WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jul 8, 2024 – 12:22 PM EDT

PDB ID	:	8VSK
Title	:	Crystal structure of Dehaloperoxidase A in complex with substrate 2,4-dibromophenol
Authors	:	Aktar, M.S.; de Serrano, V.S.; Ghiladi, R.A.; Franzen, S.
Deposited on	:	2024-01-24
Resolution	:	1.51 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

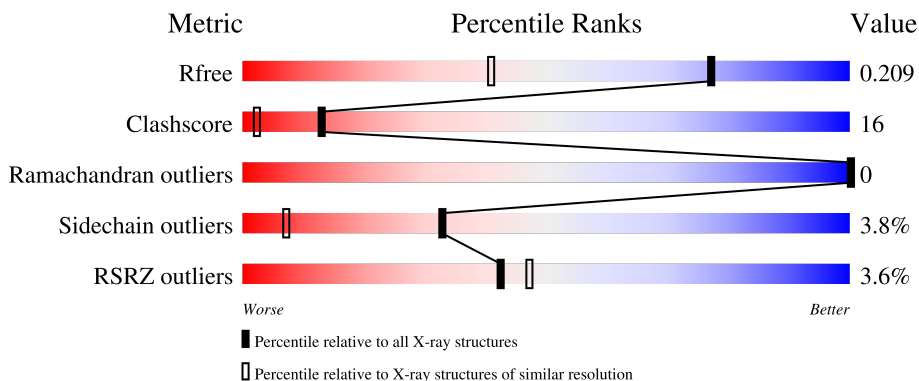|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.209
Clashscore		16
Ramachandran outliers		0
Sidechain outliers		3.8%
RSRZ outliers		3.6%

Worse ... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

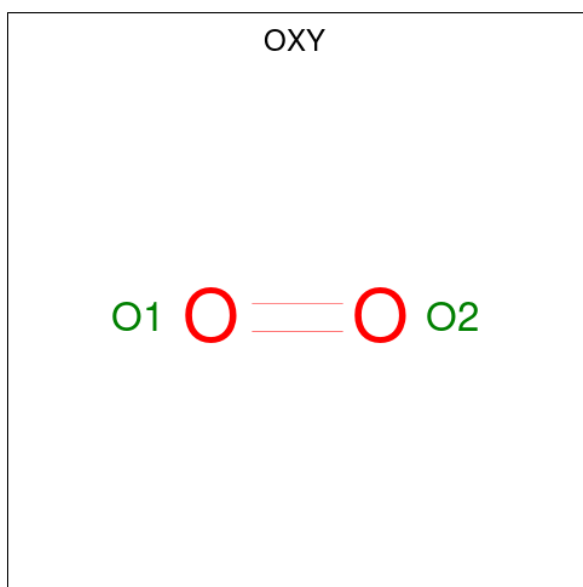| Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	137	4% / 84% / 16%
1	BBB	137	4% / 80% / 18% / •

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
4	GOL	AAA	203	-	-	X	-
6	Y8I	BBB	202	-	-	X	-
7	PEG	BBB	203	-	-	X	-
7	PEG	BBB	204	-	-	X	-

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 2912 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 A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	137	Total	C	N	O	S	0	25	0
			1295	808	222	256	9			
1	BBB	137	Total	C	N	O	S	9	22	0
			1263	790	221	244	8			

- 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).

HEM

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

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).

OXY

O1 O ═══ O O2

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	1	Total 2	O 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3
OH O3

C1   C2

HO
O1

OH
O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total 6	C 3	O 3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

