W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 13, 2023 – 10:23 AM JST

PDB ID	:	5WV3
Title	:	Crystal structure of bovine lactoperoxidase with a partial Glu258-heme linkage at 2.07 A resolution.
Authors	:	Singh, P.K.; Sirohi, H.V.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2016-12-21
Resolution	:	2.07 Å(reported)

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

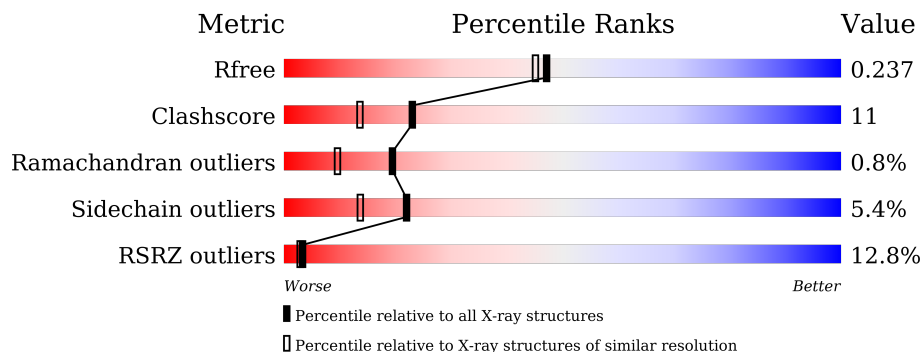|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
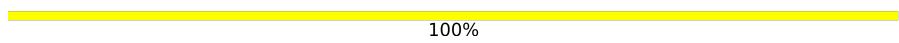*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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		0.237
Clashscore		11
Ramachandran outliers		0.8%
Sidechain outliers		5.4%
RSRZ outliers		12.8%

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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	A	595	13% / 78% / 19% / ··
2	B	2	100%

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:

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wwPDB
PROTEIN DATA BANK

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	A	198	-	X	X	-
7	OSM	A	609	-	-	X	-
7	OSM	A	611	-	-	X	-
7	OSM	A	613	-	-	X	-
7	OSM	A	614	-	-	X	-
7	OSM	A	617	-	-	X	-
7	OSM	A	622	-	-	X	-
8	GOL	A	623	-	-	X	-

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 5214 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 Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total 4775	C 3035	N 848	O 864	P 1	S 27	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	SER	PHE	conflict	UNP P80025
A	410	LYS	ASP	conflict	UNP P80025
A	547	MET	VAL	conflict	UNP P80025

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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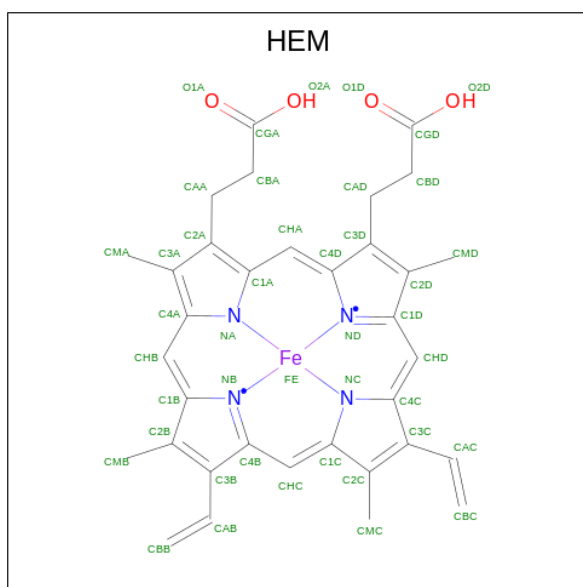
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
4	A	1	43	34	1	4	4	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG
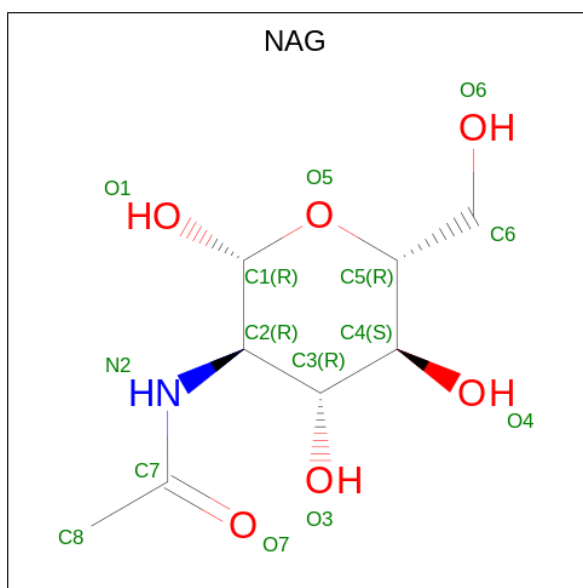
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	A	1	14	8	1	5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	I 3	0	0

