



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2021 – 09:09 pm GMT

PDB ID : 7OUY  
Title : Crystal structure of dimeric chlorite dismutase variant R127A (CCld R127A) from *Cyanothece* sp. PCC7425 in complex with nitrite  
Authors : Schmidt, D.; Mlynek, G.; Djinovic-Carugo, K.; Obinger, C.  
Deposited on : 2021-06-14  
Resolution : 1.50 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](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

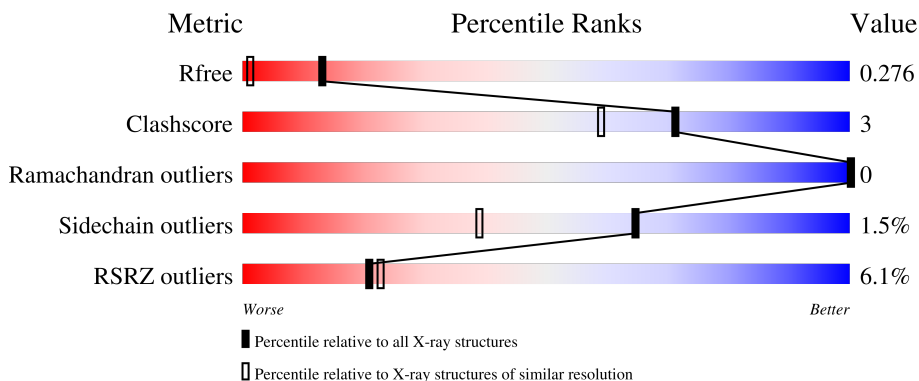
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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  $\leq 5\%$ . 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	188	 6% 89% 5% 6%
1	B	188	 4% 88% 5% 6%
1	C	188	 5% 87% 7% 6%
1	D	188	 8% 85% 8% 6%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12987 atoms, of which 5996 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	176	2882	927	1433	261	257	4	0	0	0
1	B	176	2905	933	1445	265	258	4	0	1	0
1	C	176	2882	927	1433	261	257	4	0	0	0
1	D	176	2906	933	1446	265	258	4	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

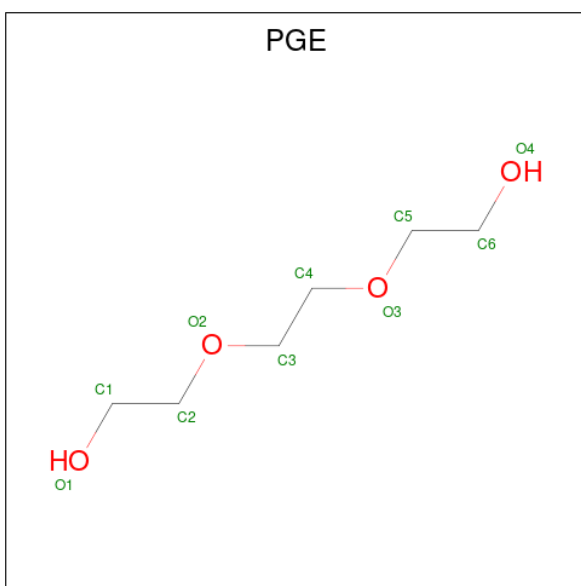
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP B8HNS6
A	-4	PRO	-	expression tag	UNP B8HNS6
A	-3	GLY	-	expression tag	UNP B8HNS6
A	-2	TYR	-	expression tag	UNP B8HNS6
A	-1	GLN	-	expression tag	UNP B8HNS6
A	0	ASP	-	expression tag	UNP B8HNS6
A	1	PRO	-	expression tag	UNP B8HNS6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

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

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



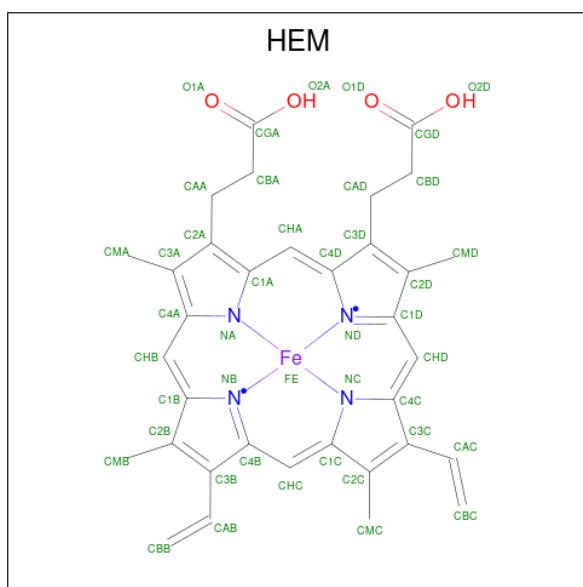
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	Total	C	H	O	0	0
			24	6	14	4		
2	B	1	Total	C	H	O	0	0
			24	6	14	4		
2	B	1	Total	C	H	O	0	0
			24	6	14	4		
2	C	1	Total	C	H	O	0	0
			24	6	14	4		
2	D	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



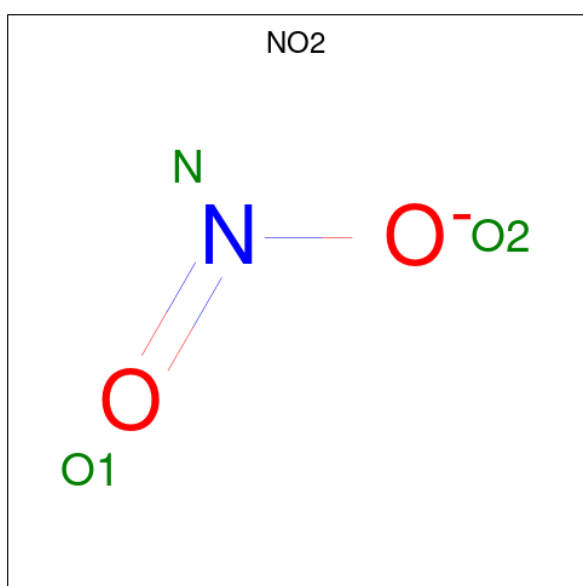
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	9	3	3	3	0	0
3	A	1	9	3	3	3	0	0
3	C	1	9	3	3	3	0	0
3	C	1	9	3	3	3	0	0
3	C	1	13	3	7	3	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



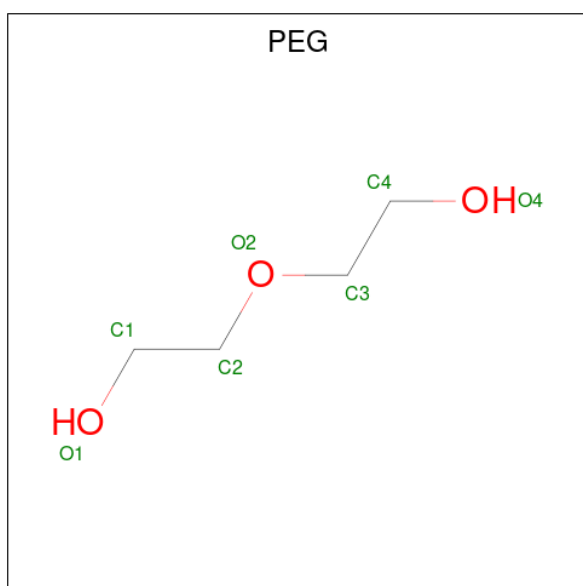
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Fe	H	N			O
4	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
4	B	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
4	C	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
4	D	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- Molecule 5 is NITRITE ION (three-letter code: NO2) (formula: NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 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
6	A	1	Total	C	H	O	0	0
			17	4	10	3		
6	C	1	Total	C	H	O	0	0
			17	4	10	3		
6	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

- Molecule 8 is water.

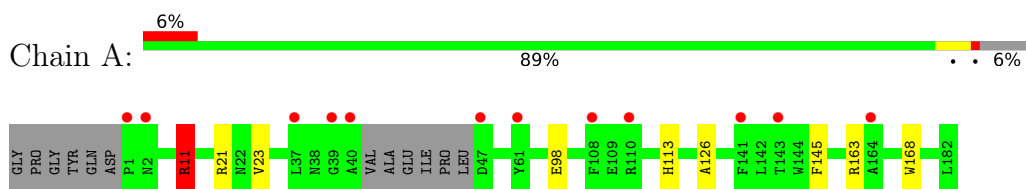
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	194	Total	O	0	0
			194	194		
8	B	245	Total	O	0	0
			245	245		
8	C	256	Total	O	0	0
			256	256		
8	D	183	Total	O	0	0
			183	183		



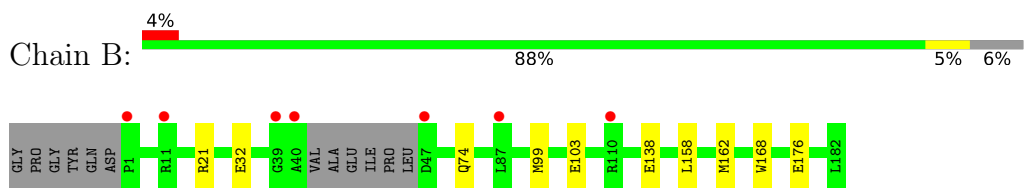
### 3 Residue-property plots [i](#)

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 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.