• Molecule 6 is 2,4-bis(bromanyl)phenol (three-letter code: Y8I) (formula: $C_6H_4Br_2O$).
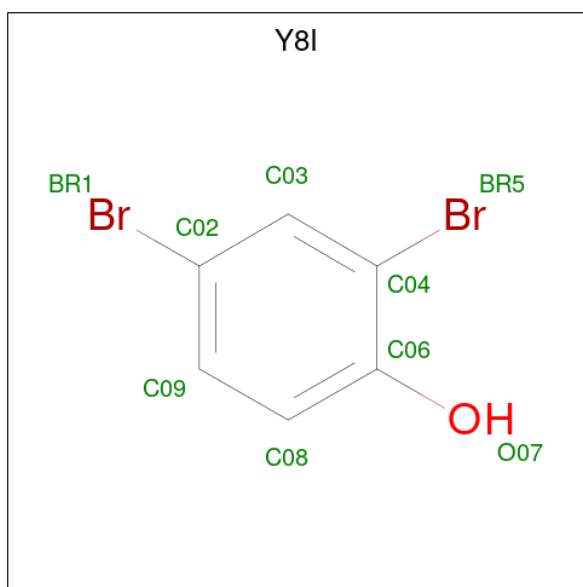
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	BBB	1	Total 9	Br 2	C 6	O 1	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
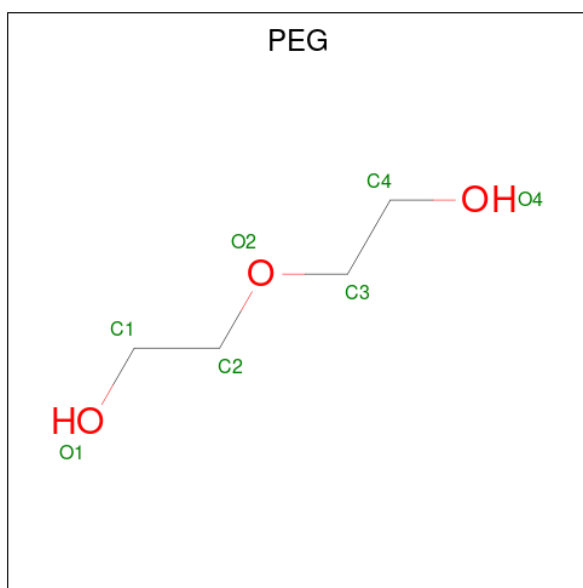
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	BBB	1	Total 7	C 4	O 3	0	0
7	BBB	1	Total 7	C 4	O 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	104	Total 104	O 104	0	0
8	BBB	118	Total 118	O 118	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Dehaloperoxidase A

Chain AAA:

• Molecule 1: Dehaloperoxidase A

Chain BBB:
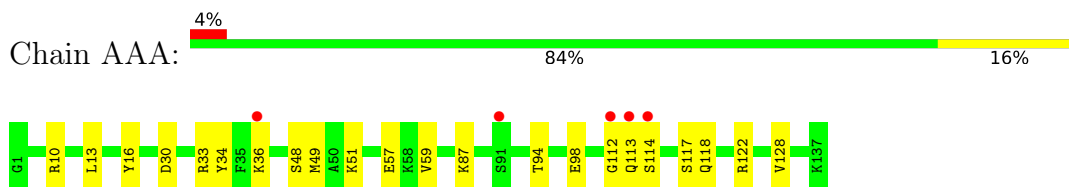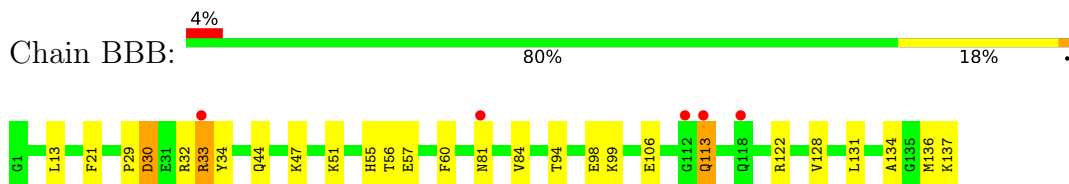
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.17Å 66.18Å 69.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.69 – 1.51 36.66 – 1.52	Depositor EDS
% Data completeness (in resolution range)	99.6 (36.69-1.51) 99.6 (36.66-1.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.181 , 0.205 0.191 , 0.209	Depositor DCC
R_{free} test set	2050 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	14.7	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 42.5	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.025 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2912	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, HEM, PEG, SO4, OXY, Y8I

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	AAA	0.78	0/1324	0.88	1/1768 (0.1%)
1	BBB	0.79	0/1297	0.86	0/1736
All	All	0.79	0/2621	0.87	1/3504 (0.0%)

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	AAA	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	122	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	112	GLY	Peptide

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	AAA	1295	0	1263	28	2
1	BBB	1263	0	1226	53	2
2	AAA	43	0	30	1	0
2	BBB	43	0	30	2	0
3	AAA	2	0	0	0	0
4	AAA	6	0	8	11	0
5	AAA	5	0	0	0	0
5	BBB	10	0	0	0	0
6	BBB	9	0	0	13	0
7	BBB	14	0	20	16	0
8	AAA	104	0	0	4	0
8	BBB	118	0	0	7	0
All	All	2912	0	2577	87	2

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 16.