- Molecule 7 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH_5NOS).

OSM

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 4	C 1	N 1	O 1	S 1	0	0
7	A	1	Total 4	C 1	N 1	O 1	S 1	0	0
7	A	1	Total 4	C 1	N 1	O 1	S 1	0	0
7	A	1	Total 4	C 1	N 1	O 1	S 1	0	0
7	A	1	Total 4	C 1	N 1	O 1	S 1	0	0
7	A	1	Total 4	C 1	N 1	O 1	S 1	0	0
7	A	1	Total 4	C 1	N 1	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 4	C 1	N 1	O 1	S 1	0	0
7	A	1	Total 4	C 1	N 1	O 1	S 1	0	0
7	A	1	Total 4	C 1	N 1	O 1	S 1	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
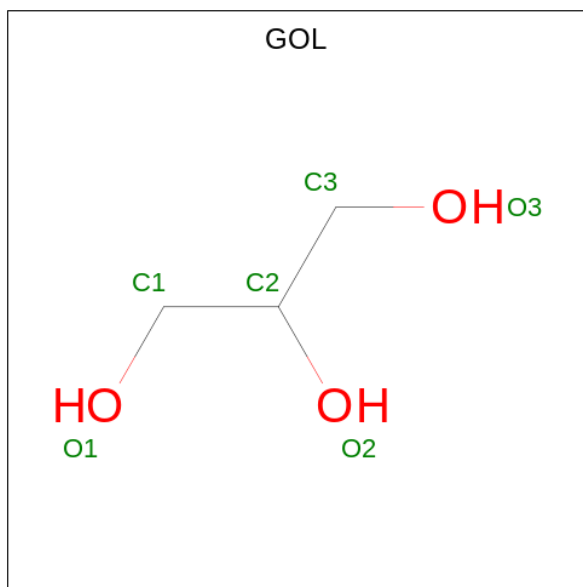
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 6	C 3	O 3	0	0
8	A	1	Total 6	C 3	O 3	0	0

- Molecule 9 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total 1	Br 1	0	0

- Molecule 10 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	269	Total 269	O 269	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: Lactoperoxidase

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
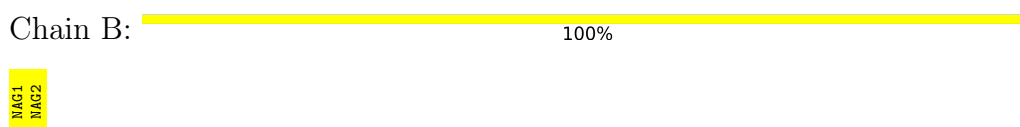
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.01Å 79.81Å 66.11Å 90.00° 93.01° 90.00°	Depositor
Resolution (Å)	34.17 – 2.07 34.15 – 2.07	Depositor EDS
% Data completeness (in resolution range)	94.4 (34.17-2.07) 94.5 (34.15-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.167 , 0.236 0.178 , 0.237	Depositor DCC
R_{free} test set	1001 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 61.3	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5214	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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 $< \lvert L \rvert >$, $< L^2 >$ 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: SEP, NAG, BR, OSM, HEM, IOD, GOL, CA

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	1.00	4/4896 (0.1%)	1.04	15/6638 (0.2%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	GLU	CD-OE2	7.28	1.33	1.25
1	A	503	GLU	CD-OE1	-6.96	1.18	1.25
1	A	503	GLU	CD-OE2	-5.99	1.19	1.25
1	A	46	TRP	CG-CD1	5.27	1.44	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ASP	CB-CG-OD2	-8.85	110.33	118.30
1	A	418	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	108	ASP	CB-CG-OD1	6.87	124.48	118.30
1	A	255	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	551	ARG	NE-CZ-NH1	6.19	123.39	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	THR	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	A	4775	0	4693	108	0
2	B	28	0	25	0	0
3	A	1	0	0	0	0
4	A	43	0	30	11	0
5	A	42	0	39	4	0
6	A	3	0	0	0	0
7	A	40	0	48	22	0
8	A	12	0	16	5	0
9	A	1	0	0	0	0
10	A	269	0	0	5	0
All	All	5214	0	4851	112	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 11.