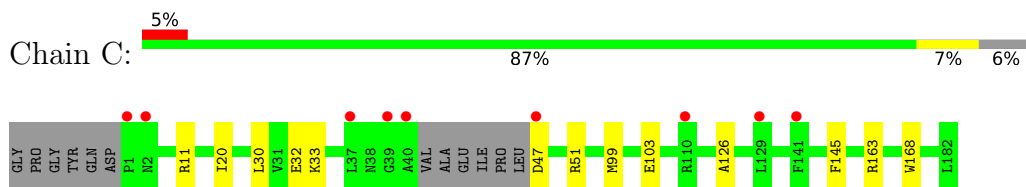
- Molecule 1: Chlorite dismutase



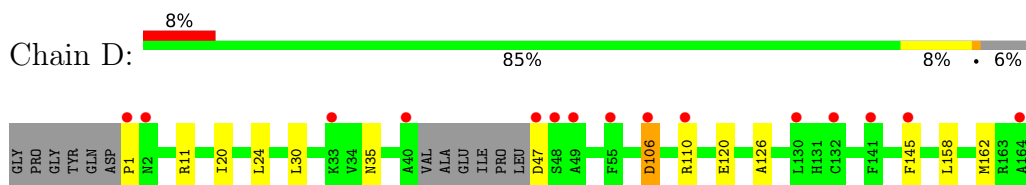
- Molecule 1: Chlorite dismutase



- Molecule 1: Chlorite dismutase



- Molecule 1: Chlorite dismutase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.25Å 54.96Å 93.89Å 99.51° 94.81° 98.38°	Depositor
Resolution (Å)	30.44 – 1.50 30.44 – 1.50	Depositor EDS
% Data completeness (in resolution range)	90.8 (30.44-1.50) 90.8 (30.44-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 1.50Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.249 , 0.275 0.251 , 0.276	Depositor DCC
$R_{free}$ test set	1515 reflections (1.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtrriage
Anisotropy	0.316	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>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12987	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 87.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5850e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NO2, PEG, PGE, GOL, HEM

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	0.37	0/1483	0.56	0/2004
1	B	0.41	0/1494	0.59	0/2018
1	C	0.40	0/1483	0.58	0/2004
1	D	0.39	0/1494	0.58	0/2018
All	All	0.39	0/5954	0.57	0/8044

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ARG	Sidechain

### 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	1449	1433	1434	5	0
1	B	1460	1445	1446	6	0
1	C	1449	1433	1434	9	0
1	D	1460	1446	1446	13	0
2	A	10	14	14	0	0
2	B	20	28	28	0	0
2	C	10	14	14	0	0
2	D	10	14	14	0	0
3	A	12	6	16	0	0
3	C	18	13	24	0	0
4	A	43	30	30	3	0
4	B	43	30	30	1	0
4	C	43	30	30	3	0
4	D	43	30	30	2	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
5	C	3	0	0	0	0
5	D	3	0	0	0	0
6	A	7	10	10	0	0
6	C	7	10	10	0	0
6	D	7	10	10	0	0
7	A	5	0	0	0	0
7	D	5	0	0	0	0
8	A	194	0	0	3	4
8	B	245	0	0	2	3
8	C	256	0	0	5	3
8	D	183	0	0	7	4
All	All	6991	5996	6020	42	7

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.

All (42) 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:11:ARG:NH2	8:A:301:HOH:O	2.06	0.89
1:B:138:GLU:OE1	8:B:301:HOH:O	2.10	0.69
4:C:203:HEM:HHC	4:C:203:HEM:HBB2	1.76	0.67
1:D:20:ILE:HD12	1:D:30:LEU:HA	1.83	0.61
1:D:47:ASP:N	8:D:310:HOH:O	2.34	0.61
1:D:1:PRO:N	8:D:311:HOH:O	2.34	0.59
4:A:203:HEM:HBB2	4:A:203:HEM:HHC	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:202:HEM:HBB2	4:B:202:HEM:HHC	1.87	0.56
1:B:99:MET:HE3	1:B:103:GLU:HB3	1.87	0.56
4:D:202:HEM:HHC	4:D:202:HEM:HBB2	1.89	0.55
1:C:32:GLU:OE1	8:C:302:HOH:O	2.18	0.55
1:B:99:MET:HE3	1:B:103:GLU:CB	2.37	0.54
1:D:35:ASN:ND2	8:D:313:HOH:O	2.40	0.54
1:C:47:ASP:N	8:C:310:HOH:O	2.43	0.52
1:B:32:GLU:OE1	8:B:302:HOH:O	2.19	0.51
1:D:120:GLU:OE2	8:D:302:HOH:O	2.20	0.50
1:D:24:LEU:N	8:D:314:HOH:O	2.45	0.49
1:D:165:SER:O	8:D:301:HOH:O	2.19	0.48
1:A:98:GLU:OE2	8:A:302:HOH:O	2.20	0.48
1:A:113:HIS:ND1	8:A:311:HOH:O	2.35	0.47
1:C:99:MET:HE3	1:C:103:GLU:HB3	1.97	0.45
1:A:21:ARG:HD3	1:A:23:VAL:HG22	1.98	0.45
1:A:126:ALA:O	1:A:145:PHE:HA	2.16	0.45
1:D:11:ARG:HH11	1:D:11:ARG:HG2	1.81	0.45
4:C:203:HEM:HBB2	4:C:203:HEM:CHC	2.45	0.45
1:C:33:LYS:NZ	8:C:319:HOH:O	2.49	0.43
1:C:126:ALA:O	1:C:145:PHE:HA	2.19	0.43
1:D:11:ARG:HH11	1:D:11:ARG:CG	2.32	0.43
1:C:99:MET:CE	1:C:103:GLU:HB3	2.48	0.43
1:D:47:ASP:N	8:D:317:HOH:O	2.51	0.43
1:C:20:ILE:HD12	1:C:30:LEU:HA	2.02	0.42
1:B:21:ARG:HD3	1:B:176:GLU:OE1	2.20	0.41
4:D:202:HEM:HBC2	4:D:202:HEM:CMC	2.50	0.41
1:B:158:LEU:O	1:B:162:MET:HG3	2.20	0.41
1:C:163:ARG:NH1	8:C:321:HOH:O	2.50	0.41
1:D:106:ASP:OD1	1:D:110:ARG:NE	2.53	0.41
4:A:203:HEM:HBC2	4:A:203:HEM:CMC	2.51	0.41
1:D:158:LEU:O	1:D:162:MET:HG3	2.21	0.41
1:C:51:ARG:NH2	8:C:307:HOH:O	2.38	0.41
4:C:203:HEM:HHC	4:C:203:HEM:CBB	2.48	0.40
1:D:126:ALA:O	1:D:145:PHE:HA	2.21	0.40
4:A:203:HEM:HHC	4:A:203:HEM:CBB	2.50	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:431:HOH:O	8:B:448:HOH:O[1_545]	1.96	0.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:484:HOH:O	8:C:335:HOH:O[1_565]	1.99	0.21
8:A:462:HOH:O	8:D:469:HOH:O[1_656]	2.07	0.13
8:C:443:HOH:O	8:D:394:HOH:O[1_545]	2.10	0.10
8:A:433:HOH:O	8:D:452:HOH:O[1_556]	2.11	0.09
8:A:439:HOH:O	8:D:335:HOH:O[1_556]	2.15	0.05
8:B:465:HOH:O	8:C:440:HOH:O[1_565]	2.15	0.05

## 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	172/188 (92%)	168 (98%)	4 (2%)	0	100	100
1	B	173/188 (92%)	168 (97%)	5 (3%)	0	100	100
1	C	172/188 (92%)	167 (97%)	5 (3%)	0	100	100
1	D	173/188 (92%)	168 (97%)	5 (3%)	0	100	100
All	All	690/752 (92%)	671 (97%)	19 (3%)	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	149/158 (94%)	146 (98%)	3 (2%)	55	25
1	B	150/158 (95%)	148 (99%)	2 (1%)	69	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	149/158 (94%)	147 (99%)	2 (1%)	69	44
1	D	150/158 (95%)	148 (99%)	2 (1%)	69	44
All	All	598/632 (95%)	589 (98%)	9 (2%)	65	39

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	163	ARG
1	A	168	TRP
1	B	74	GLN
1	B	168	TRP
1	C	11	ARG
1	C	168	TRP
1	D	106	ASP
1	D	168	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	71	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](#)