The worst 5 of 87 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:BBB:60[A]:PHE:HE1	6:BBB:202:Y8I:C02	1.31	1.41
1:BBB:60[A]:PHE:CE1	6:BBB:202:Y8I:C02	2.08	1.33
1:AAA:49[A]:MET:CE	1:AAA:51[A]:LYS:HE2	1.66	1.25
1:AAA:49[A]:MET:HE2	1:AAA:51[A]:LYS:CE	1.88	1.03
1:BBB:60[A]:PHE:CZ	6:BBB:202:Y8I:BR1	1.02	1.03

All (2) 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)
1:AAA:33:ARG:NE	1:BBB:30[B]:ASP:OD2[4_455]	2.00	0.20
1:AAA:33:ARG:CD	1:BBB:30[B]:ASP:OD2[4_455]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	162/137 (118%)	158 (98%)	4 (2%)	0	100	100
1	BBB	157/137 (115%)	156 (99%)	1 (1%)	0	100	100
All	All	319/274 (116%)	314 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	144/117 (123%)	136 (94%)	8 (6%)	21	2
1	BBB	139/117 (119%)	132 (95%)	7 (5%)	24	3
All	All	283/234 (121%)	268 (95%)	15 (5%)	33	3

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	87[B]	LYS
1	BBB	113[B]	GLN
1	BBB	30[A]	ASP
1	BBB	137	LYS
1	BBB	33[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	AAA	201	3,1	41,50,50	1.21	3 (7%)	45,82,82	1.52	9 (20%)
7	PEG	BBB	204	-	6,6,6	0.57	0	5,5,5	0.32	0
5	SO4	BBB	205	-	4,4,4	0.47	0	6,6,6	0.30	0
3	OXY	AAA	202	2	1,1,1	0.42	0	-		
6	Y8I	BBB	202	-	9,9,9	0.41	0	12,12,12	1.33	2 (16%)
4	GOL	AAA	203	-	5,5,5	0.25	0	5,5,5	0.52	0
7	PEG	BBB	203	-	6,6,6	0.40	0	5,5,5	0.29	0
5	SO4	BBB	206	-	4,4,4	0.17	0	6,6,6	0.57	0
5	SO4	AAA	204	-	4,4,4	0.42	0	6,6,6	0.22	0
2	HEM	BBB	201	8,1	41,50,50	1.39	7 (17%)	45,82,82	1.83	10 (22%)

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	AAA	201	3,1	-	3/12/54/54	-
7	PEG	BBB	204	-	-	2/4/4/4	-
6	Y8I	BBB	202	-	-	-	0/1/1/1
4	GOL	AAA	203	-	-	2/4/4/4	-
7	PEG	BBB	203	-	-	4/4/4/4	-
2	HEM	BBB	201	8,1	-	5/12/54/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	201	HEM	C1B-NB	-3.21	1.34	1.40
2	BBB	201	HEM	CAA-C2A	2.73	1.56	1.52
2	AAA	201	HEM	FE-NB	2.62	2.09	1.96
2	BBB	201	HEM	O2A-CGA	-2.55	1.22	1.30
2	AAA	201	HEM	CHB-C1B	2.32	1.40	1.35

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	201	HEM	CAD-CBD-CGD	-5.46	101.85	113.60
2	BBB	201	HEM	C4B-C3B-C2B	-3.35	104.46	107.11
2	AAA	201	HEM	C1B-NB-C4B	3.14	108.31	105.07
2	BBB	201	HEM	CMA-C3A-C4A	-3.13	123.65	128.46
2	BBB	201	HEM	CMA-C3A-C2A	2.96	130.52	124.94

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	203	GOL	O1-C1-C2-C3
2	AAA	201	HEM	C3D-CAD-CBD-CGD
7	BBB	204	PEG	O1-C1-C2-O2
2	BBB	201	HEM	C3D-CAD-CBD-CGD
7	BBB	203	PEG	O2-C3-C4-O4