The worst 5 of 112 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:108:ASP:OD2	4:A:602:HEM:CMD	1.78	1.28
1:A:258[A]:GLU:OE2	4:A:602:HEM:CMB	1.83	1.27
1:A:258[A]:GLU:OE2	4:A:602:HEM:HMB1	0.96	1.12
1:A:108:ASP:OD2	4:A:602:HEM:HMD1	0.84	1.01
1:A:335:VAL:HG22	5:A:607:NAG:C8	1.92	0.98

There are no symmetry-related clashes.

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	A	593/595 (100%)	557 (94%)	31 (5%)	5 (1%)	19	9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PRO
1	A	167	CYS
1	A	168	PRO
1	A	174	SER
1	A	56	ALA

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	A	518/517 (100%)	490 (95%)	28 (5%)	22	14

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	594	GLU
1	A	218	GLU
1	A	551	ARG
1	A	212	LEU

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	63	GLN
1	A	138	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#|Z| > 2$
1	SEP	A	198	1	8,9,10	1.70	2 (25%)	8,12,14	4.54	5 (62%)

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
1	SEP	A	198	1	-	5/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-OG	3.38	1.71	1.60
1	A	198	SEP	P-O2P	-2.22	1.46	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	SEP	OG-CB-CA	11.15	118.99	108.14
1	A	198	SEP	P-OG-CB	3.81	128.78	118.30
1	A	198	SEP	OG-P-O1P	-3.19	97.54	106.47
1	A	198	SEP	O2P-P-OG	2.33	112.92	106.73
1	A	198	SEP	O3P-P-OG	-2.24	100.77	106.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	N-CA-CB-OG
1	A	198	SEP	CA-CB-OG-P
1	A	198	SEP	CB-OG-P-O2P
1	A	198	SEP	CB-OG-P-O3P
1	A	198	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	4	0

5.5 Carbohydrates (i)

2 monosaccharides 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	NAG	B	1	1,2	14,14,15	0.54	0	17,19,21	2.58	3 (17%)
2	NAG	B	2	2	14,14,15	0.71	0	17,19,21	2.70	9 (52%)

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	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	O5-C1-C2	-8.62	97.68	111.29
2	B	2	NAG	C1-C2-N2	-5.13	101.73	110.49
2	B	2	NAG	C3-C4-C5	4.02	117.41	110.24
2	B	2	NAG	C1-O5-C5	4.01	117.63	112.19
2	B	1	NAG	C1-C2-N2	3.82	117.01	110.49

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C4-C5-C6-O6

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 oligosaccharide.

