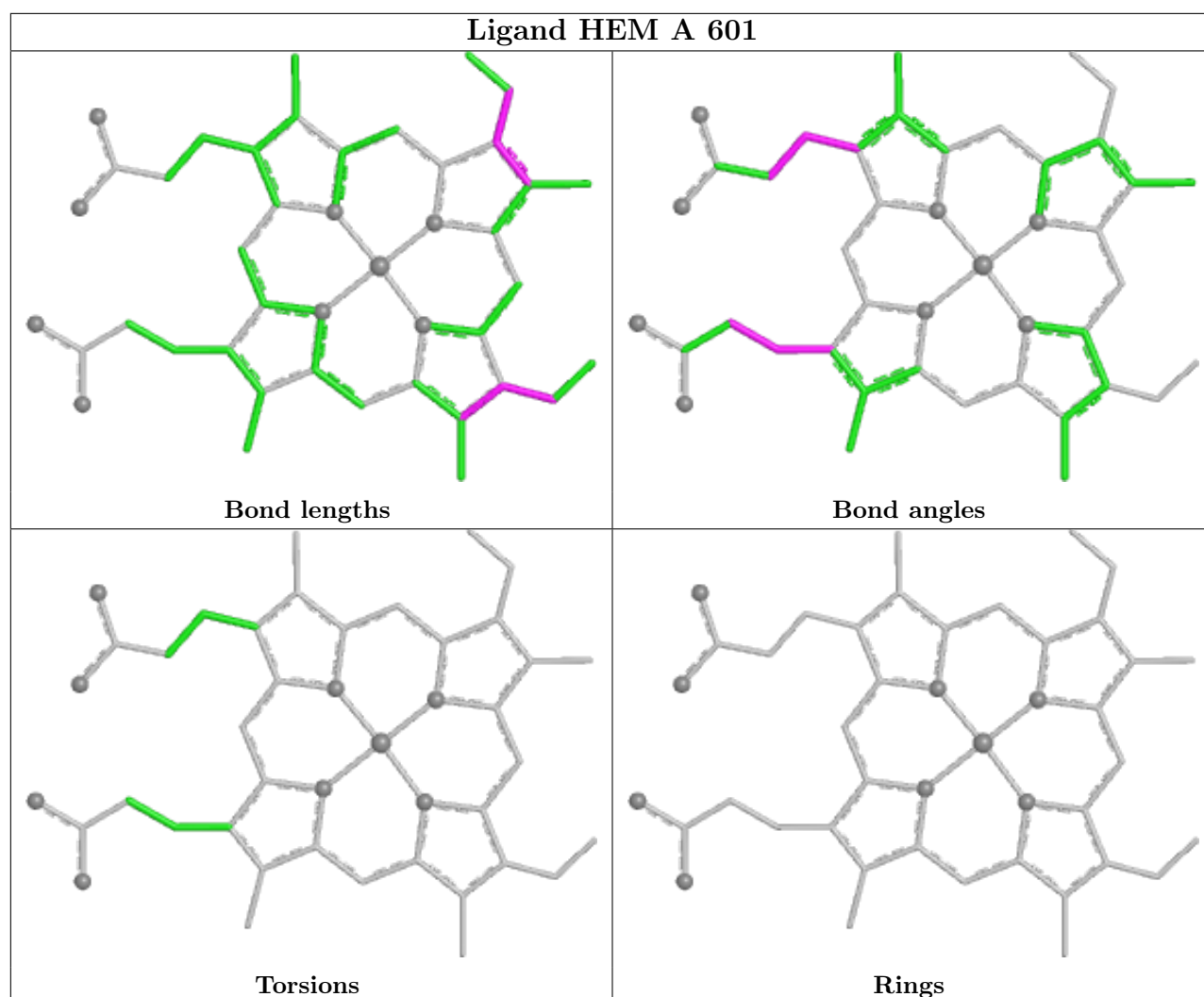
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	HEM	5	0
2	A	601	HEM	5	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

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

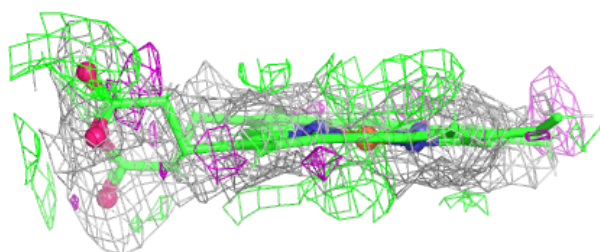
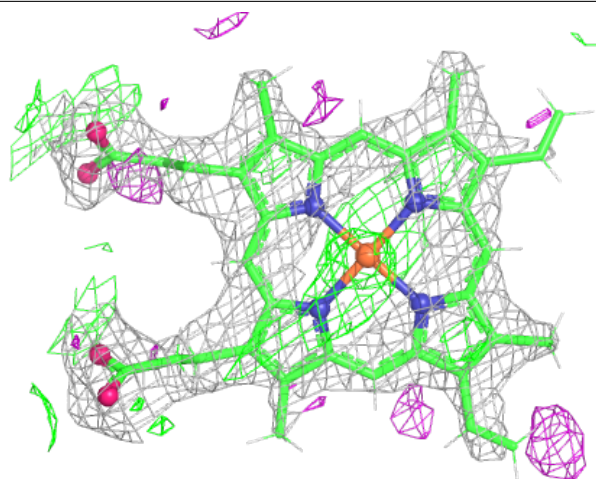
### 6.4 Ligands