There are no ring outliers.
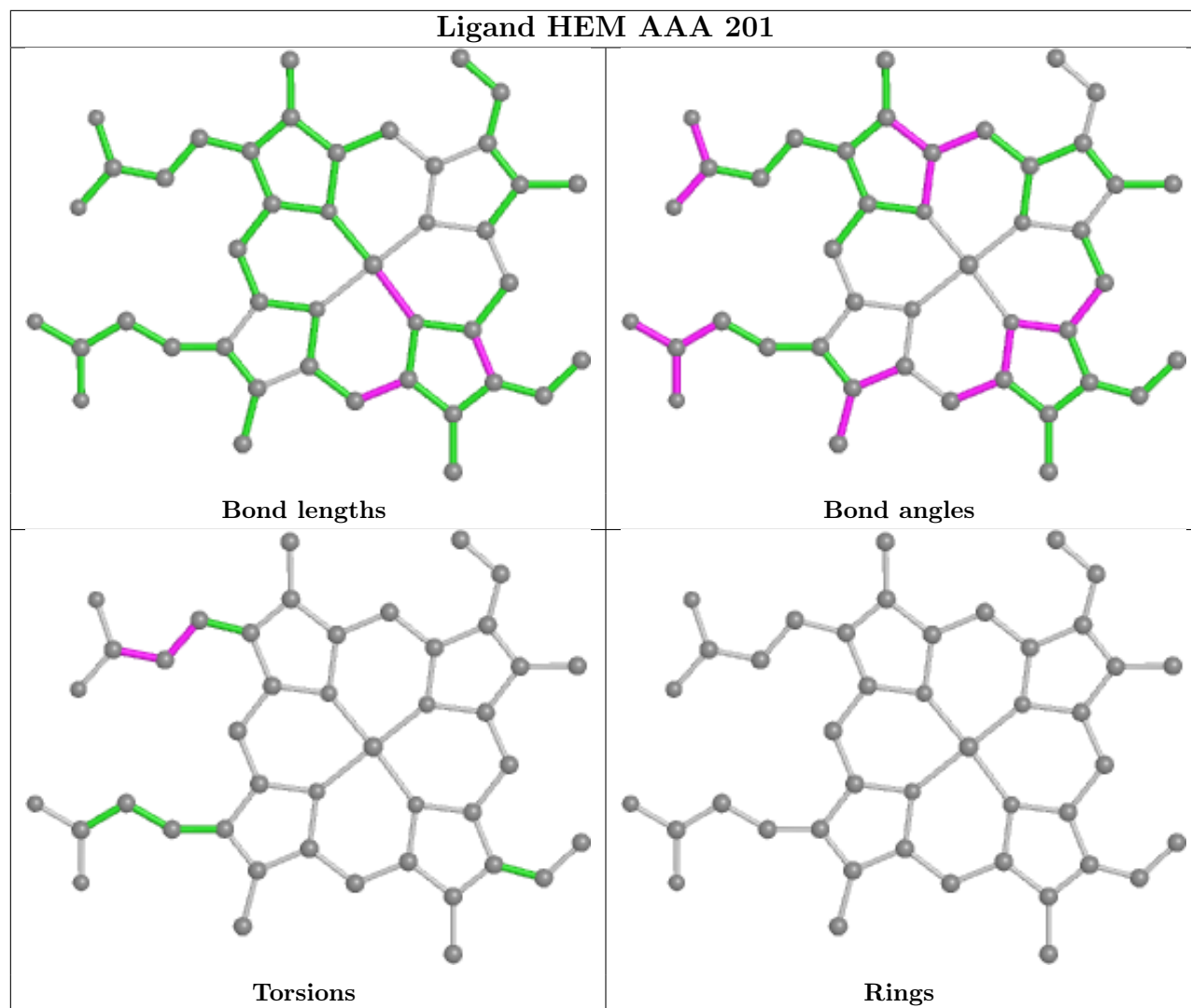
6 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	201	HEM	1	0
7	BBB	204	PEG	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	BBB	202	Y8I	13	0
4	AAA	203	GOL	11	0
7	BBB	203	PEG	9	0
2	BBB	201	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEM AAA 201

