

Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 09:39 PM JST

PDB ID	:	7DLH
Title	:	Crystallization of Cationic Peroxidase from Proso Millet and Identification of
		Its Phosphatase Active Sites
Authors	:	Cui, x.d.; Wang, t.f.; Wang, k.
Deposited on		
Resolution	:	1.79 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 (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 (1)) were used in the production of this report:

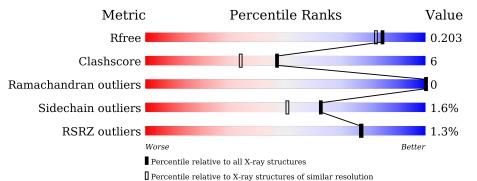
MolProbity Mogul Xtriage (Phenix) EDS	:	4.02b-467 1.8.5 (274361), CSD as541be (2020) 1.13 2.36
buster-report Percentile statistics Refmac	: : :	1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.79 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	А	337	.%	81%	8% 10%
2	В	2	50%		50%
3	С	3	33%	33%	33%



7DLH

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 2815 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 peroxidase.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	302	Total 2324	C 1447	N 431	O 436	S 10	0	4	0

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

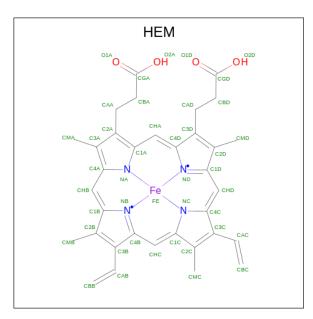
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	В	2	Total C N O 28 16 2 10	0	0	0

• Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(2-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf	Trace
3	С	3	Total 37	C 22	N 2	0 13	0	0	0

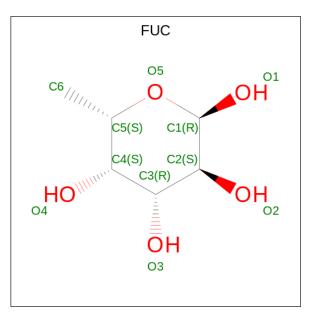
• Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
4	Δ	1	Total	С	Fe	Ν	0	0	0
4	Л	1	43	34	1	4	4	0	0

• Molecule 5 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	А	1	Total 10	С 6	0 4	0	0

• Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

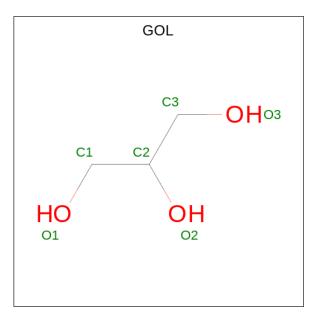


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0

• Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	Total Na 1 1	0	0

• Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	3	Total Cl 3 3	0	0

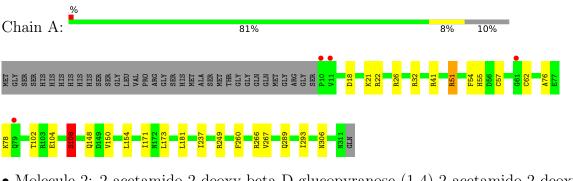
• Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	362	Total O 362 362	0	0



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: peroxidase

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

Chain B:	50%	50%
NAG2 NAG2		

• Molecule 3: alpha-D-mannopyranose-(2-3)-[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	C 2 2 21	Depositor
Cell constants	56.30Å 112.67Å 111.58Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.64 - 1.79	Depositor
Resolution (A)	39.64 - 1.79	EDS
% Data completeness	98.0 (39.64-1.79)	Depositor
(in resolution range)	98.0(39.64-1.79)	EDS
R _{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.82 (at 1.79 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
D D.	0.171 , 0.205	Depositor
R, R_{free}	0.173 , 0.203	DCC
R_{free} test set	2000 reflections (6.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	12.7	Xtriage
Anisotropy	0.708	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 42.5	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2815	wwPDB-VP
Average B, all atoms $(Å^2)$	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: HEM, GOL, NA, NAG, CA, FUC, MAN, CL

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	Bo	nd lengths	Bond angles	
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.55	1/2367~(0.0%)	0.58	0/3210