23 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	HEM	B	202	1,5	27,50,50	2.02	9 (33%)	17,82,82	1.67	5 (29%)
4	HEM	C	203	1,5	27,50,50	2.02	7 (25%)	17,82,82	1.56	2 (11%)
6	PEG	C	206	-	6,6,6	0.11	0	5,5,5	0.14	0
6	PEG	A	206	-	6,6,6	0.10	0	5,5,5	0.07	0
7	SO4	A	207	-	4,4,4	0.14	0	6,6,6	0.05	0
4	HEM	A	203	1,5	27,50,50	1.96	6 (22%)	17,82,82	1.55	4 (23%)
3	GOL	A	202	-	5,5,5	0.75	0	5,5,5	1.03	0
5	NO2	C	204	4	1,2,2	4.66	1 (100%)	0,1,1	-	-
3	GOL	C	205	-	5,5,5	0.88	0	5,5,5	0.93	0
2	PGE	D	201	-	9,9,9	0.31	0	8,8,8	0.25	0
5	NO2	D	203	4	1,2,2	4.80	1 (100%)	0,1,1	-	-
2	PGE	C	201	-	9,9,9	0.37	0	8,8,8	0.44	0
3	GOL	C	202	-	5,5,5	0.89	0	5,5,5	0.98	0
5	NO2	B	203	4	1,2,2	5.03	1 (100%)	0,1,1	-	-
3	GOL	A	205	-	5,5,5	0.97	0	5,5,5	0.91	0
2	PGE	B	201	-	9,9,9	0.39	0	8,8,8	0.29	0
2	PGE	B	204	-	9,9,9	0.32	0	8,8,8	0.31	0
7	SO4	D	205	-	4,4,4	0.12	0	6,6,6	0.04	0
2	PGE	A	201	-	9,9,9	0.34	0	8,8,8	0.42	0
6	PEG	D	204	-	6,6,6	0.12	0	5,5,5	0.11	0
4	HEM	D	202	1,5	27,50,50	2.03	6 (22%)	17,82,82	1.48	3 (17%)
5	NO2	A	204	4	1,2,2	4.98	1 (100%)	0,1,1	-	-
3	GOL	C	207	-	5,5,5	0.78	0	5,5,5	1.00	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
4	HEM	A	203	1,5	-	0/6/54/54	-
3	GOL	A	205	-	-	3/4/4/4	-
3	GOL	C	202	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGE	B	204	-	-	4/7/7/7	-
3	GOL	C	205	-	-	4/4/4/4	-
2	PGE	D	201	-	-	2/7/7/7	-
4	HEM	B	202	1,5	-	0/6/54/54	-
2	PGE	C	201	-	-	3/7/7/7	-
4	HEM	C	203	1,5	-	0/6/54/54	-
2	PGE	A	201	-	-	4/7/7/7	-
6	PEG	A	206	-	-	1/4/4/4	-
6	PEG	C	206	-	-	1/4/4/4	-
6	PEG	D	204	-	-	2/4/4/4	-
4	HEM	D	202	1,5	-	0/6/54/54	-
2	PGE	B	201	-	-	2/7/7/7	-
3	GOL	A	202	-	-	2/4/4/4	-
3	GOL	C	207	-	-	2/4/4/4	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203	HEM	C3B-C2B	-5.42	1.32	1.40
4	D	202	HEM	C3B-C2B	-5.10	1.33	1.40
5	B	203	NO2	O1-N	5.03	1.47	1.22
5	A	204	NO2	O1-N	4.98	1.47	1.22
4	D	202	HEM	C3C-C2C	-4.91	1.33	1.40
4	C	203	HEM	C3B-C2B	-4.88	1.33	1.40
5	D	203	NO2	O1-N	4.80	1.46	1.22
5	C	204	NO2	O1-N	4.66	1.45	1.22
4	C	203	HEM	C3C-C2C	-4.52	1.34	1.40
4	A	203	HEM	C3C-C2C	-4.37	1.34	1.40
4	B	202	HEM	C3B-C2B	-4.23	1.34	1.40
4	B	202	HEM	C3C-C2C	-4.02	1.34	1.40
4	D	202	HEM	C3B-CAB	4.00	1.56	1.47
4	C	203	HEM	C3B-CAB	3.78	1.55	1.47
4	D	202	HEM	C3C-CAC	3.46	1.54	1.47
4	B	202	HEM	C3B-CAB	3.46	1.55	1.47
4	B	202	HEM	C4B-NB	3.42	1.43	1.36
4	B	202	HEM	C3C-CAC	3.34	1.54	1.47
4	A	203	HEM	C3B-CAB	3.27	1.54	1.47
4	C	203	HEM	C3C-CAC	3.26	1.54	1.47
4	A	203	HEM	C3C-CAC	2.79	1.53	1.47
4	B	202	HEM	CAD-C3D	2.76	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203	HEM	CAA-C2A	2.69	1.56	1.52
4	A	203	HEM	CAD-C3D	2.37	1.56	1.52
4	C	203	HEM	C1A-NA	2.30	1.40	1.36
4	D	202	HEM	CAA-C2A	2.25	1.55	1.52
4	C	203	HEM	CAA-C2A	2.19	1.55	1.52
4	B	202	HEM	C1A-NA	2.13	1.40	1.36
4	B	202	HEM	CAA-C2A	2.12	1.55	1.52
4	C	203	HEM	CMC-C2C	2.05	1.56	1.51
4	B	202	HEM	CMC-C2C	2.03	1.56	1.51
4	D	202	HEM	CAD-C3D	2.02	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	203	HEM	CBD-CAD-C3D	-3.55	105.93	112.48
4	B	202	HEM	CBD-CAD-C3D	-3.11	106.75	112.48
4	D	202	HEM	CAA-CBA-CGA	-2.74	108.07	112.67
4	B	202	HEM	CAA-CBA-CGA	-2.67	108.19	112.67
4	C	203	HEM	CAA-CBA-CGA	-2.51	108.45	112.67
4	B	202	HEM	CMA-C3A-C4A	-2.49	124.64	128.46
4	B	202	HEM	CMD-C2D-C1D	-2.44	124.71	128.46
4	A	203	HEM	CBD-CAD-C3D	-2.37	108.10	112.48
4	B	202	HEM	C3C-C4C-NC	-2.31	106.57	110.94
4	A	203	HEM	CMD-C2D-C1D	-2.29	124.94	128.46
4	D	202	HEM	CMA-C3A-C4A	-2.29	124.95	128.46
4	D	202	HEM	CMD-C2D-C1D	-2.29	124.95	128.46
4	A	203	HEM	CBA-CAA-C2A	-2.19	108.45	112.49
4	A	203	HEM	C3B-C4B-NB	-2.03	106.58	109.21

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	202	GOL	O1-C1-C2-C3
3	A	205	GOL	C1-C2-C3-O3
3	A	205	GOL	O2-C2-C3-O3
3	A	202	GOL	O1-C1-C2-O2
3	C	205	GOL	O2-C2-C3-O3
3	C	207	GOL	O1-C1-C2-O2
6	D	204	PEG	O2-C3-C4-O4
2	C	201	PGE	O1-C1-C2-O2
6	D	204	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	205	GOL	O1-C1-C2-C3
3	C	205	GOL	O1-C1-C2-C3
3	C	205	GOL	C1-C2-C3-O3
3	C	207	GOL	O1-C1-C2-C3
2	A	201	PGE	O2-C3-C4-O3
2	B	204	PGE	O2-C3-C4-O3
2	A	201	PGE	O1-C1-C2-O2
2	B	204	PGE	O1-C1-C2-O2
2	C	201	PGE	C3-C4-O3-C5
6	A	206	PEG	C1-C2-O2-C3
2	A	201	PGE	C3-C4-O3-C5
2	B	204	PGE	C3-C4-O3-C5
3	C	205	GOL	O1-C1-C2-O2
2	B	204	PGE	O3-C5-C6-O4
6	C	206	PEG	C4-C3-O2-C2
2	D	201	PGE	C6-C5-O3-C4
2	B	201	PGE	C6-C5-O3-C4
2	D	201	PGE	O2-C3-C4-O3
2	B	201	PGE	O2-C3-C4-O3
2	A	201	PGE	C1-C2-O2-C3
2	C	201	PGE	O2-C3-C4-O3

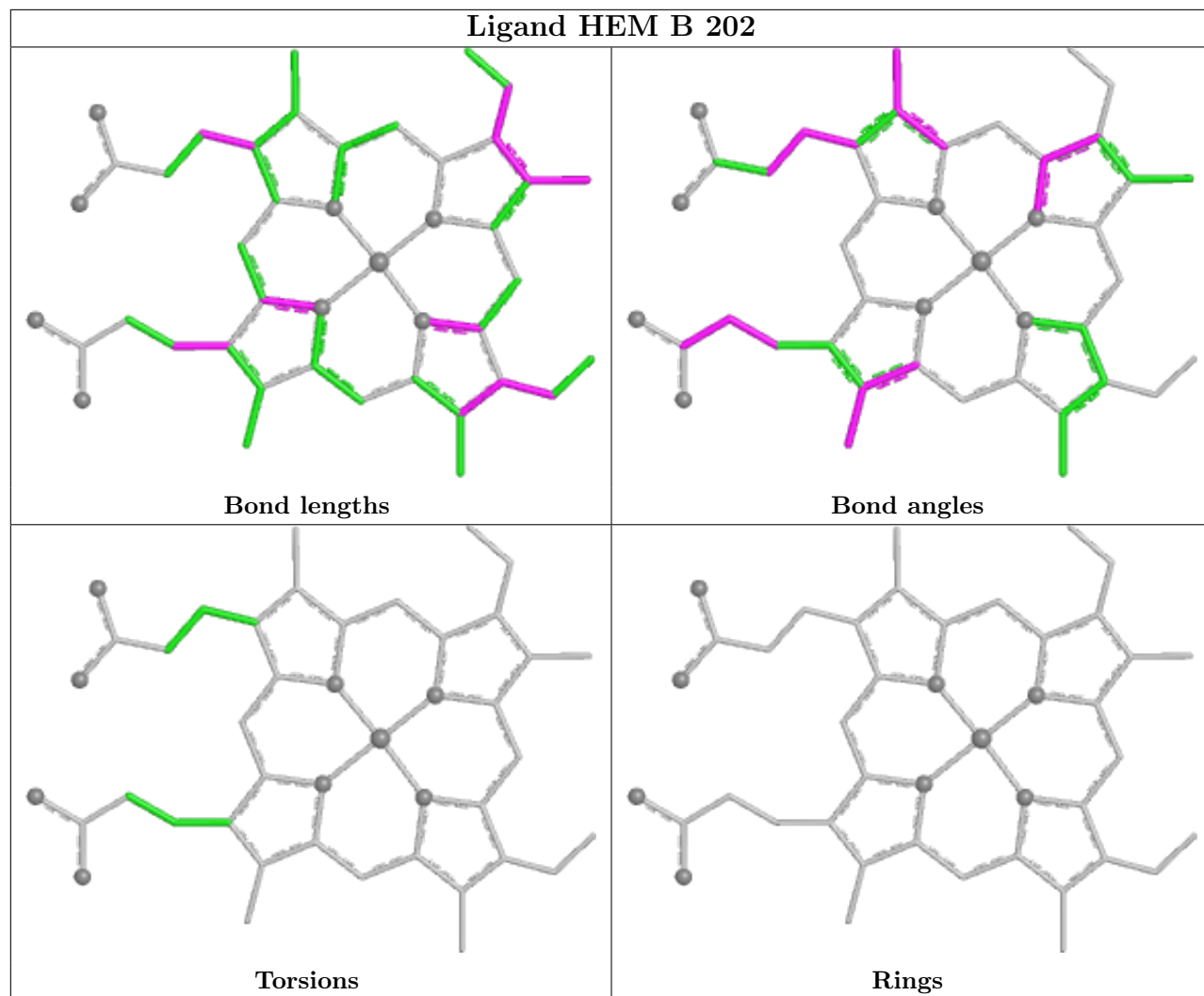
There are no ring outliers.