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings
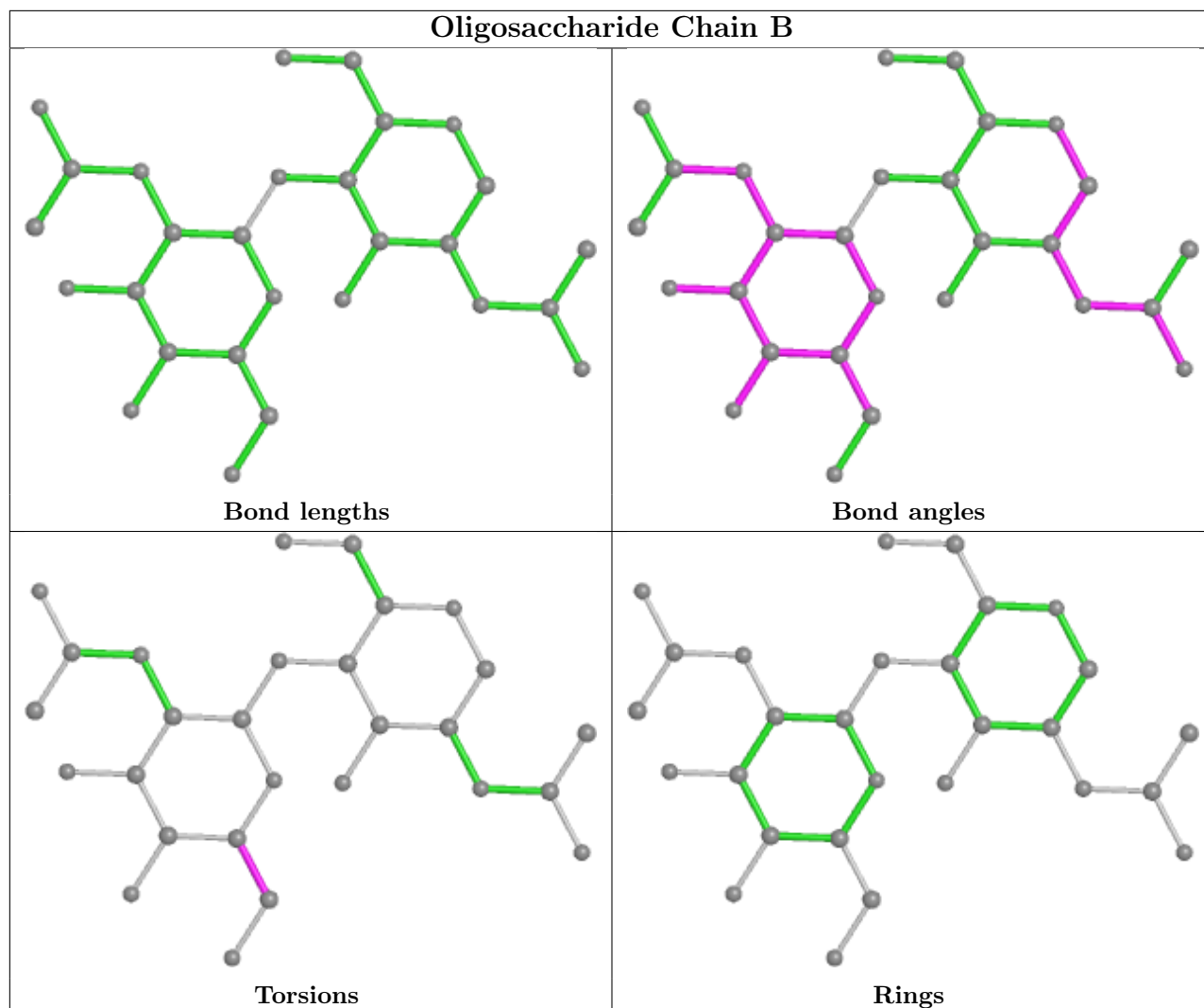
5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 5 are monoatomic - leaving 16 for Mogul analysis.

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	#$|Z| > 2$
5	NAG	A	606	1	14,14,15	1.29	1 (7%)	17,19,21	1.97	5 (29%)
7	OSM	A	622	-	1,3,3	0.06	0	0,2,2	-	-
7	OSM	A	610	-	1,3,3	0.11	0	0,2,2	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
7	OSM	A	615	-	1,3,3	0.01	0	0,2,2	-	-
7	OSM	A	616	-	1,3,3	0.18	0	0,2,2	-	-
4	HEM	A	602	10,1	41,50,50	1.65	10 (24%)	45,82,82	1.85	10 (22%)
7	OSM	A	609	-	1,3,3	0.01	0	0,2,2	-	-
7	OSM	A	611	-	1,3,3	0.06	0	0,2,2	-	-
7	OSM	A	613	-	1,3,3	0.03	0	0,2,2	-	-
5	NAG	A	607	1	14,14,15	0.27	0	17,19,21	0.59	0
8	GOL	A	618	-	5,5,5	0.45	0	5,5,5	0.49	0
7	OSM	A	617	-	1,3,3	0.11	0	0,2,2	-	-
8	GOL	A	623	-	5,5,5	0.81	0	5,5,5	1.14	0
7	OSM	A	612	-	1,3,3	0.16	0	0,2,2	-	-
5	NAG	A	603	1	14,14,15	0.47	0	17,19,21	2.02	5 (29%)
7	OSM	A	614	-	1,3,3	0.25	0	0,2,2	-	-

