



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 10:19 PM JST

PDB ID : 7DN7
Title : Crystal structure of ternary complexes of lactoperoxidase with hydrogen peroxide at 1.70 Å resolution
Authors : Singh, P.K.; Singh, A.K.; Singh, R.P.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2020-12-09
Resolution : 1.70 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 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

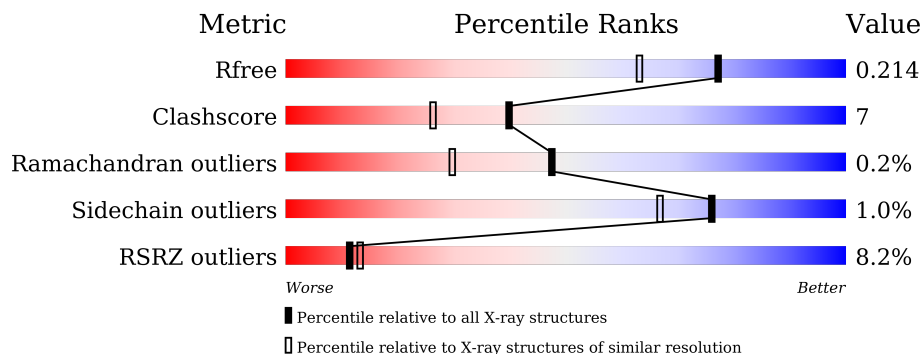
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

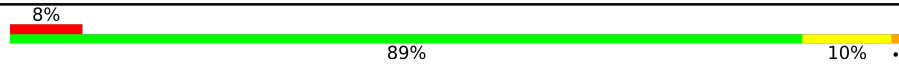
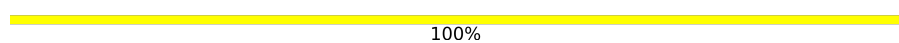
The reported resolution of this entry is 1.70 Å.

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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 $\leq 5\%$. 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	595	 8% 89% 10%
2	C	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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PEO	A	628	-	-	X	-
9	OSM	A	616	-	-	X	-
9	OSM	A	618	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5605 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.

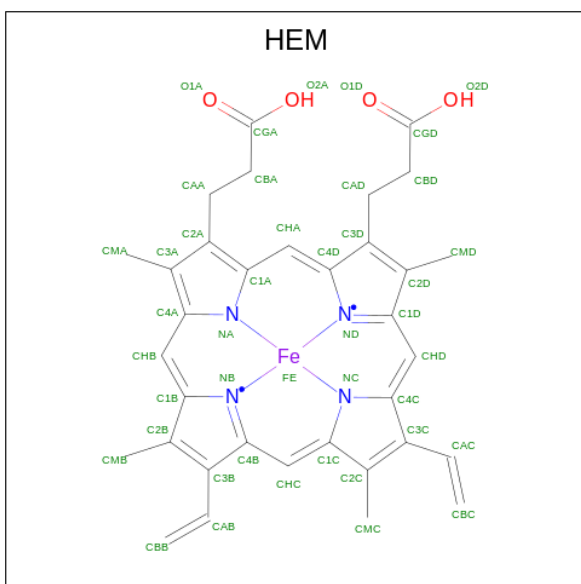
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	595	4808	3059	857	864	28	0	4	0

- 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
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

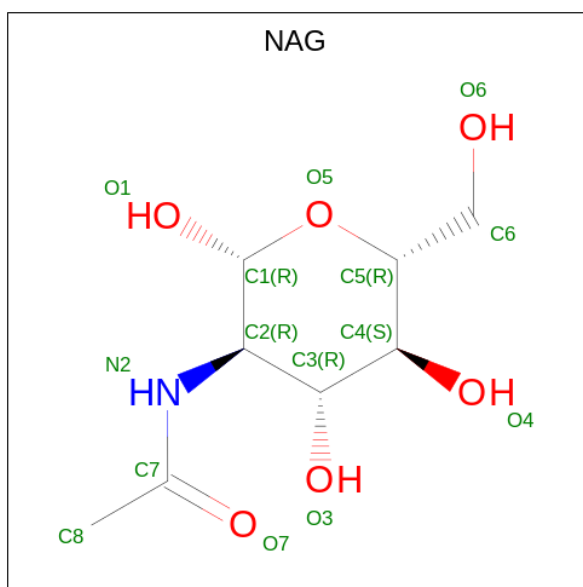


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
3	A	1	43	34	1	4	4	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
6	A	19	19	19	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