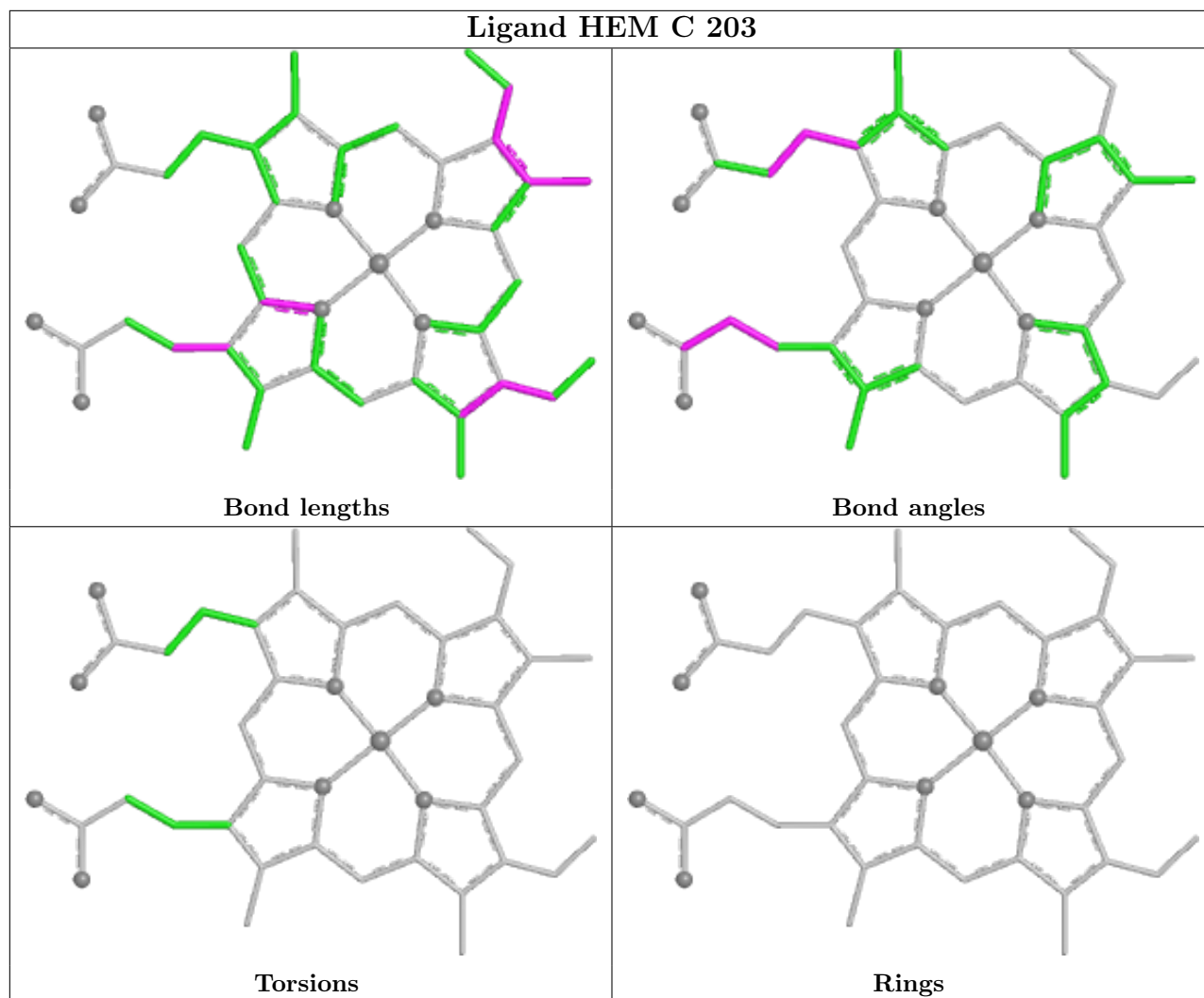
4 monomers are involved in 9 short contacts:

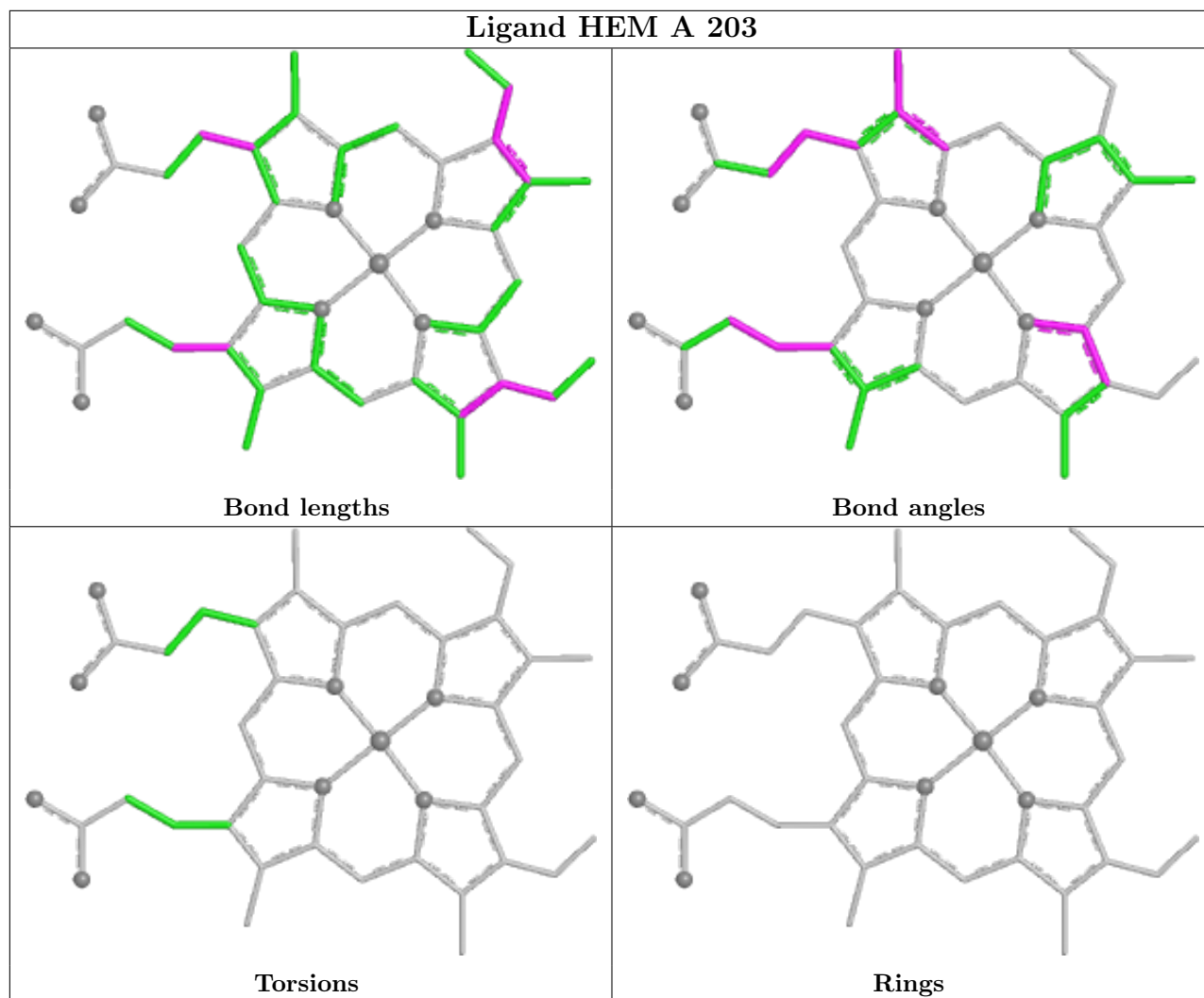
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	HEM	1	0
4	C	203	HEM	3	0
4	A	203	HEM	3	0
4	D	202	HEM	2	0

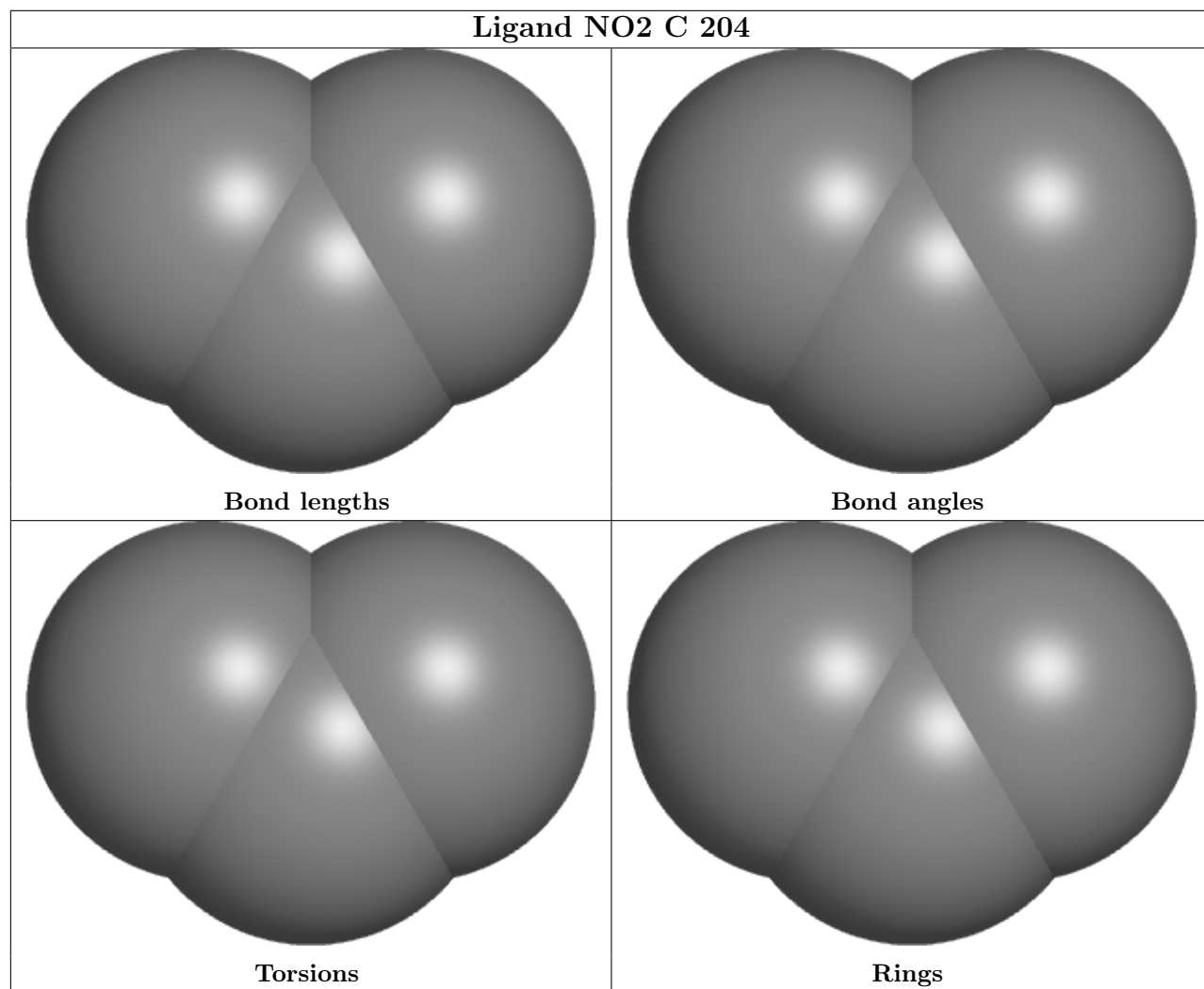
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