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	108	SER	C-O	-5.24	1.13	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2324	0	2317	28	0
2	В	28	0	25	4	0
3	С	37	0	30	1	0
4	А	43	0	30	2	0
5	А	10	0	10	1	0
6	А	1	0	0	0	0
7	А	1	0	0	0	0
8	А	6	0	8	0	0
9	А	3	0	0	0	0
10	А	362	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2815	0	2420	29	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 6.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:41:ARG:NH2	10:A:501:HOH:O	2.15	0.79
1:A:306:ASN:HD21	2:B:1:NAG:C1	2.05	0.69
1:A:78:LYS:NZ	10:A:503:HOH:O	2.25	0.69
1:A:32[B]:ARG:NH2	10:A:505:HOH:O	2.30	0.63
1:A:26:ARG:NH1	1:A:104:GLU:OE2	2.33	0.61
1:A:171:ILE:HD13	1:A:293:ILE:CD1	2.31	0.60
1:A:306:ASN:HD21	2:B:1:NAG:C2	2.16	0.58
1:A:267:VAL:HG13	10:A:507:HOH:O	2.03	0.58
1:A:267:VAL:HG22	10:A:692:HOH:O	2.05	0.56
1:A:237:ILE:HG12	10:A:764:HOH:O	2.07	0.54
1:A:76:ALA:O	1:A:78:LYS:HE2	2.09	0.53
1:A:108:SER:OG	1:A:108:SER:O	2.27	0.51
1:A:289:GLN:NE2	10:A:509:HOH:O	2.40	0.51
1:A:55:HIS:CE1	1:A:154:LEU:HD11	2.46	0.51
1:A:51:ARG:HB2	4:A:401:HEM:C2D	2.48	0.48
1:A:18:ASP:HB2	1:A:21:LYS:HE2	1.94	0.47
1:A:306:ASN:ND2	2:B:1:NAG:C1	2.76	0.47
1:A:57:CYS:CB	1:A:62:CYS:SG	3.03	0.47
1:A:306:ASN:ND2	10:A:515:HOH:O	2.47	0.47
1:A:171:ILE:HD12	1:A:173:LEU:HG	1.98	0.46
1:A:260:PHE:O	1:A:266:ARG:NE	2.50	0.45
1:A:102:THR:HG21	10:A:739:HOH:O	2.16	0.45
1:A:150:VAL:HG13	1:A:154:LEU:HD12	1.99	0.44
1:A:78:LYS:HA	1:A:78:LYS:HD3	1.87	0.44
1:A:249:ARG:HH11	3:C:1:NAG:H81	1.83	0.44
5:A:402:FUC:O5	2:B:1:NAG:H3	2.18	0.43
1:A:181:LEU:HB3	4:A:401:HEM:HMC3	2.01	0.43
1:A:22:ARG:HA	1:A:22:ARG:HD2	1.78	0.42
1:A:32[B]:ARG:NH1	10:A:521:HOH:O	2.50	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	А	304/337~(90%)	301 (99%)	3 (1%)	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	А	255/278~(92%)	251~(98%)	4 (2%)	62 51

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	51	ARG
1	А	54	PHE
1	А	108	SER
1	А	148	GLN

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

Mol	Chain	Res	Type	
1	А	306	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)

5 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	Dog	Res Link Bond lengths				Bond angles		
10101	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	В	1	2	14,14,15	1.77	2 (14%)	17,19,21	1.29	2 (11%)
2	NAG	В	2	2	14,14,15	1.21	1 (7%)	17,19,21	2.15	3 (17%)
3	NAG	С	1	1,3	14,14,15	0.20	0	17,19,21	0.71	1 (5%)
3	MAN	С	2	3	10,10,12	0.63	0	13,13,17	1.92	2 (15%)
3	NAG	С	3	3	13,13,15	0.42	0	14,17,21	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	В	1	2	-	0/6/23/26	0/1/1/1
2	NAG	В	2	2	-	0/6/23/26	0/1/1/1
3	NAG	С	1	1,3	-	2/6/23/26	0/1/1/1
3	MAN	С	2	3	-	2/2/16/22	0/1/1/1
3	NAG	С	3	3	-	0/6/19/26	0/1/1/1

All (3) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	В	1	NAG	O5-C1	-5.95	1.34	1.43
2	В	2	NAG	C2-N2	-3.21	1.40	1.46
2	В	1	NAG	C1-C2	-2.74	1.48	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	2	NAG	C1-O5-C5	6.58	121.11	112.19
3	С	2	MAN	C3-C4-C5	-5.59	104.40	109.97
2	В	2	NAG	C6-C5-C4	-3.52	104.75	113.00
2	В	1	NAG	C3-C4-C5	3.36	116.23	110.24
2	В	1	NAG	C1-O5-C5	-2.81	108.38	112.19
2	В	2	NAG	O5-C1-C2	-2.61	107.17	111.29
3	С	1	NAG	C1-O5-C5	2.26	115.25	112.19
3	С	2	MAN	C2-C3-C4	-2.15	108.69	111.16

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	2	MAN	O5-C5-C6-O6
3	С	1	NAG	C8-C7-N2-C2
3	С	1	NAG	O7-C7-N2-C2
3	С	2	MAN	C4-C5-C6-O6