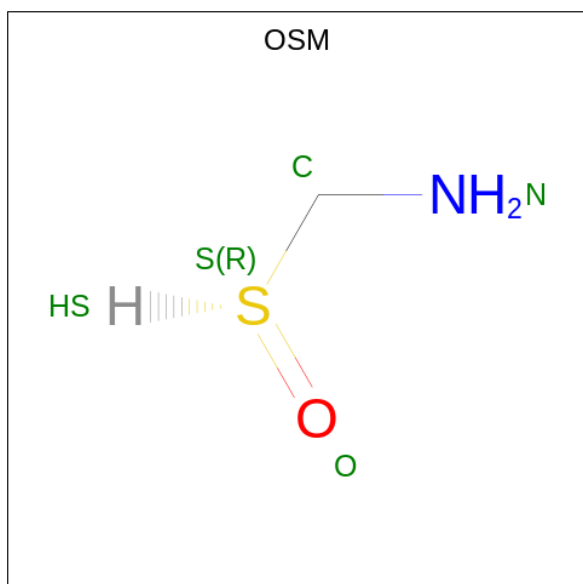


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

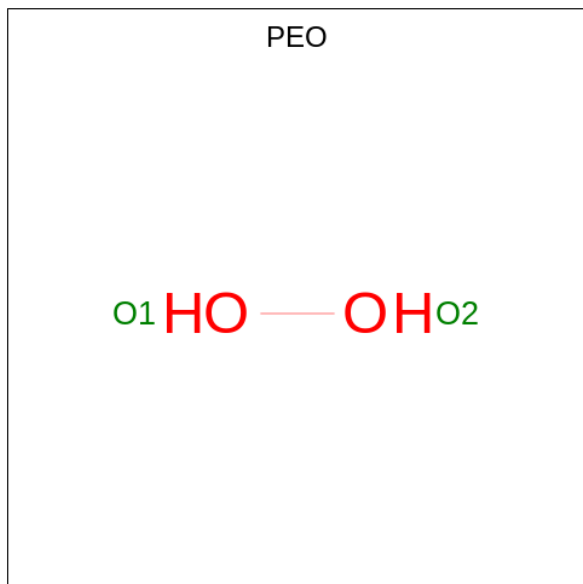
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Zn 1 1	0	0

- Molecule 9 is 1-(OXIDOSULFANYL)METHANAMINE (three-letter code: OSM) (formula: CH₅NOS).



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

- Molecule 10 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H₂O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	O	0	0
			2	2		

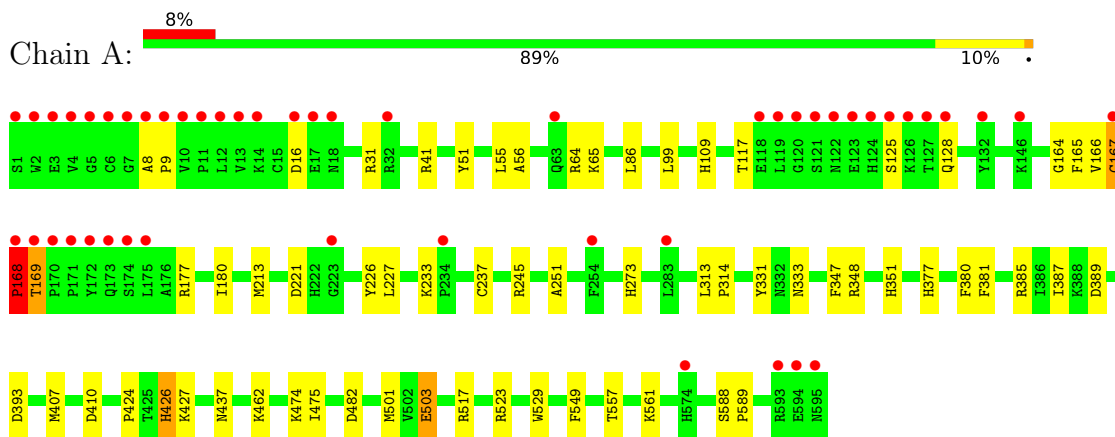
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	659	Total	O	0	0
			659	659		

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: Lactoperoxidase



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.92Å 79.50Å 77.72Å 90.00° 102.25° 90.00°	Depositor
Resolution (Å)	26.71 – 1.70 26.71 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (26.71-1.70) 95.0 (26.71-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.01 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.181 , 0.204 0.191 , 0.214	Depositor DCC
R_{free} test set	3384 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5605	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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: IOD, CA, ZN, EDO, HEM, PEO, NAG, OSM

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	0.74	0/4936	0.91	5/6693 (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	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	177	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	426	HIS	CB-CA-C	7.36	125.11	110.40
1	A	168	PRO	N-CA-CB	-5.54	96.51	102.60
1	A	348	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	56	ALA	N-CA-CB	-5.15	102.89	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	CYS	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	4808	0	4729	66	0
2	C	28	0	25	0	0
3	A	43	0	30	0	0
4	A	1	0	0	0	0
5	A	28	0	26	0	0
6	A	19	0	0	6	0
7	A	4	0	5	0	0
8	A	1	0	0	0	0
9	A	12	0	15	5	0
10	A	2	0	0	2	0
11	A	659	0	0	23	0
All	All	5605	0	4830	71	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.