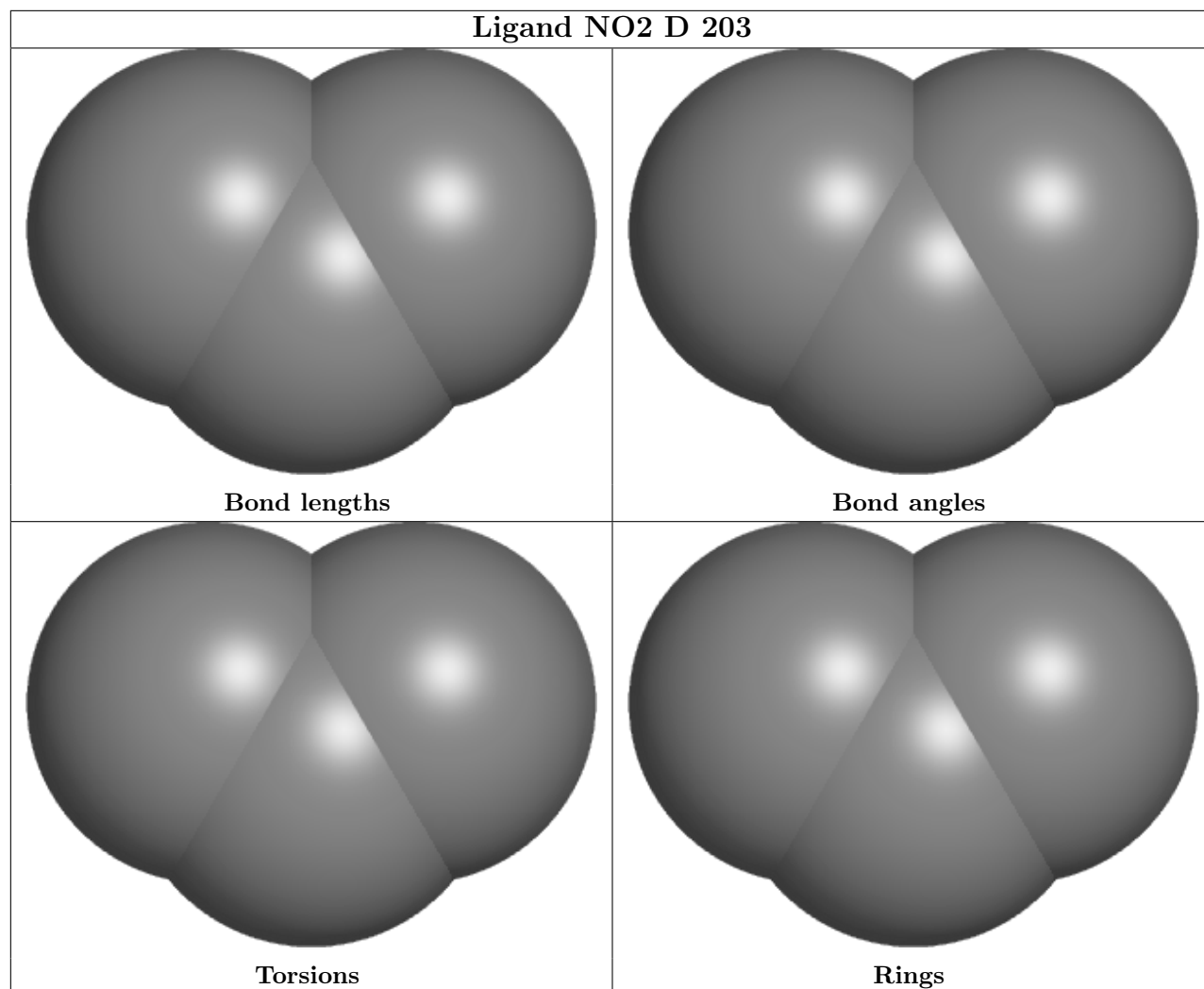
equivalents in the CSD to analyse the geometry.