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
5	NAG	A	606	1	-	0/6/23/26	0/1/1/1
7	OSM	A	622	-	-	0/0/1/1	-
7	OSM	A	610	-	-	0/0/1/1	-
7	OSM	A	615	-	-	0/0/1/1	-
7	OSM	A	616	-	-	0/0/1/1	-
4	HEM	A	602	10,1	-	4/12/54/54	-
7	OSM	A	609	-	-	0/0/1/1	-
7	OSM	A	611	-	-	0/0/1/1	-
7	OSM	A	613	-	-	0/0/1/1	-
5	NAG	A	607	1	-	3/6/23/26	0/1/1/1
8	GOL	A	618	-	-	2/4/4/4	-
7	OSM	A	617	-	-	0/0/1/1	-
8	GOL	A	623	-	-	4/4/4/4	-
7	OSM	A	612	-	-	0/0/1/1	-
5	NAG	A	603	1	-	2/6/23/26	0/1/1/1
7	OSM	A	614	-	-	0/0/1/1	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	HEM	C3D-C2D	-3.76	1.28	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	HEM	FE-NB	3.44	2.13	1.96
4	A	602	HEM	C4D-C3D	2.94	1.50	1.45
4	A	602	HEM	CBD-CGD	2.92	1.57	1.50
4	A	602	HEM	C4D-ND	-2.87	1.35	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	602	HEM	CBA-CAA-C2A	-5.95	102.47	112.62
5	A	606	NAG	C4-C3-C2	4.48	117.59	111.02
4	A	602	HEM	CMD-C2D-C1D	4.19	131.42	125.04
5	A	606	NAG	C2-N2-C7	4.18	128.85	122.90
5	A	603	NAG	C1-C2-N2	3.79	116.97	110.49

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	607	NAG	C8-C7-N2-C2
5	A	607	NAG	O7-C7-N2-C2
8	A	623	GOL	C1-C2-C3-O3
5	A	607	NAG	C1-C2-N2-C7
5	A	603	NAG	C4-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	622	OSM	2	0
7	A	616	OSM	1	0
4	A	602	HEM	11	0
7	A	609	OSM	2	0
7	A	611	OSM	2	0
7	A	613	OSM	3	0
5	A	607	NAG	4	0
8	A	618	GOL	1	0
7	A	617	OSM	7	0
8	A	623	GOL	4	0
7	A	612	OSM	1	0
7	A	614	OSM	4	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 A 602