Bond lengths

Bond angles

Torsions

Rings

Ligand Y8I BBB 202

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM BBB 201

Bond lengths

Bond angles

Torsions

Rings
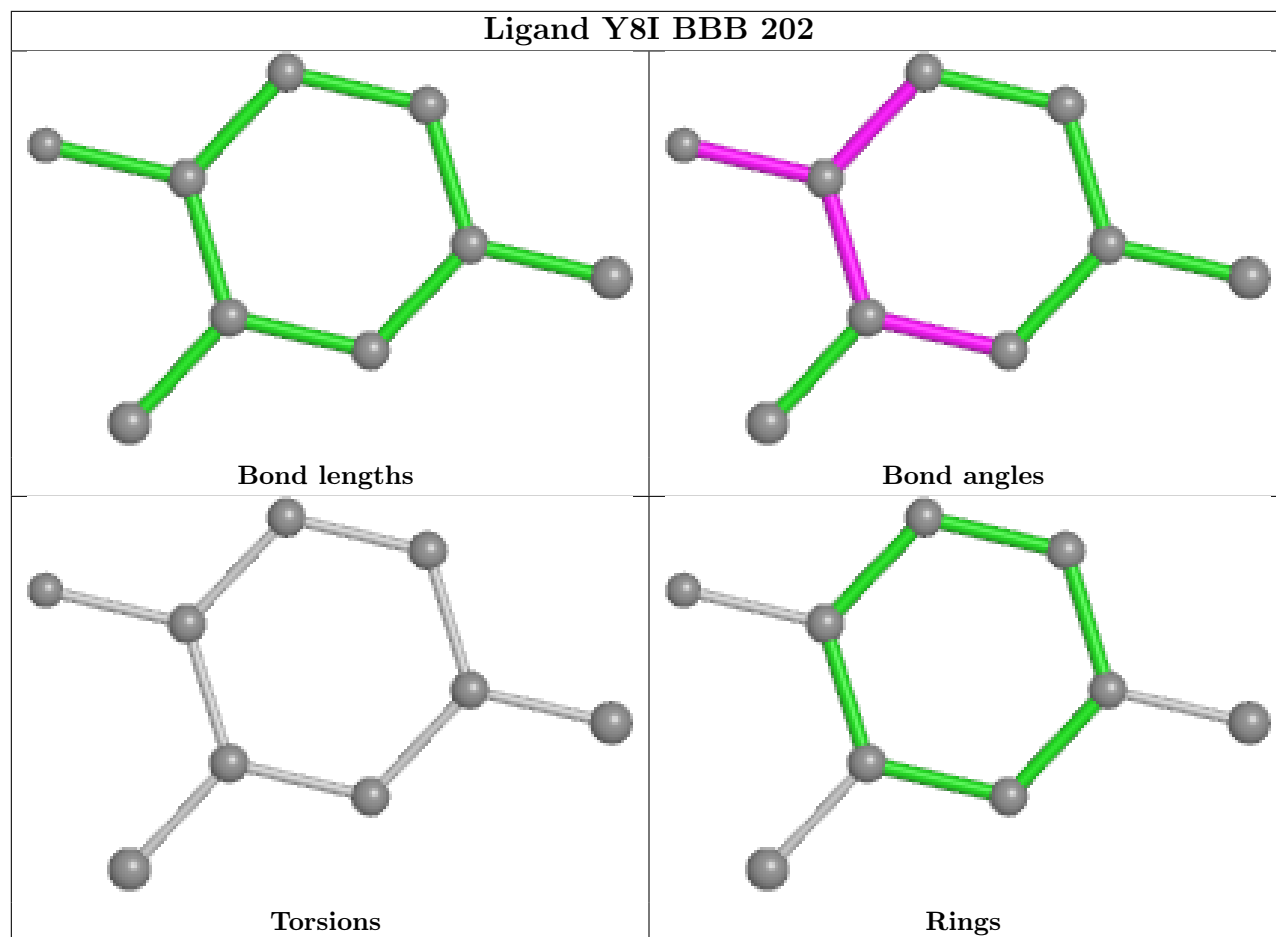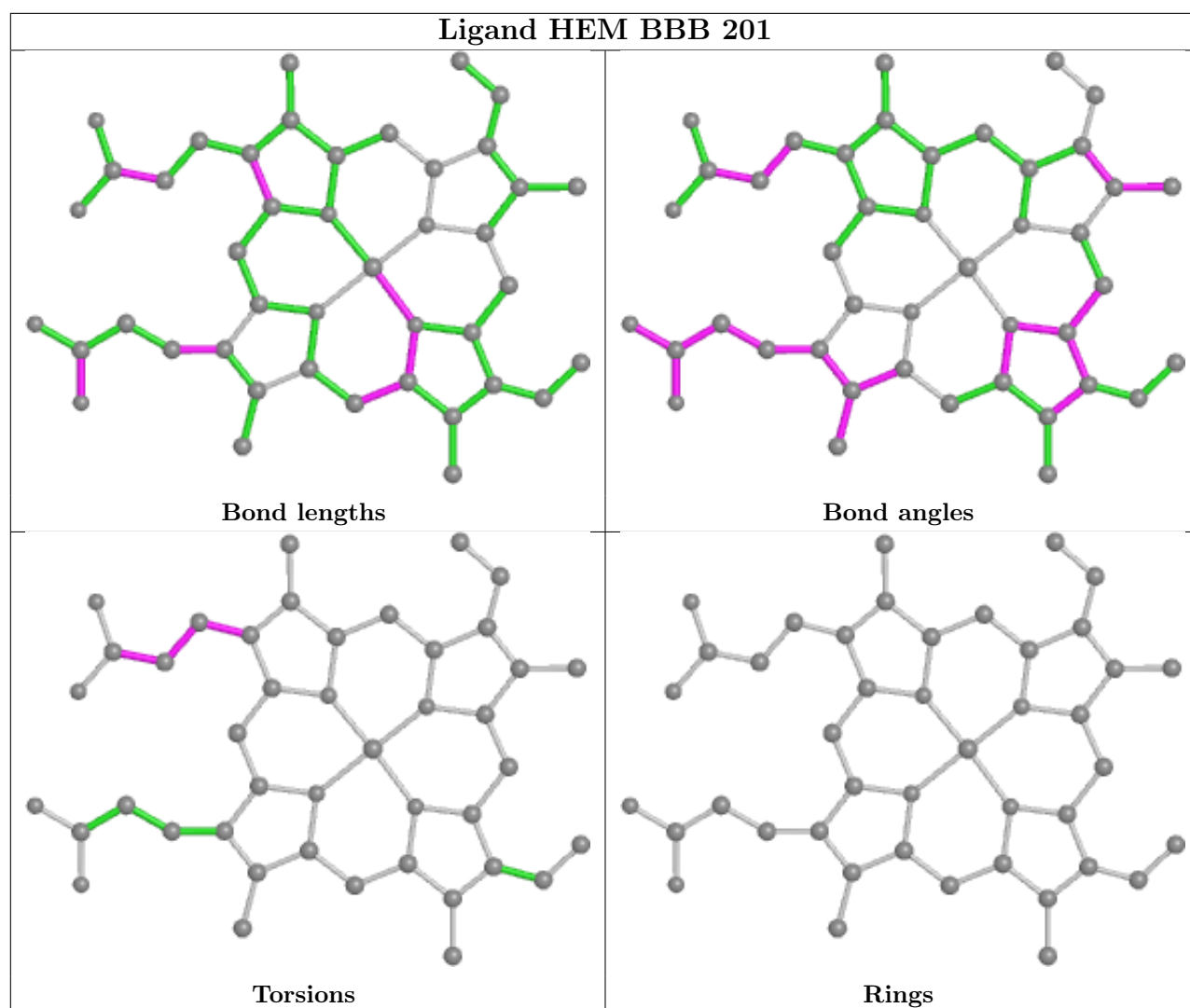
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	137/137 (100%)	-0.00	5 (3%)	42	47	10, 16, 28, 33	0
1	BBB	137/137 (100%)	-0.02	5 (3%)	42	47	9, 13, 28, 40	2 (1%)
All	All	274/274 (100%)	-0.01	10 (3%)	42	47	9, 15, 28, 40	2 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	118[A]	GLN	4.9
1	AAA	112	GLY	4.7
1	BBB	112	GLY	4.0
1	BBB	81[A]	ASN	3.2
1	BBB	33[A]	ARG	3.1