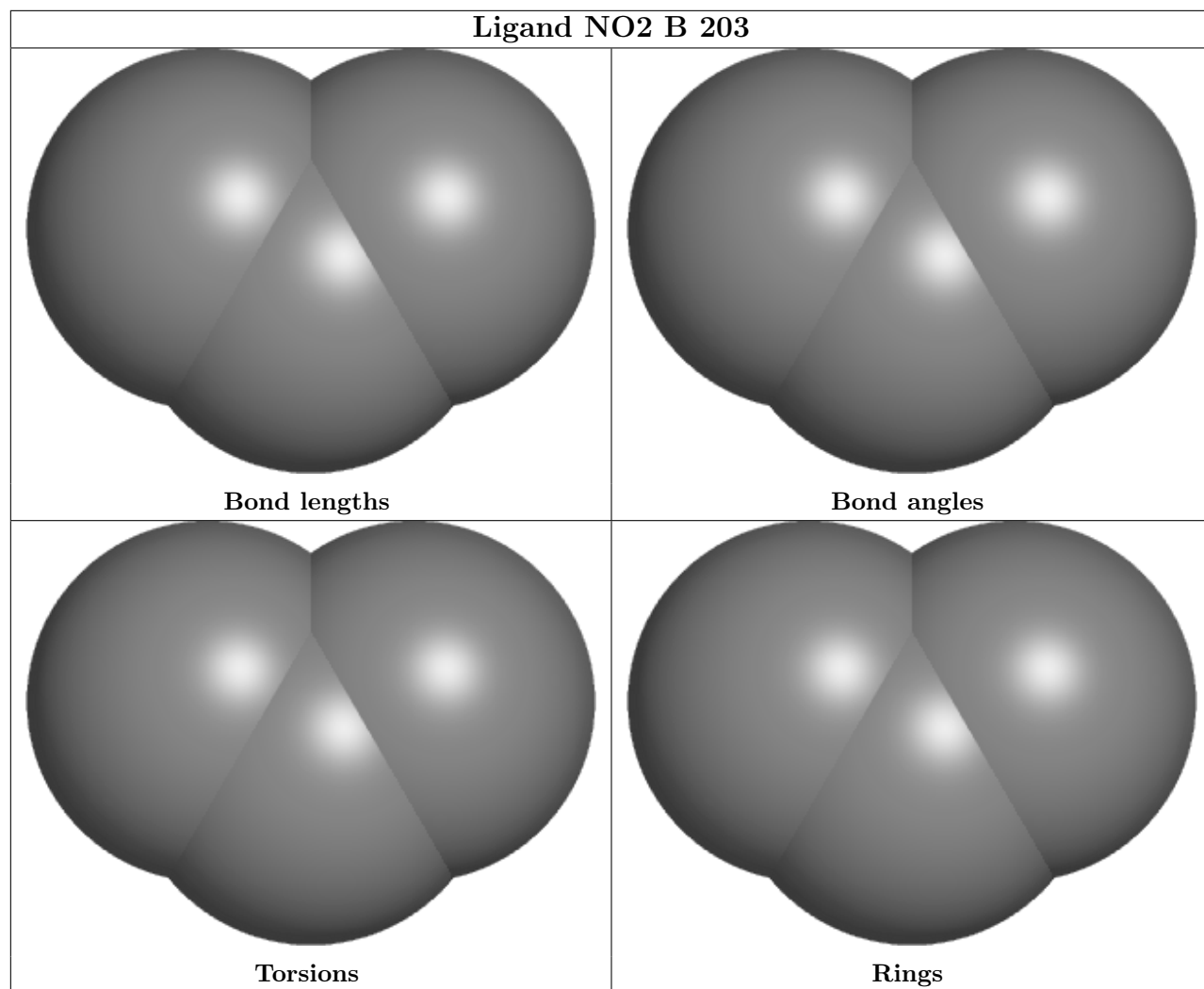


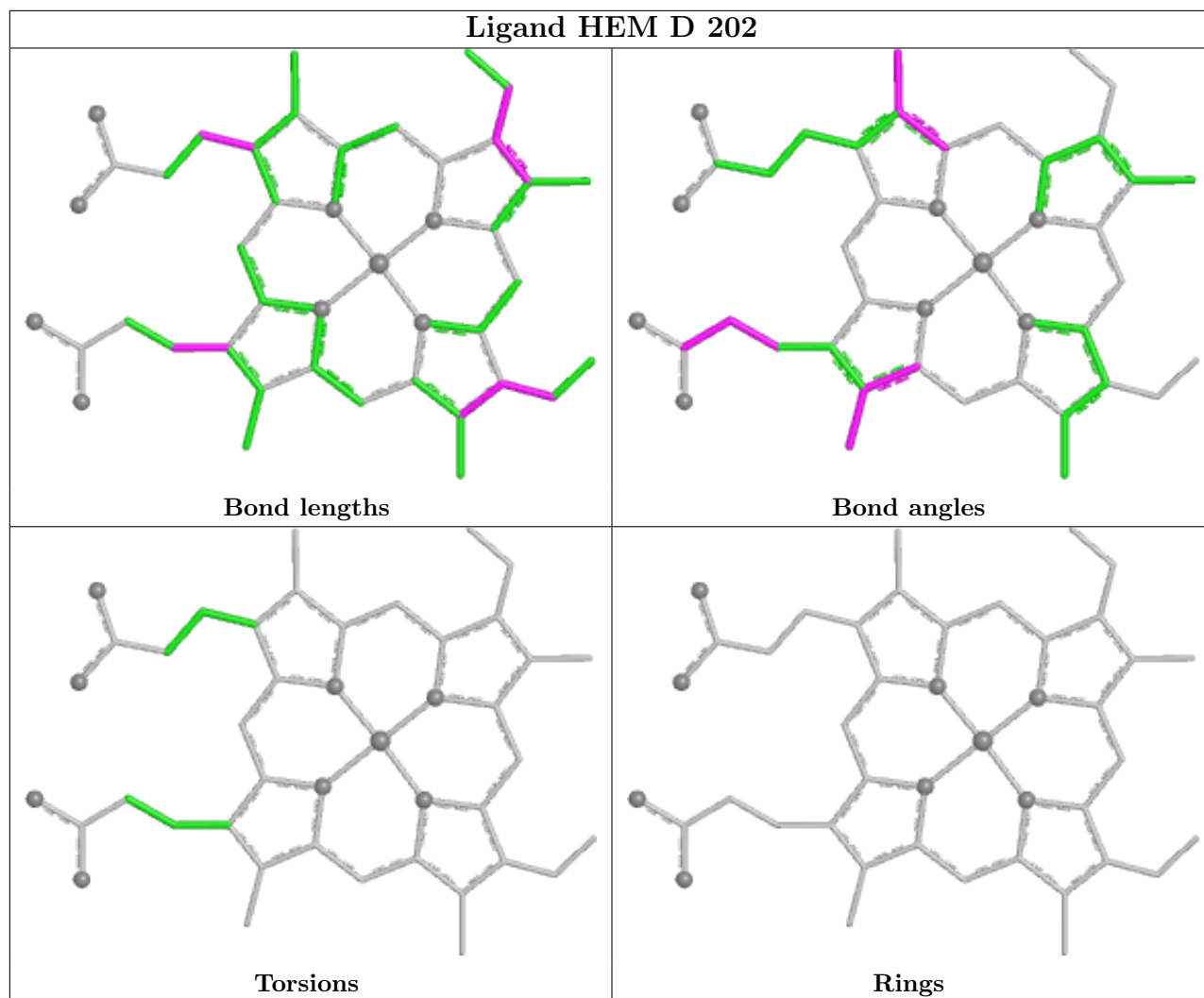


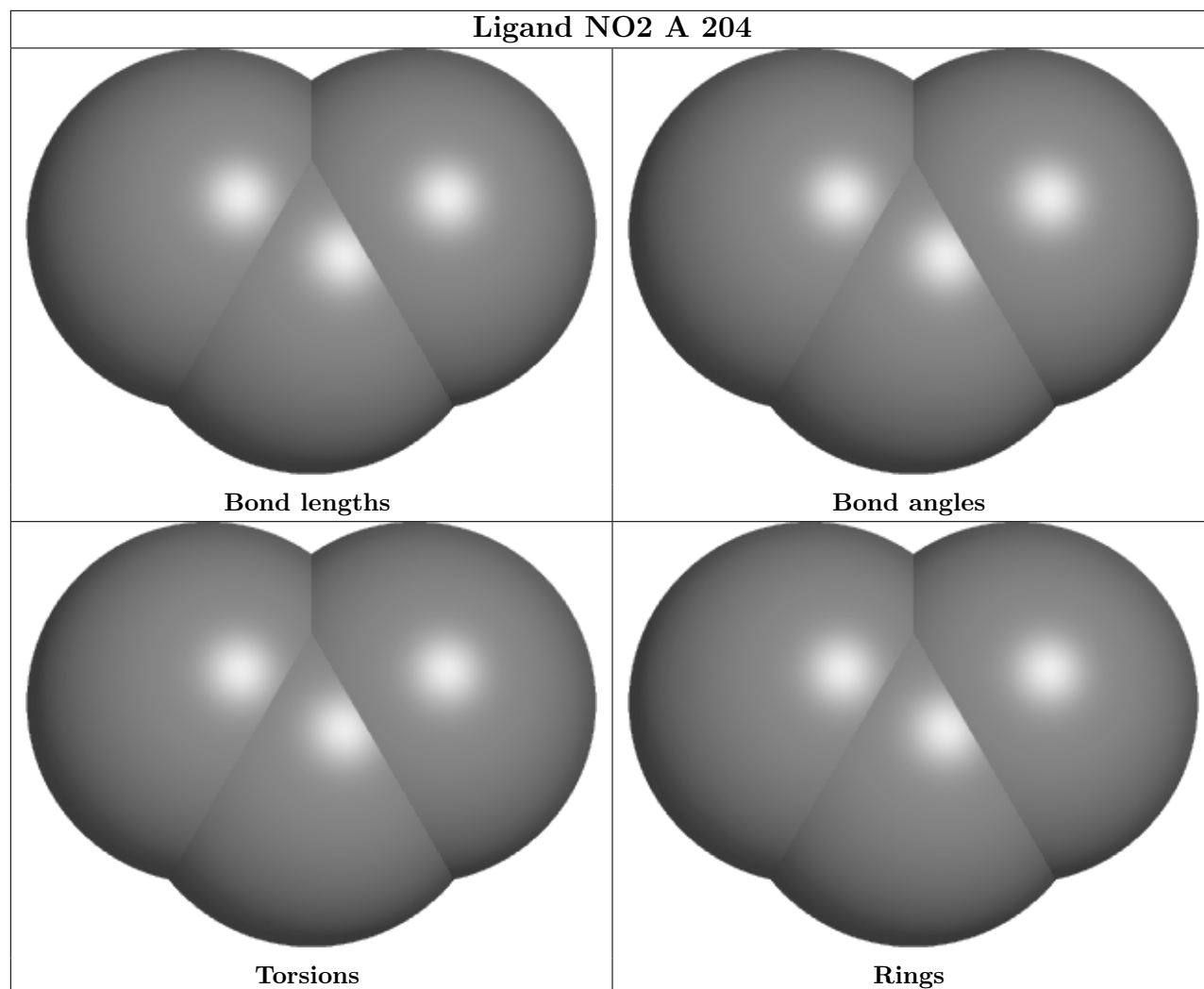












## 5.7 Other polymers [i](#)

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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	176/188 (93%)	0.56	12 (6%) 17 18	17, 37, 56, 88	0
1	B	176/188 (93%)	0.28	7 (3%) 38 42	16, 32, 46, 79	0
1	C	176/188 (93%)	0.35	9 (5%) 28 30	17, 32, 50, 81	0
1	D	176/188 (93%)	0.58	15 (8%) 10 11	17, 36, 54, 95	0
All	All	704/752 (93%)	0.44	43 (6%) 21 23	16, 34, 54, 95	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	40	ALA	7.0
1	D	1	PRO	6.6
1	B	1	PRO	6.4
1	C	1	PRO	5.4
1	D	49	ALA	5.4
1	D	40	ALA	5.3
1	D	47	ASP	5.3
1	B	40	ALA	5.1
1	A	40	ALA	4.4
1	A	47	ASP	4.3
1	C	39	GLY	3.8
1	C	47	ASP	3.7
1	A	1	PRO	3.6
1	A	110	ARG	3.5
1	A	141	PHE	3.5
1	A	2	ASN	3.4
1	B	47	ASP	3.4
1	A	37	LEU	3.0
1	A	39	GLY	3.0
1	C	110	ARG	2.9
1	A	61	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	141	PHE	2.7
1	B	39	GLY	2.7
1	D	130	LEU	2.5
1	B	11	ARG	2.5
1	B	110	ARG	2.4
1	D	55	PHE	2.4
1	D	141	PHE	2.3
1	C	37	LEU	2.2
1	A	143	THR	2.2
1	D	106	ASP	2.2
1	D	2	ASN	2.2
1	D	132	CYS	2.2
1	A	164	ALA	2.2
1	D	145	PHE	2.1
1	B	87	LEU	2.1
1	D	48	SER	2.1
1	C	2	ASN	2.1
1	A	108	PHE	2.1
1	D	164	ALA	2.1
1	D	110	ARG	2.0
1	C	129	LEU	2.0
1	D	33	LYS	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PGE	B	204	10/10	0.75	0.23	40,78,109,119	0