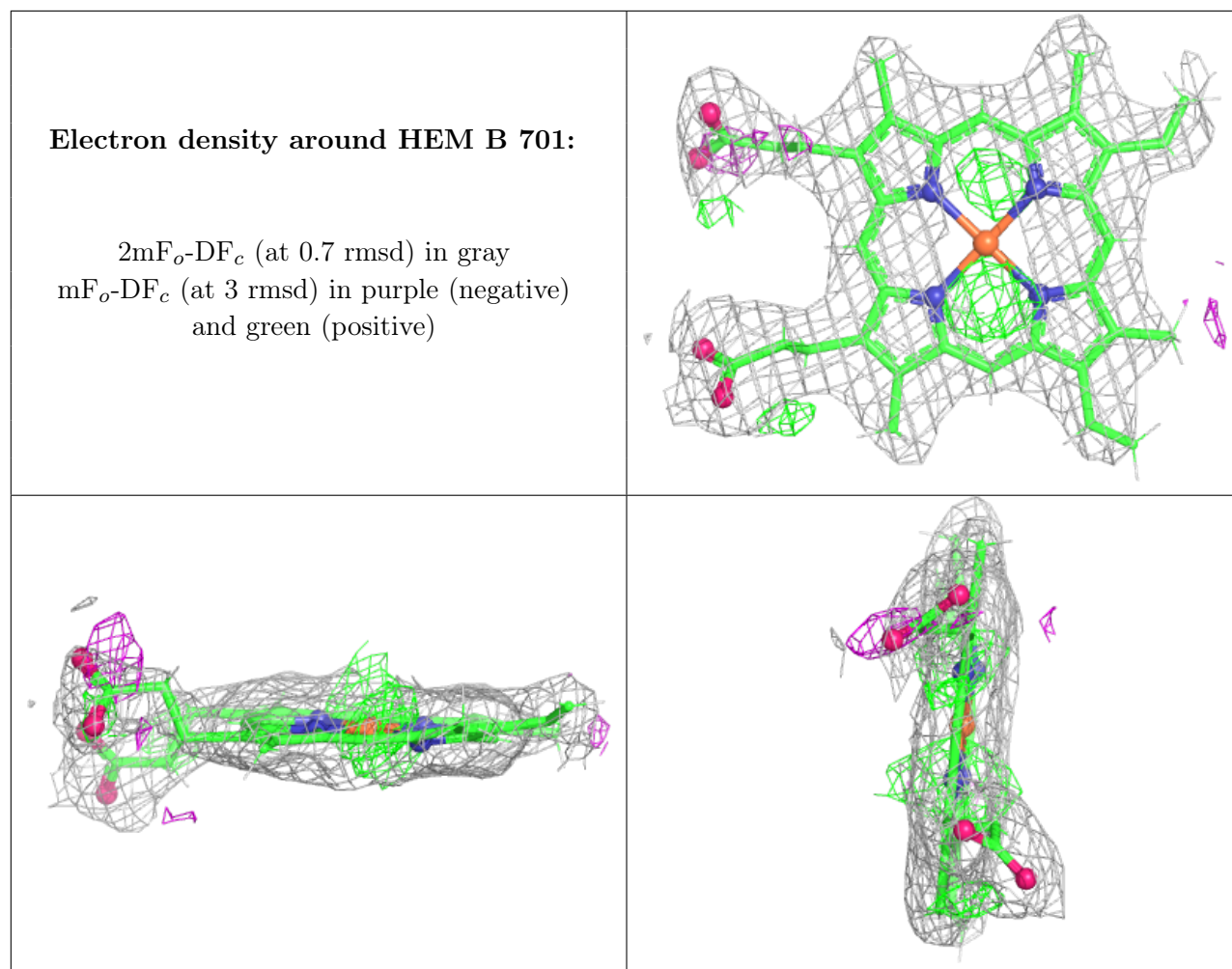
Unable to reproduce the depositors R factor - this section is therefore empty.

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 HEM A 601:**

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





## 6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.