All (71) 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:517[B]:ARG:HB3	1:A:517[B]:ARG:NH2	1.54	1.22
1:A:407[B]:MET:HG3	1:A:501:MET:HE3	1.30	1.10
1:A:517[B]:ARG:NH2	1:A:517[B]:ARG:CB	2.27	0.98
1:A:517[B]:ARG:CB	1:A:517[B]:ARG:HH21	1.78	0.96
6:A:622:IOD:I	11:A:1167:HOH:O	2.54	0.93
1:A:109:HIS:NE2	10:A:628:PEO:O1	2.04	0.89
1:A:517[B]:ARG:HB3	1:A:517[B]:ARG:CZ	2.06	0.85
1:A:407[B]:MET:HG3	1:A:501:MET:CE	2.05	0.84
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.22	0.84
1:A:517[B]:ARG:HH21	1:A:517[B]:ARG:CG	1.90	0.84
6:A:621:IOD:I	11:A:1339:HOH:O	2.70	0.79
6:A:619:IOD:I	10:A:628:PEO:O1	2.75	0.75
1:A:86:LEU:O	11:A:701:HOH:O	2.06	0.74
1:A:407[B]:MET:CG	1:A:501:MET:HE3	2.15	0.73
1:A:462:LYS:HD2	11:A:742:HOH:O	1.89	0.73
1:A:65:LYS:HD3	11:A:1135:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ASP:OD1	11:A:702:HOH:O	2.08	0.72
1:A:165:PHE:CZ	1:A:169:THR:O	2.43	0.71
1:A:517[A]:ARG:NE	11:A:703:HOH:O	2.16	0.70
1:A:503:GLU:HG3	11:A:1120:HOH:O	1.93	0.69
1:A:245:ARG:NH2	11:A:706:HOH:O	2.22	0.68
1:A:407[B]:MET:CG	1:A:501:MET:CE	2.70	0.67
1:A:407[A]:MET:HB3	1:A:501:MET:CE	2.23	0.67
9:A:616:OSM:H2	11:A:984:HOH:O	1.95	0.66
9:A:616:OSM:N	11:A:709:HOH:O	2.27	0.65
1:A:65:LYS:HE2	11:A:1135:HOH:O	1.98	0.63
1:A:333:ASN:HD22	9:A:618:OSM:HS	1.45	0.63
1:A:517[B]:ARG:HH21	1:A:517[B]:ARG:HG2	1.67	0.60
1:A:407[A]:MET:HB3	1:A:501:MET:HE2	1.83	0.60
1:A:125:SER:HA	1:A:128:GLN:HB3	1.84	0.59
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.38	0.59
1:A:65:LYS:CE	11:A:1135:HOH:O	2.51	0.58
1:A:333:ASN:ND2	9:A:618:OSM:HS	2.02	0.57
1:A:165:PHE:HZ	1:A:169:THR:O	1.85	0.57
1:A:51:TYR:CD2	1:A:55:LEU:O	2.62	0.53
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.44	0.52
1:A:517[B]:ARG:CB	1:A:517[B]:ARG:CZ	2.82	0.52
1:A:31:ARG:HD2	6:A:613:IOD:I	2.81	0.51
1:A:385:ARG:O	1:A:389:ASP:HB3	2.11	0.51
1:A:16:ASP:OD1	1:A:16:ASP:C	2.51	0.49
1:A:117:THR:HG22	1:A:164:GLY:HA2	1.94	0.49
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.95	0.49
1:A:424:PRO:C	1:A:426:HIS:H	2.15	0.49
1:A:166:VAL:HG12	1:A:180:ILE:HG12	1.95	0.48
1:A:407[B]:MET:C	1:A:407[B]:MET:SD	2.93	0.47
1:A:313:LEU:N	1:A:314:PRO:CD	2.78	0.46
1:A:99:LEU:HD21	1:A:549:PHE:CD1	2.51	0.45
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.52	0.45
1:A:588:SER:OG	1:A:589:PRO:HD3	2.18	0.44
1:A:407[B]:MET:CG	1:A:501:MET:HE2	2.45	0.44
1:A:482:ASP:OD2	11:A:705:HOH:O	2.21	0.43
1:A:588:SER:N	1:A:589:PRO:CD	2.82	0.43
1:A:387:ILE:HG21	6:A:610:IOD:I	2.89	0.43
1:A:407[B]:MET:HE3	1:A:407[B]:MET:HB2	1.83	0.43
1:A:65:LYS:NZ	11:A:745:HOH:O	2.50	0.42
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.53	0.42
1:A:427:LYS:HE2	11:A:747:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:GLU:HG3	1:A:503:GLU:H	1.55	0.42
1:A:233:LYS:CE	11:A:859:HOH:O	2.67	0.42
1:A:167:CYS:O	1:A:168:PRO:O	2.38	0.42
1:A:237:CYS:HA	1:A:381:PHE:O	2.19	0.42
1:A:393:ASP:OD1	1:A:557:THR:HB	2.20	0.41
1:A:227:LEU:CD2	1:A:251:ALA:HB2	2.49	0.41
1:A:331:TYR:HE2	9:A:618:OSM:HN1	1.68	0.41
1:A:561:LYS:HE2	6:A:625:IOD:I	2.91	0.41
1:A:427:LYS:HG2	11:A:1153:HOH:O	2.21	0.41
1:A:41:ARG:NH1	11:A:743:HOH:O	2.50	0.41
1:A:65:LYS:CD	11:A:1135:HOH:O	2.54	0.41
1:A:233:LYS:HE3	11:A:859:HOH:O	2.21	0.41
1:A:64:ARG:NH2	11:A:730:HOH:O	2.45	0.40
1:A:475:ILE:HG23	11:A:1103:HOH:O	2.21	0.40