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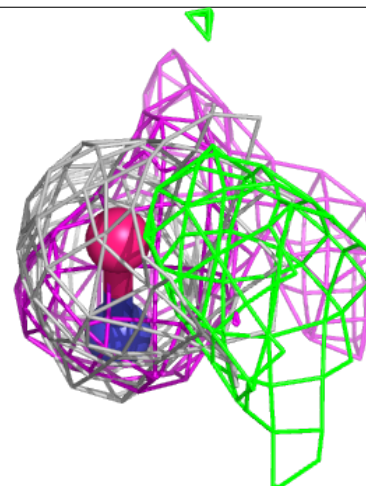
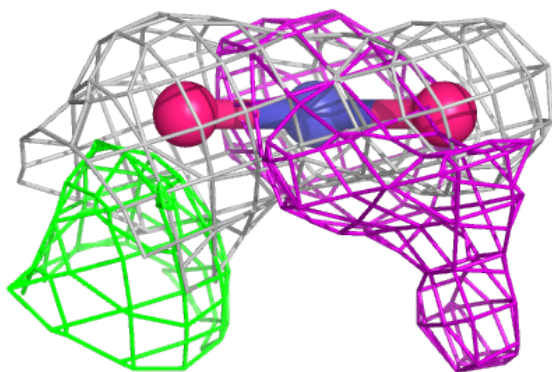
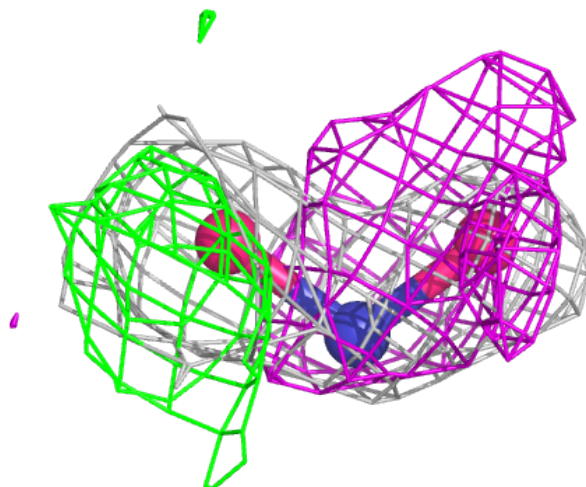
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	PEG	D	204	7/7	0.78	0.36	51,63,80,90	0
3	GOL	A	202	6/6	0.80	0.16	33,40,44,47	0
6	PEG	C	206	7/7	0.82	0.21	37,46,56,56	0
2	PGE	C	201	10/10	0.83	0.17	34,44,52,72	0
3	GOL	C	207	6/6	0.83	0.15	33,44,56,57	0
5	NO2	A	204	3/3	0.85	0.13	27,27,31,31	0
3	GOL	C	202	6/6	0.85	0.13	34,40,45,45	0
3	GOL	A	205	6/6	0.85	0.16	30,38,46,46	0
6	PEG	A	206	7/7	0.86	0.22	43,53,63,66	0
2	PGE	A	201	10/10	0.88	0.13	25,41,52,62	0
2	PGE	B	201	10/10	0.88	0.15	29,37,45,54	0
2	PGE	D	201	10/10	0.90	0.14	28,37,49,54	0
5	NO2	C	204	3/3	0.92	0.15	24,24,29,33	0
5	NO2	D	203	3/3	0.93	0.15	20,20,27,36	0
3	GOL	C	205	6/6	0.93	0.11	30,39,47,47	0
5	NO2	B	203	3/3	0.95	0.11	21,21,22,31	0
7	SO4	A	207	5/5	0.96	0.15	54,54,64,65	0
4	HEM	A	203	43/43	0.97	0.13	16,23,33,34	0
4	HEM	B	202	43/43	0.97	0.10	15,22,33,34	0
4	HEM	C	203	43/43	0.97	0.12	17,22,31,32	0
4	HEM	D	202	43/43	0.97	0.11	17,24,32,35	0
7	SO4	D	205	5/5	0.98	0.17	54,60,64,66	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.

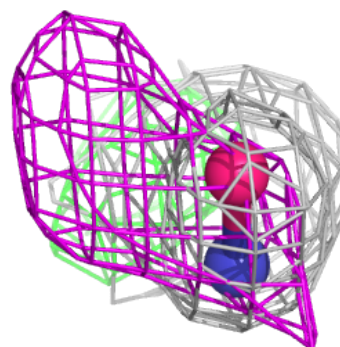
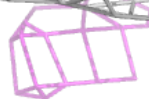
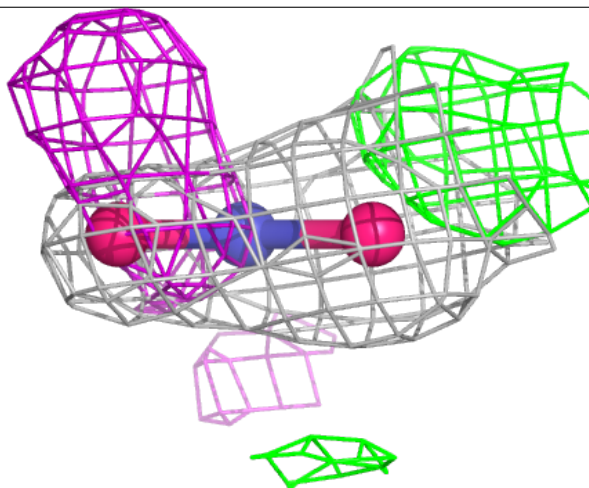
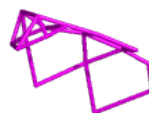
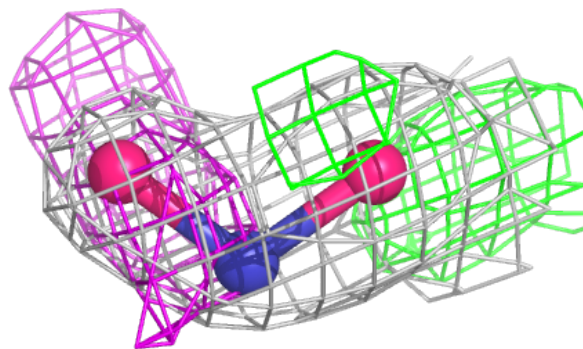
**Electron density around NO2 A 204:**

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



**Electron density around NO2 C 204:**

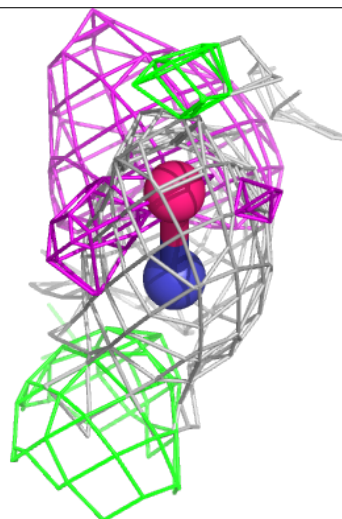
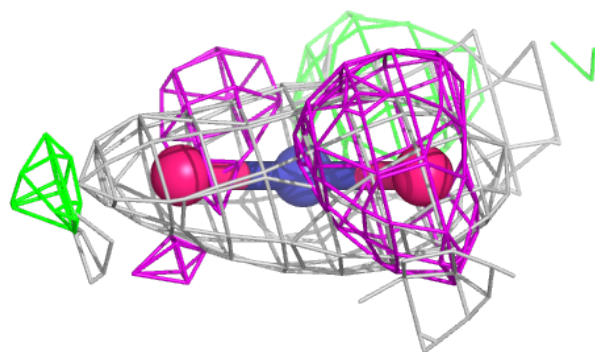
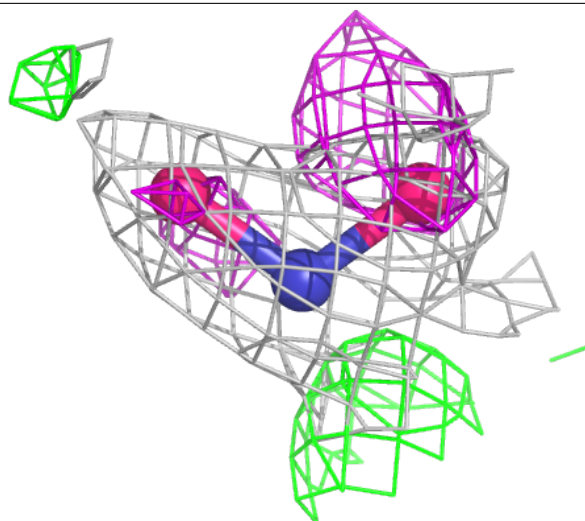
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





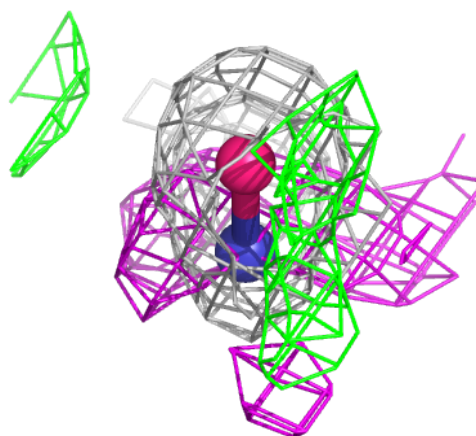
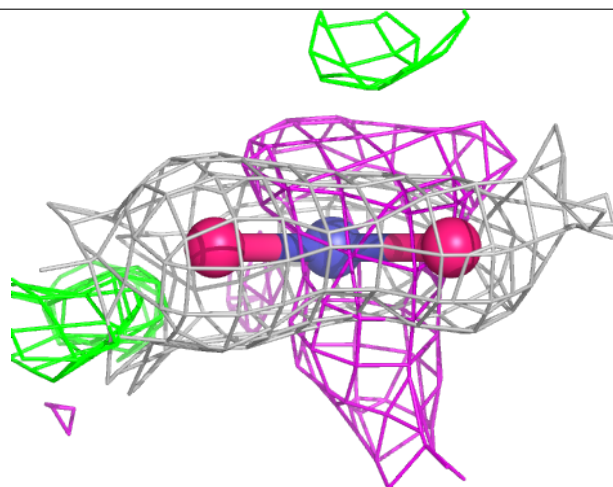
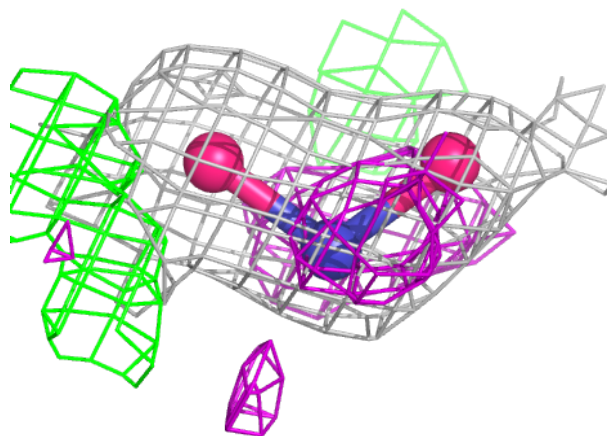
**Electron density around NO2 D 203:**