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

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

6.3 Carbohydrates ⓘ
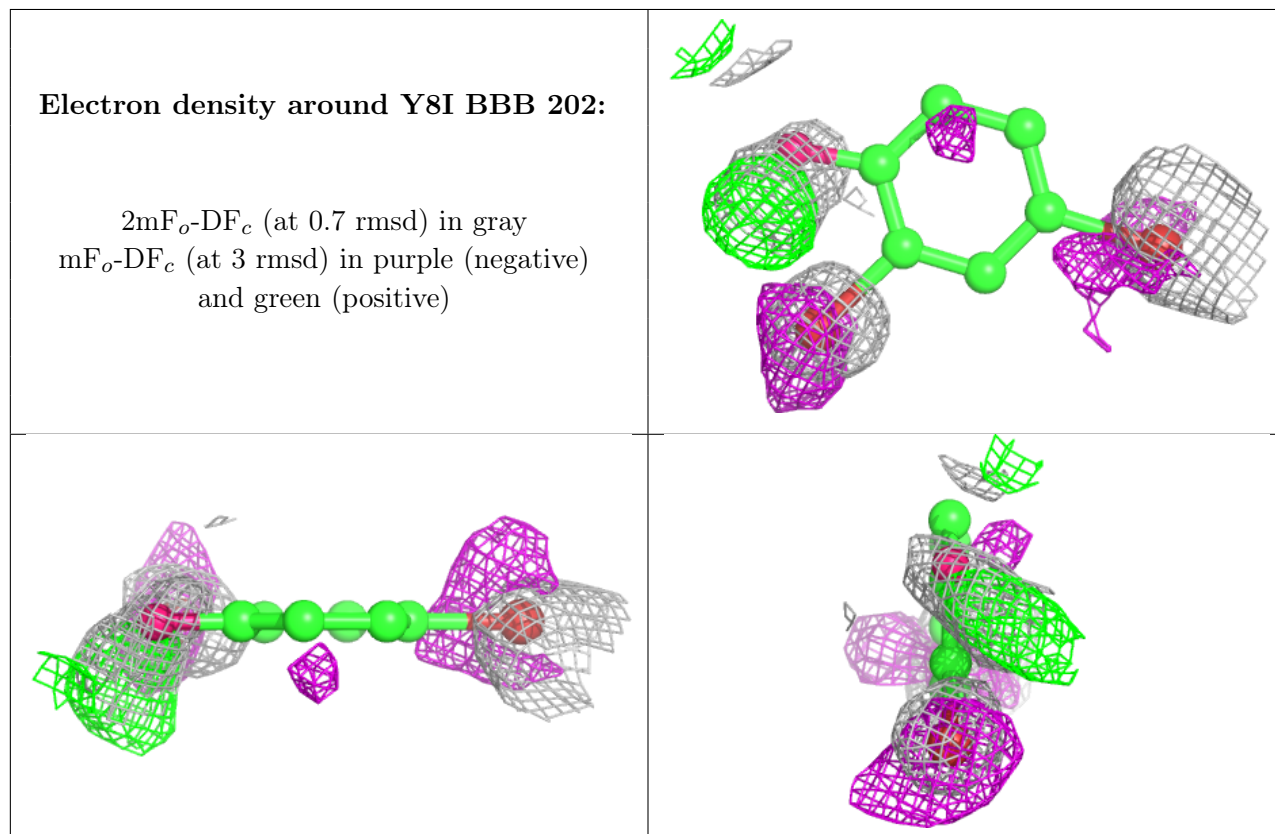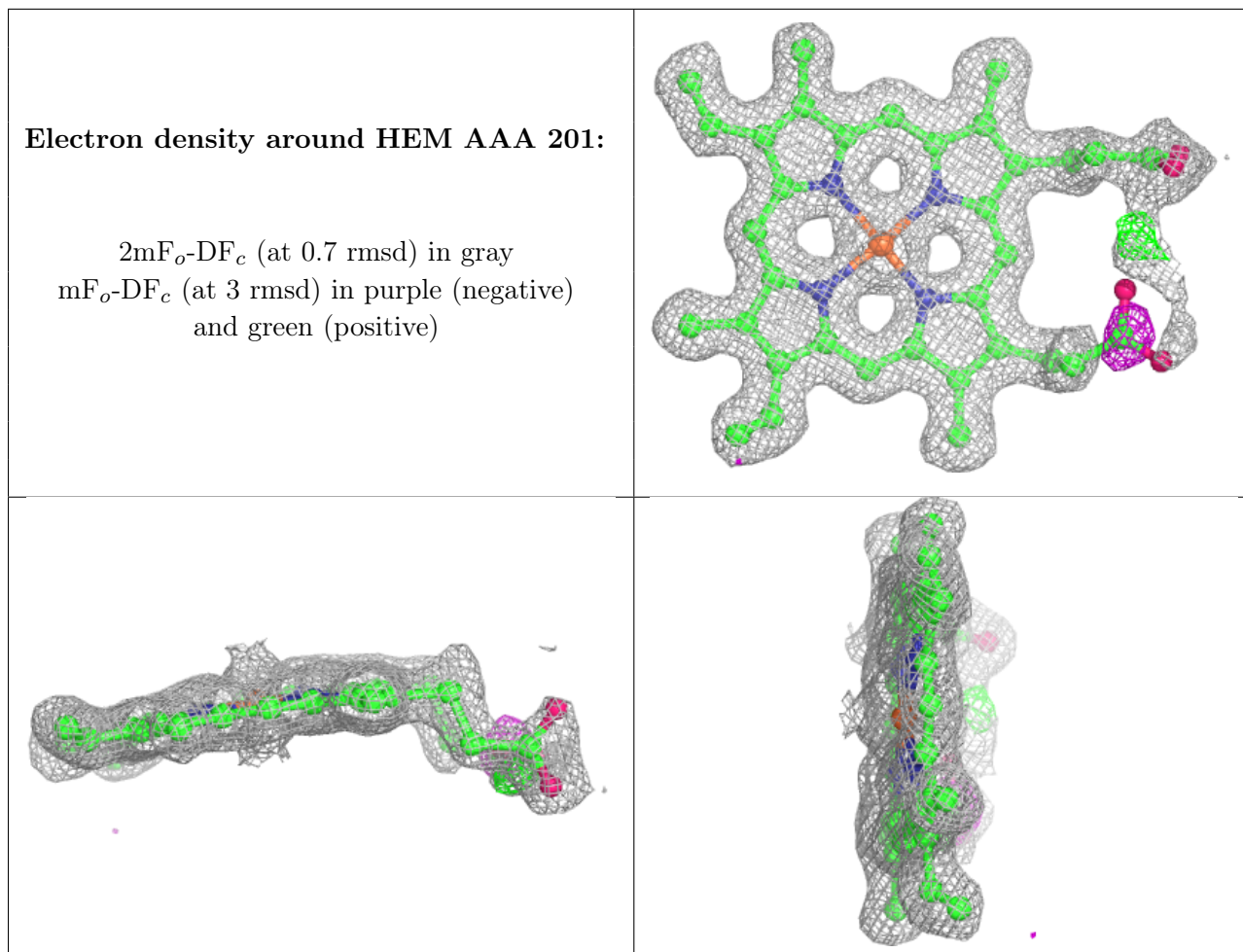
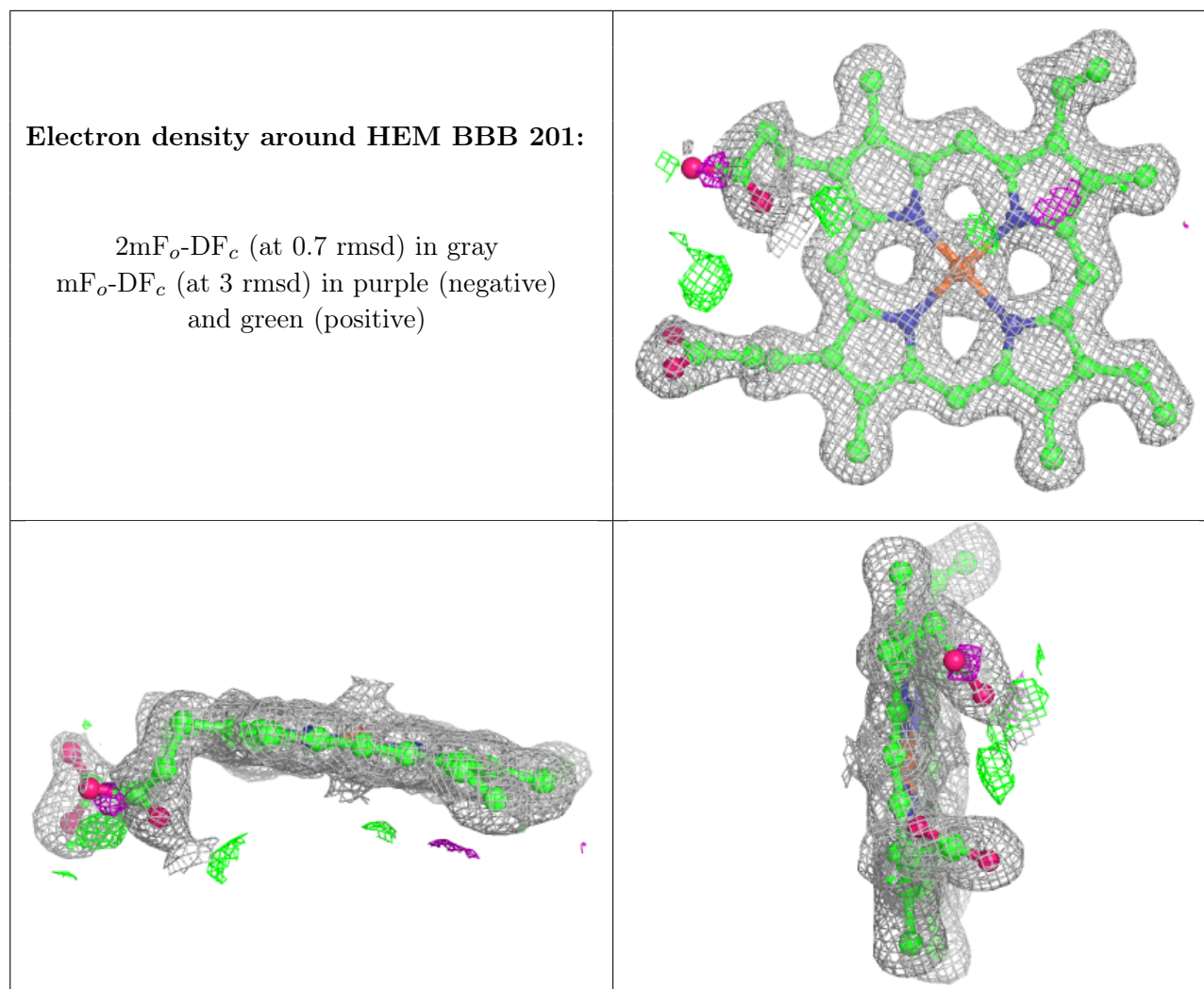There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OXY	AAA	202	2/2	0.83	0.13	20,20,20,23	0
4	GOL	AAA	203	6/6	0.83	0.19	28,36,37,47	0
7	PEG	BBB	203	7/7	0.86	0.19	30,38,60,62	0
7	PEG	BBB	204	7/7	0.88	0.17	17,31,44,48	0
6	Y8I	BBB	202	9/9	0.89	0.57	30,33,36,48	9
5	SO4	BBB	206	5/5	0.96	0.17	20,22,24,30	0
2	HEM	AAA	201	43/43	0.96	0.11	13,17,40,61	0
2	HEM	BBB	201	43/43	0.98	0.09	10,13,26,50	3
5	SO4	AAA	204	5/5	0.99	0.04	12,12,15,16	0
5	SO4	BBB	205	5/5	0.99	0.04	14,15,17,17	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 Y8I BBB 202:

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

Electron density around HEM AAA 201:

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

Electron density around HEM BBB 201:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.