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	597/595 (100%)	567 (95%)	29 (5%)	1 (0%)	47 30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	PRO

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	522/518 (101%)	517 (99%)	5 (1%)	76 67

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	PRO
1	A	169	THR
1	A	347	PHE
1	A	474	LYS
1	A	503	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	147	ASN
1	A	333	ASN

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](#)

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	C	1	1,2	14,14,15	1.02	2 (14%)	17,19,21	1.21	2 (11%)
2	NAG	C	2	2	14,14,15	0.74	0	17,19,21	2.70	3 (17%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	-2.21	1.40	1.43
2	C	1	NAG	O4-C4	2.17	1.48	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	8.60	123.84	112.19
2	C	2	NAG	C4-C3-C2	-4.43	104.53	111.02
2	C	2	NAG	O3-C3-C2	3.14	115.96	109.47
2	C	1	NAG	C6-C5-C4	2.73	119.41	113.00
2	C	1	NAG	O5-C5-C6	-2.45	103.37	107.20

There are no chirality outliers.

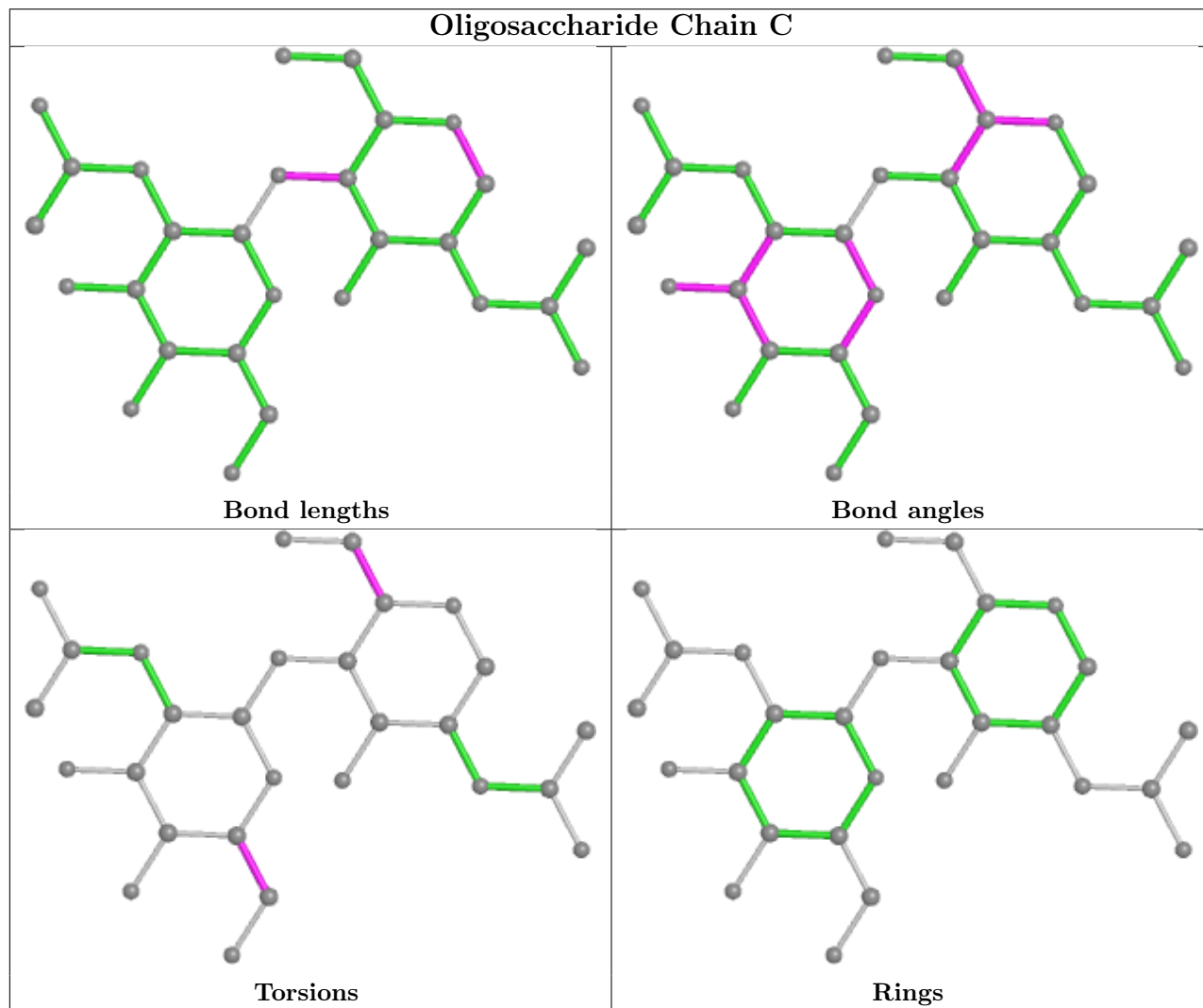
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-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.