Bond lengths

Bond angles

Torsions

Rings
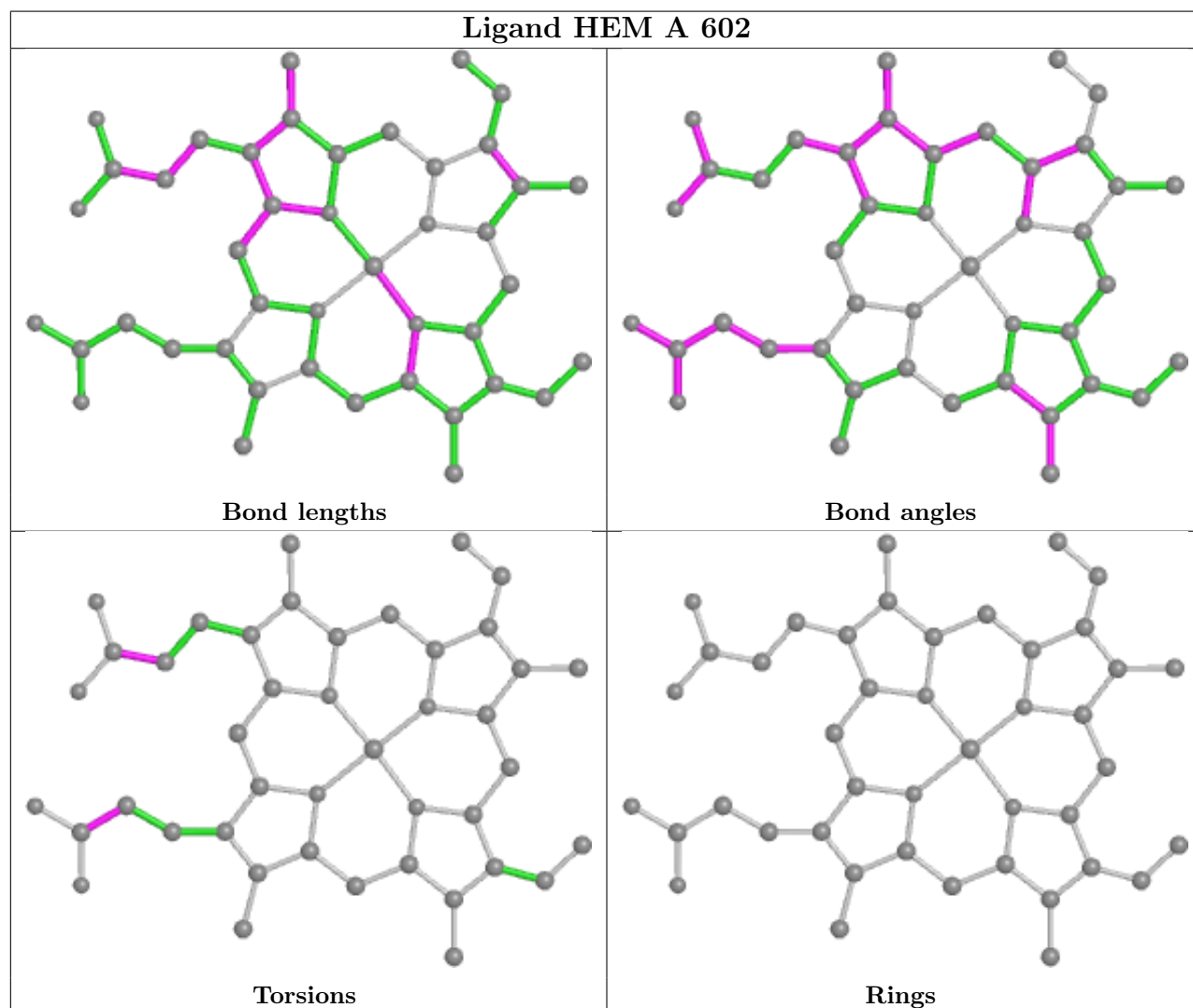
5.7 Other polymers ⓘ

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, 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(Å²)	Q<0.9
1	A	594/595 (99%)	0.66	76 (12%)	3	3	24, 50, 105, 157	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	173	GLN	14.8
1	A	172	TYR	13.3
1	A	121	SER	11.8
1	A	2	TRP	11.1
1	A	10	VAL	11.1

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

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(Å²)	Q<0.9
1	SEP	A	198	10/11	0.94	0.14	56,60,66,69	0