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



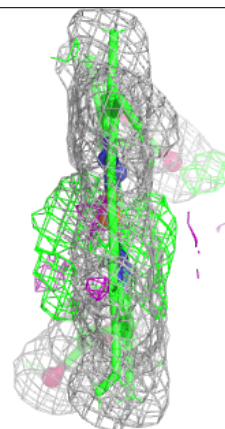
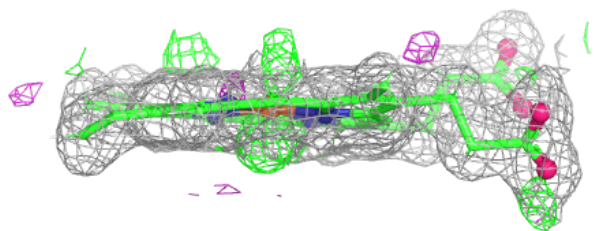
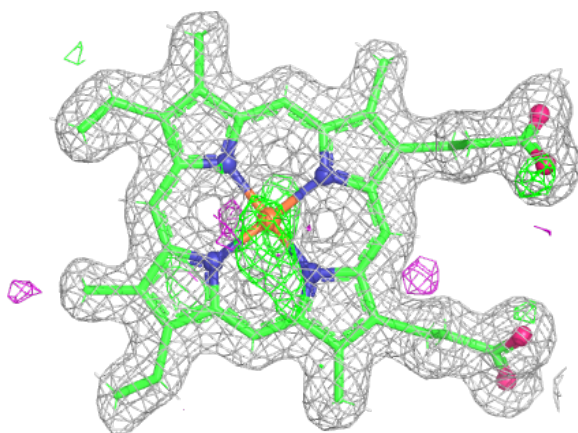
**Electron density around NO2 B 203:**

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



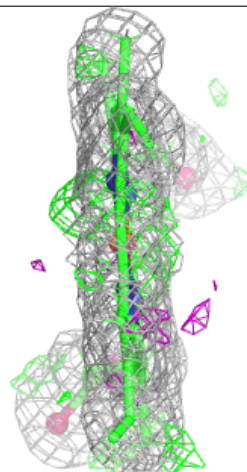
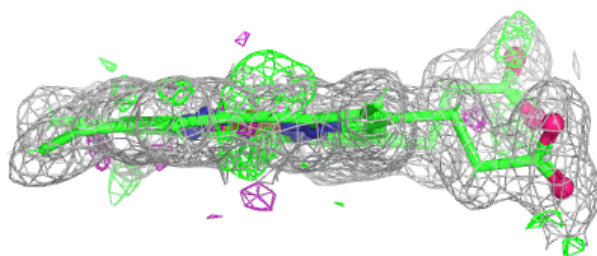
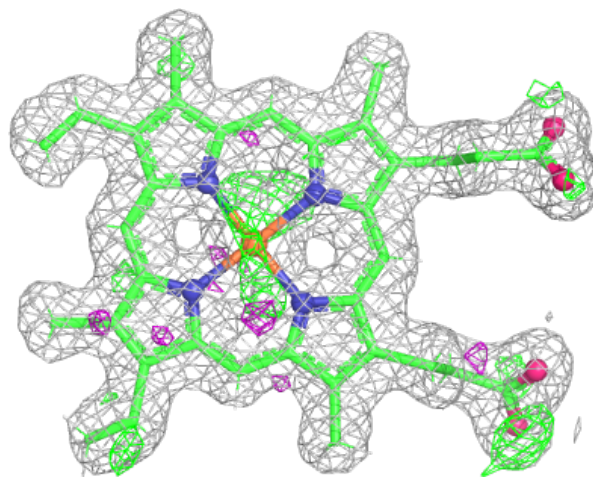
**Electron density around HEM A 203:**

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



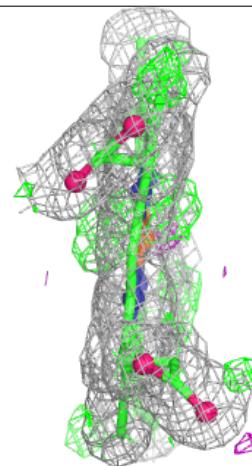
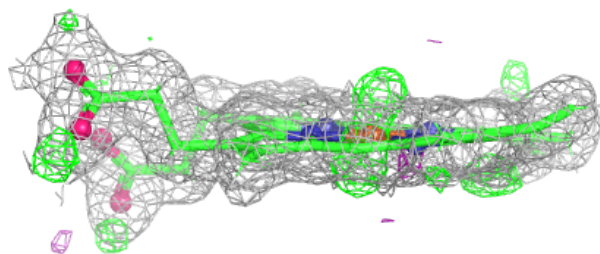
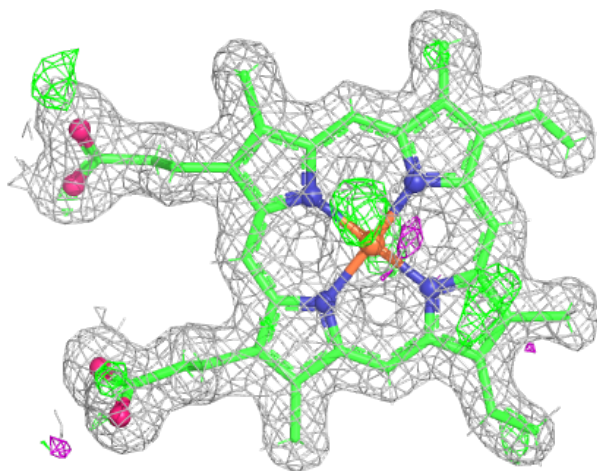
**Electron density around HEM B 202:**

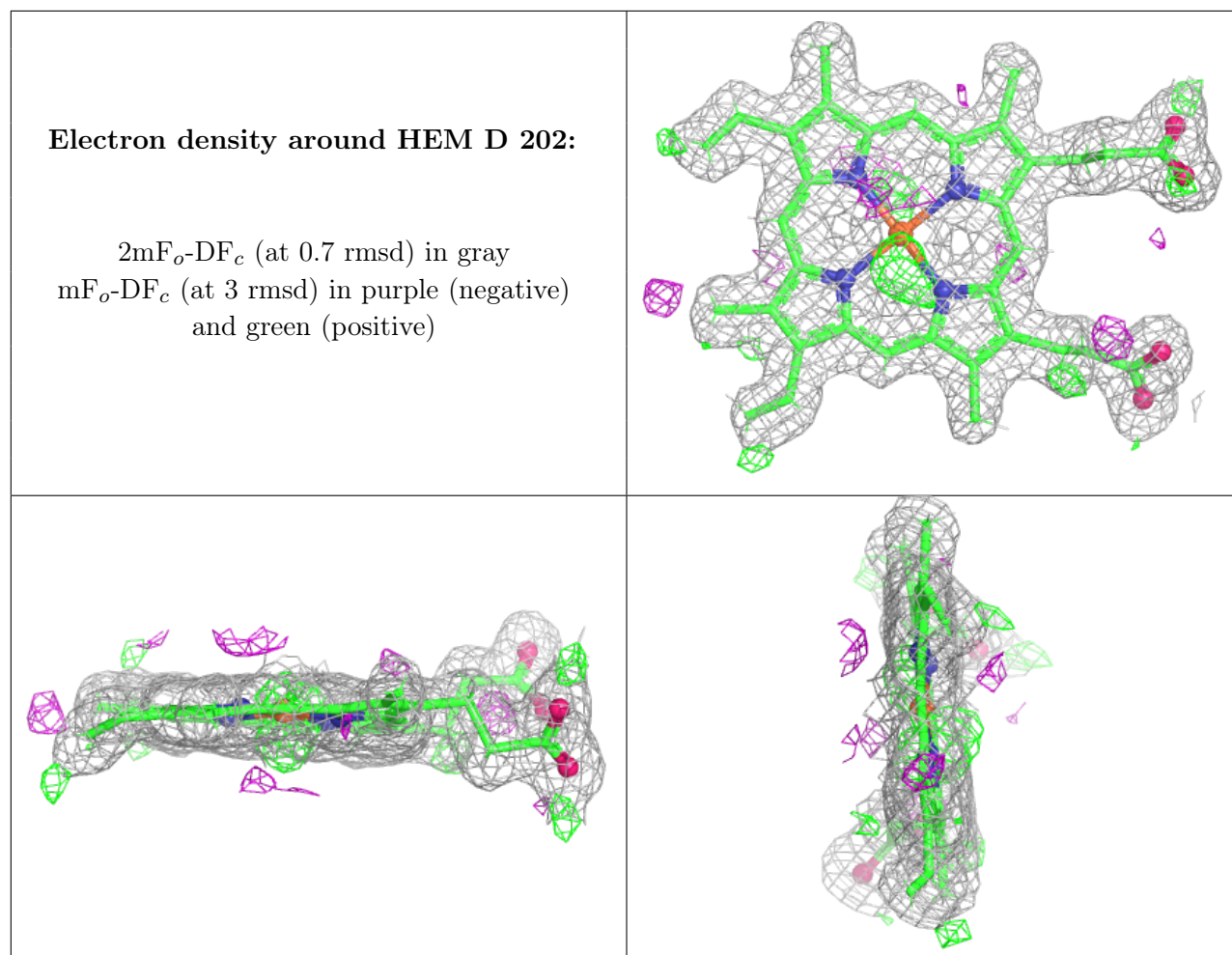
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 203:**

$2mF_o-DF_c$  (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.