5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 21 are monoatomic - leaving 8 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	629	1	14,14,15	0.74	0	17,19,21	1.62	4 (23%)
9	OSM	A	617	-	1,3,3	0.09	0	0,2,2	-	-
5	NAG	A	603	1	14,14,15	0.59	0	17,19,21	1.27	1 (5%)
9	OSM	A	616	-	1,3,3	0.01	0	0,2,2	-	-
3	HEM	A	601	1,10	41,50,50	1.68	10 (24%)	45,82,82	2.21	16 (35%)
9	OSM	A	618	6	1,3,3	0.04	0	0,2,2	-	-
7	EDO	A	614	-	3,3,3	0.71	0	2,2,2	0.39	0
10	PEO	A	628	3	1,1,1	0.68	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
5	NAG	A	629	1	-	2/6/23/26	0/1/1/1
9	OSM	A	617	-	-	0/0/1/1	-
5	NAG	A	603	1	-	0/6/23/26	0/1/1/1
9	OSM	A	616	-	-	0/0/1/1	-
3	HEM	A	601	1,10	-	4/12/54/54	-
9	OSM	A	618	6	-	0/0/1/1	-
7	EDO	A	614	-	-	1/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	HEM	C1B-NB	-4.96	1.31	1.40
3	A	601	HEM	CBD-CGD	3.06	1.57	1.50
3	A	601	HEM	O1D-CGD	2.99	1.32	1.22
3	A	601	HEM	C3C-C2C	-2.82	1.36	1.40
3	A	601	HEM	C4D-ND	-2.81	1.35	1.40
3	A	601	HEM	FE-NB	2.59	2.09	1.96
3	A	601	HEM	C2C-C1C	-2.54	1.36	1.42
3	A	601	HEM	CBD-CAD	2.39	1.59	1.52
3	A	601	HEM	C1A-CHA	-2.35	1.34	1.41
3	A	601	HEM	C4B-NB	-2.27	1.34	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	HEM	C1B-NB-C4B	6.35	111.63	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	HEM	CHC-C4B-NB	4.61	129.44	124.43
3	A	601	HEM	CMD-C2D-C1D	4.29	131.57	125.04
3	A	601	HEM	CHD-C1D-C2D	-4.17	118.47	124.98
3	A	601	HEM	CHB-C1B-NB	3.93	129.24	124.38
3	A	601	HEM	C2D-C1D-ND	3.64	114.25	109.88
3	A	601	HEM	C4A-C3A-C2A	3.47	109.41	107.00
3	A	601	HEM	C1D-C2D-C3D	-3.18	103.61	106.96
5	A	603	NAG	O5-C1-C2	-3.02	106.51	111.29
5	A	629	NAG	C1-C2-N2	2.87	115.39	110.49
3	A	601	HEM	C3D-C4D-ND	2.74	113.22	110.17
5	A	629	NAG	C1-O5-C5	-2.70	108.53	112.19
3	A	601	HEM	CHD-C1D-ND	2.58	127.23	124.43
5	A	629	NAG	C6-C5-C4	2.41	118.64	113.00
5	A	629	NAG	O3-C3-C2	-2.32	104.67	109.47
3	A	601	HEM	O2D-CGD-CBD	2.31	121.46	114.03
3	A	601	HEM	CMA-C3A-C4A	-2.30	124.93	128.46
3	A	601	HEM	C3C-C4C-NC	-2.28	106.63	110.94
3	A	601	HEM	CAD-C3D-C4D	2.19	128.49	124.66
3	A	601	HEM	C4D-ND-C1D	-2.12	102.89	105.07
3	A	601	HEM	O1D-CGD-CBD	-2.05	116.48	123.08

There are no chirality outliers.

All (7) torsion outliers are listed below:

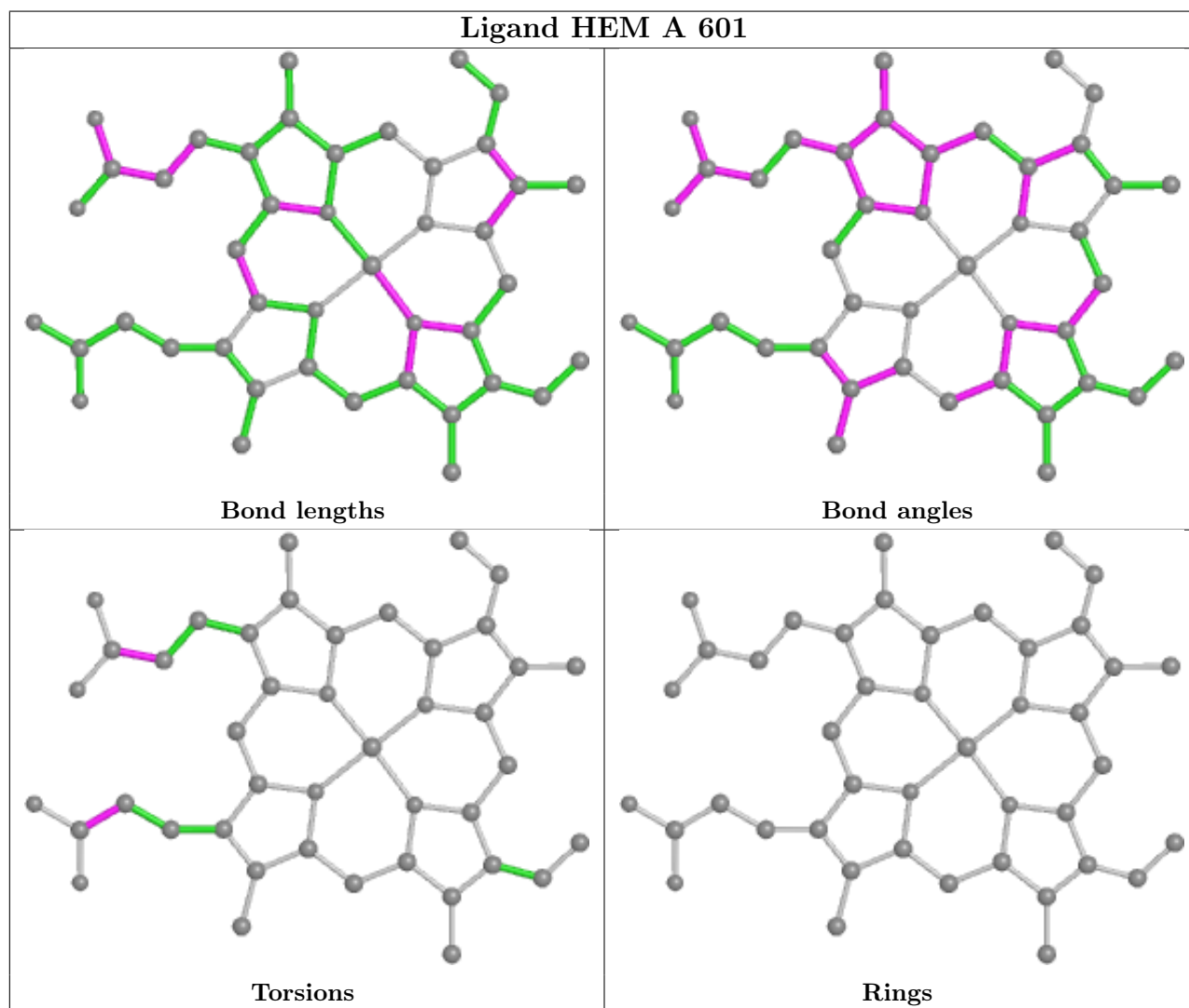
Mol	Chain	Res	Type	Atoms
5	A	629	NAG	C4-C5-C6-O6
7	A	614	EDO	O1-C1-C2-O2
5	A	629	NAG	O5-C5-C6-O6
3	A	601	HEM	CAA-CBA-CGA-O1A
3	A	601	HEM	CAD-CBD-CGD-O2D
3	A	601	HEM	CAA-CBA-CGA-O2A
3	A	601	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	616	OSM	2	0
9	A	618	OSM	3	0
10	A	628	PEO	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

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	A	595/595 (100%)	0.43	49 (8%) 11 13	11, 23, 92, 169	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	SER	31.7
1	A	172	TYR	21.6
1	A	1	SER	19.8
1	A	120	GLY	18.8
1	A	119	LEU	15.5
1	A	2	TRP	15.5
1	A	7	GLY	13.7
1	A	171	PRO	12.8
1	A	122	ASN	11.5
1	A	121	SER	11.5
1	A	595	ASN	10.8
1	A	10	VAL	10.4
1	A	13	VAL	10.3
1	A	173	GLN	10.0
1	A	8	ALA	9.6
1	A	12	LEU	8.7
1	A	125	SER	8.4
1	A	4	VAL	7.7
1	A	124	HIS	7.4
1	A	6	CYS	7.3
1	A	594	GLU	6.9
1	A	170	PRO	6.2
1	A	169	THR	6.1
1	A	168	PRO	6.0
1	A	11	PRO	5.9
1	A	593	ARG	5.7
1	A	14	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	5	GLY	5.2
1	A	118	GLU	4.6
1	A	126	LYS	4.6
1	A	9	PRO	4.0
1	A	175	LEU	3.9
1	A	123	GLU	3.8
1	A	283	LEU	3.7
1	A	132	TYR	3.5
1	A	254	PHE	3.2
1	A	127	THR	3.1
1	A	146	LYS	2.9
1	A	128	GLN	2.9
1	A	167	CYS	2.9
1	A	18	ASN	2.9
1	A	17	GLU	2.8
1	A	63	GLN	2.4
1	A	3	GLU	2.4
1	A	574	HIS	2.4
1	A	16	ASP	2.3
1	A	32	ARG	2.2
1	A	223	GLY	2.1
1	A	234	PRO	2.0