6.3 Carbohydrates ⓘ

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.
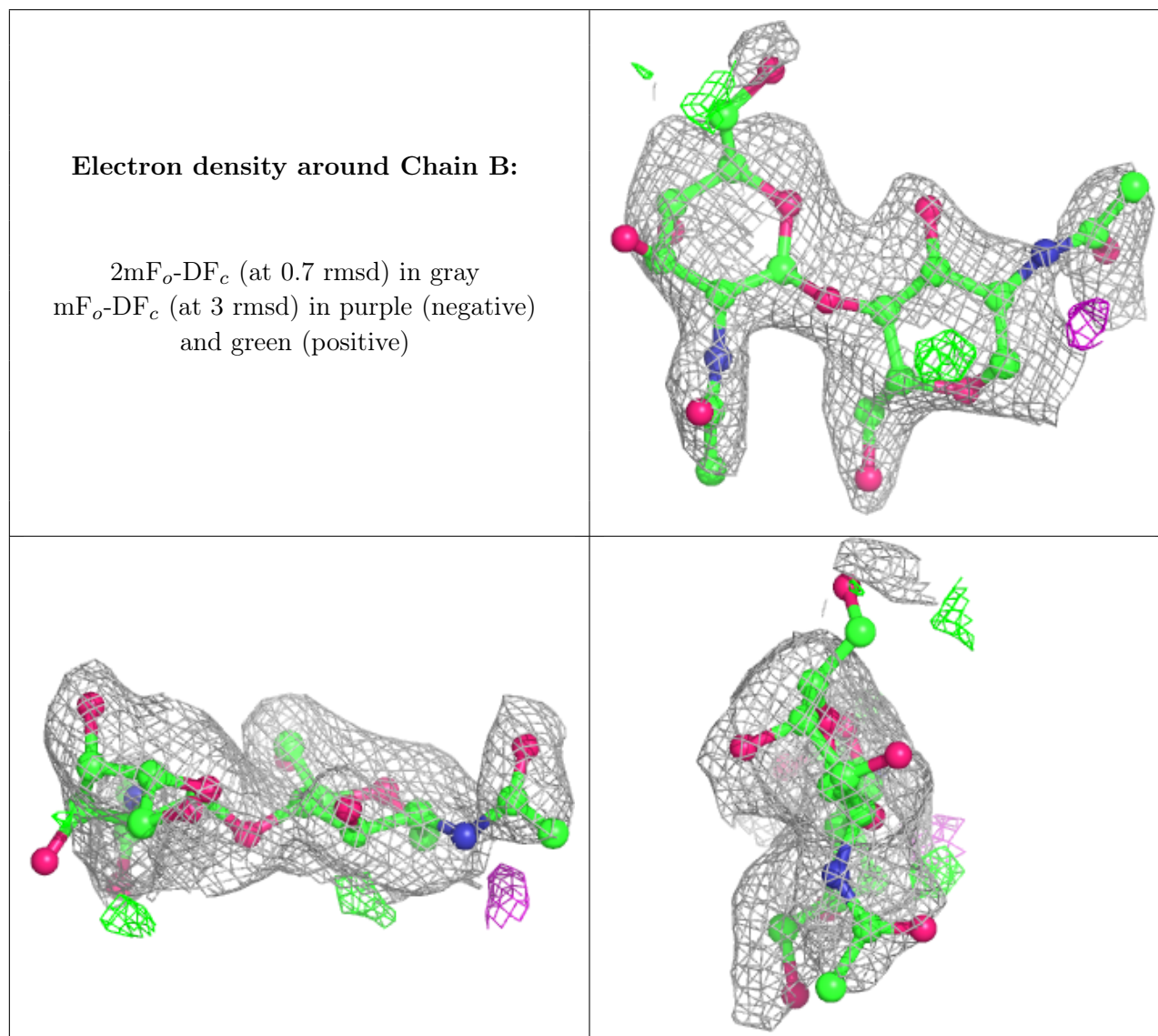
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	NAG	B	2	14/15	0.77	0.21	100,107,111,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	1	14/15	0.83	0.21	69,88,96,96	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.
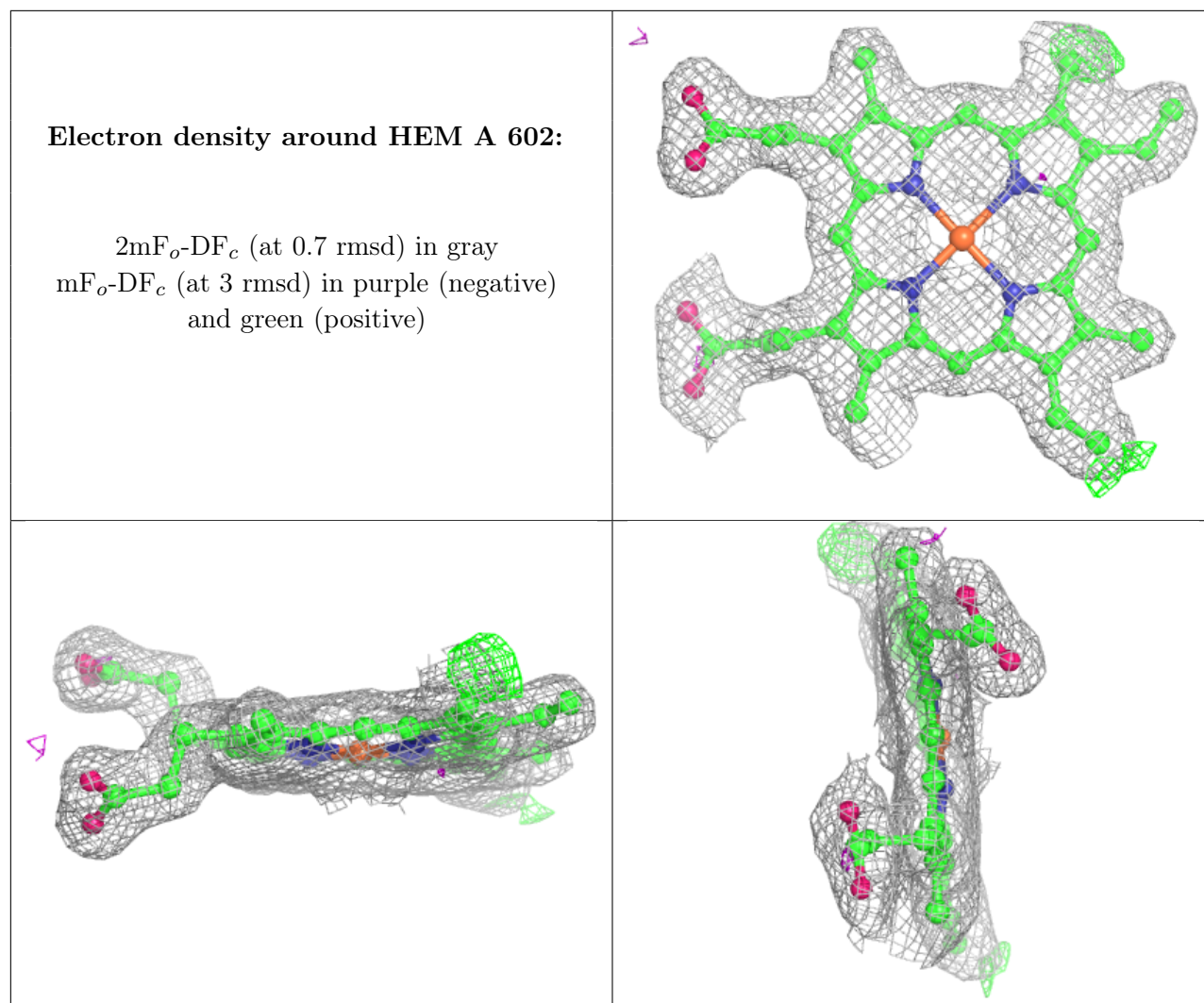