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

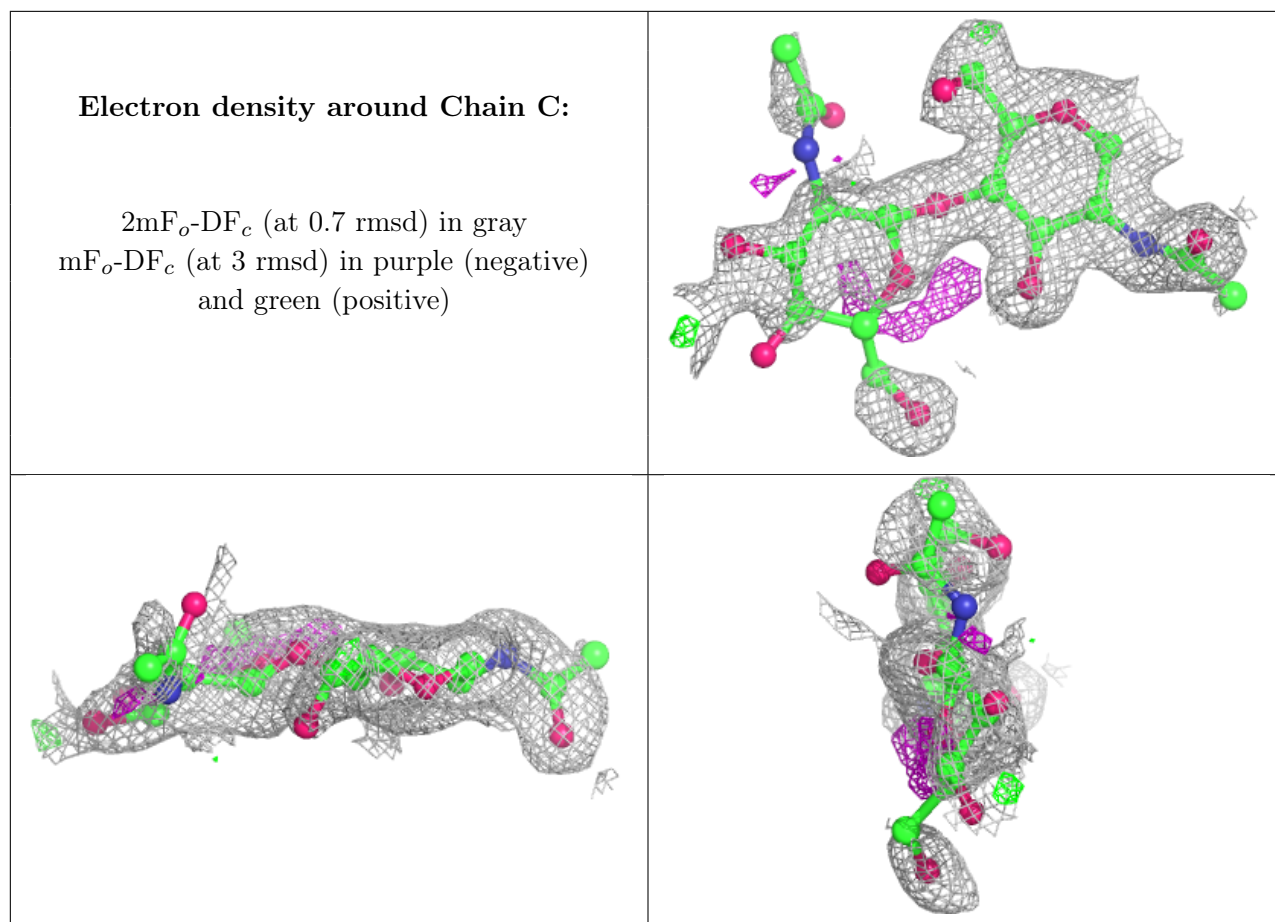
There are no non-standard protein/DNA/RNA residues in this entry.

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

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
2	NAG	C	2	14/15	0.77	0.30	52,64,78,83	0
2	NAG	C	1	14/15	0.95	0.09	24,30,38,47	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.



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, 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.