Electron density around Chain B:

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

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
7	OSM	A	614	4/4	0.69	0.27	39,39,42,43	0
5	NAG	A	606	14/15	0.77	0.18	62,67,75,76	0
5	NAG	A	607	14/15	0.81	0.27	64,70,76,80	0
5	NAG	A	603	14/15	0.85	0.31	71,76,80,80	0
8	GOL	A	623	6/6	0.90	0.13	32,36,38,41	0
6	IOD	A	619	1/1	0.95	0.06	71,71,71,71	1
8	GOL	A	618	6/6	0.95	0.12	58,59,63,63	0
7	OSM	A	610	4/4	0.95	0.15	46,47,52,53	0
7	OSM	A	611	4/4	0.96	0.13	59,60,60,68	0
7	OSM	A	615	4/4	0.96	0.11	45,48,48,52	0
7	OSM	A	617	4/4	0.97	0.07	74,75,76,77	0
4	HEM	A	602	43/43	0.97	0.20	23,26,32,33	0
7	OSM	A	616	4/4	0.97	0.15	42,44,46,47	0
9	BR	A	620	1/1	0.97	0.12	53,53,53,53	1
7	OSM	A	613	4/4	0.98	0.13	33,33,41,45	0
7	OSM	A	612	4/4	0.98	0.08	60,61,61,62	0
7	OSM	A	622	4/4	0.99	0.08	19,19,20,20	4
7	OSM	A	609	4/4	0.99	0.08	43,47,49,49	0
3	CA	A	601	1/1	0.99	0.10	34,34,34,34	0
6	IOD	A	621	1/1	0.99	0.04	42,42,42,42	1
6	IOD	A	608	1/1	1.00	0.09	31,31,31,31	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 HEM A 602:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.