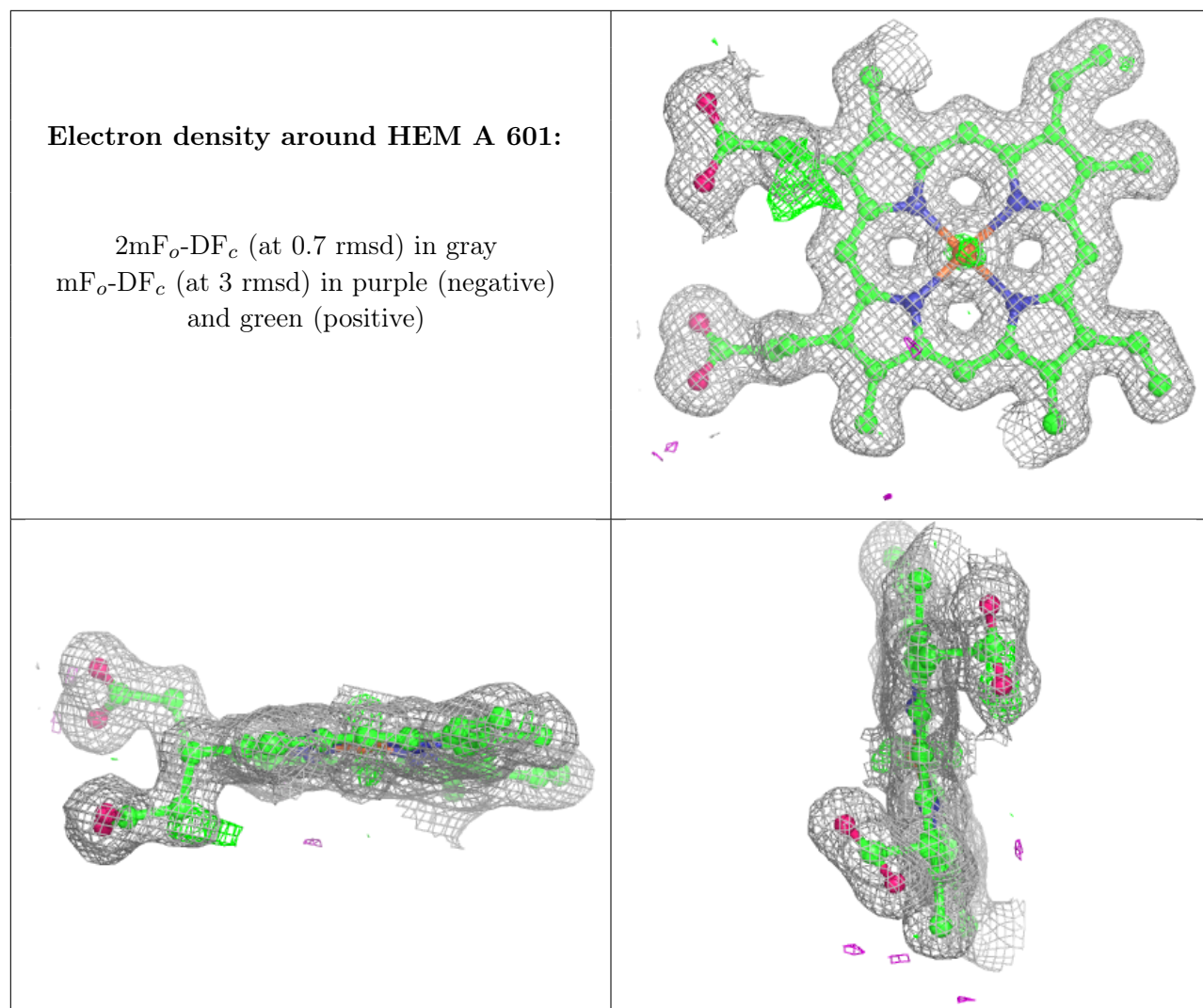
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	603	14/15	0.82	0.21	37,44,51,52	0
5	NAG	A	629	14/15	0.85	0.12	29,36,44,52	0
6	IOD	A	610	1/1	0.94	0.11	63,63,63,63	1
6	IOD	A	613	1/1	0.94	0.12	40,40,40,40	1
9	OSM	A	618	4/4	0.94	0.17	24,30,36,38	4
9	OSM	A	617	4/4	0.95	0.15	30,34,36,37	0
9	OSM	A	616	4/4	0.95	0.12	36,37,38,48	0
10	PEO	A	628	2/2	0.95	0.06	19,19,19,25	0
6	IOD	A	606	1/1	0.96	0.06	46,46,46,46	1
6	IOD	A	625	1/1	0.96	0.04	33,33,33,33	0
6	IOD	A	627	1/1	0.96	0.13	46,46,46,46	1
7	EDO	A	614	4/4	0.96	0.09	23,23,24,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	IOD	A	624	1/1	0.97	0.06	33,33,33,33	1
6	IOD	A	609	1/1	0.98	0.10	38,38,38,38	1
6	IOD	A	620	1/1	0.98	0.08	40,40,40,40	1
8	ZN	A	615	1/1	0.98	0.02	28,28,28,28	0
6	IOD	A	621	1/1	0.98	0.04	35,35,35,35	1
6	IOD	A	611	1/1	0.98	0.03	40,40,40,40	1
6	IOD	A	612	1/1	0.98	0.04	42,42,42,42	1
6	IOD	A	626	1/1	0.98	0.03	33,33,33,33	1
6	IOD	A	622	1/1	0.99	0.10	49,49,49,49	1
6	IOD	A	623	1/1	0.99	0.02	33,33,33,33	1
6	IOD	A	608	1/1	0.99	0.03	25,25,25,25	0
6	IOD	A	605	1/1	0.99	0.03	26,26,26,26	1
3	HEM	A	601	43/43	0.99	0.07	10,12,16,19	0
6	IOD	A	607	1/1	0.99	0.06	38,38,38,38	1
6	IOD	A	619	1/1	1.00	0.02	24,24,24,24	1
6	IOD	A	604	1/1	1.00	0.03	16,16,16,16	1
4	CA	A	602	1/1	1.00	0.03	14,14,14,14	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.