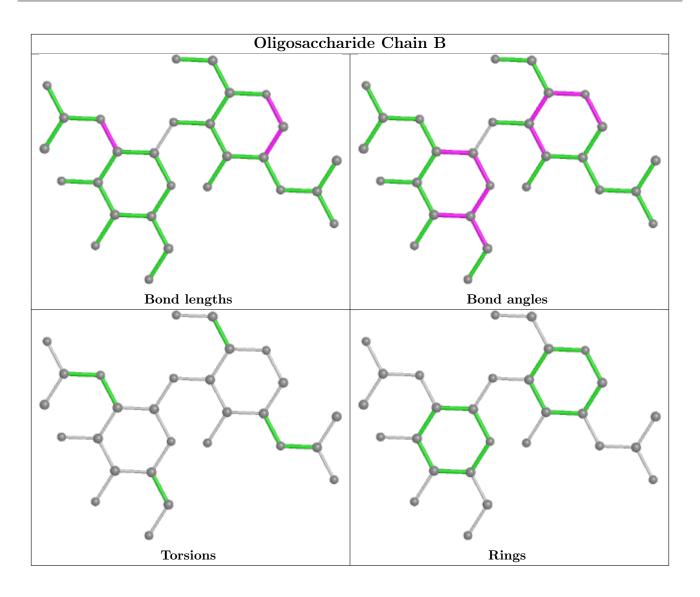
There are no ring outliers.

2 monomers are involved in 5 short contacts:

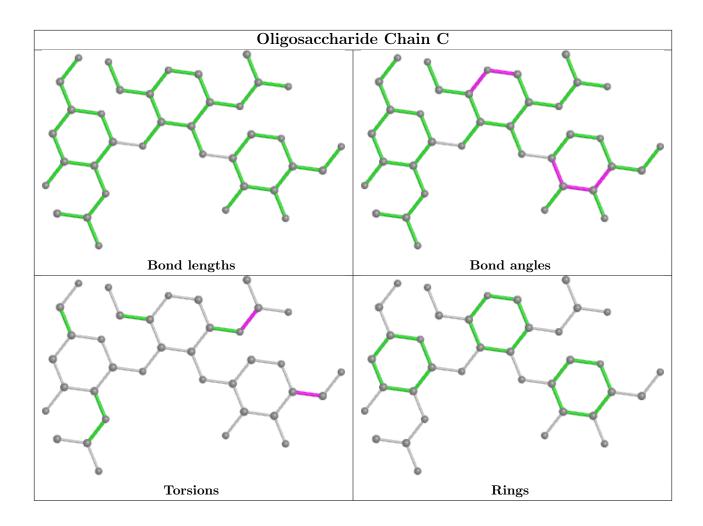
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1	NAG	4	0
3	С	1	NAG	1	0

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 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	Turne	Chain	Dec	Link Bond lengths				Bond angles		
IVIOI	Type	Unam	Res	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	FUC	А	402	-	10,10,11	1.01	0	14,14,16	1.58	4 (28%)
4	HEM	А	401	10,1	41,50,50	1.48	5 (12%)	45,82,82	1.25	6 (13%)
8	GOL	А	405	-	$5,\!5,\!5$	0.78	0	$5,\!5,\!5$	1.05	1 (20%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUC	А	402	-	-	-	0/1/1/1
4	HEM	А	401	10,1	-	4/12/54/54	-
8	GOL	А	405	-	-	2/4/4/4	-

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	401	HEM	C3C-C2C	-4.02	1.34	1.40
4	А	401	HEM	C3C-CAC	3.51	1.55	1.47
4	А	401	HEM	CAB-C3B	2.29	1.53	1.47
4	А	401	HEM	CAA-C2A	2.21	1.55	1.52
4	А	401	HEM	CMB-C2B	2.20	1.55	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
5	А	402	FUC	C1-O5-C5	3.01	119.59	112.78
5	А	402	FUC	C1-C2-C3	2.97	113.31	109.67
5	А	402	FUC	O5-C1-C2	2.71	114.95	110.77
4	А	401	HEM	CAA-CBA-CGA	-2.51	106.72	113.76
4	А	401	HEM	C4B-CHC-C1C	2.34	125.65	122.56
4	А	401	HEM	CMC-C2C-C3C	2.22	128.84	124.68
5	А	402	FUC	O5-C5-C4	2.22	113.51	109.52
4	А	401	HEM	CMA-C3A-C4A	-2.19	125.09	128.46
4	А	401	HEM	C4B-C3B-C2B	2.15	108.82	107.11
4	А	401	HEM	C1B-NB-C4B	2.10	107.25	105.07
8	А	405	GOL	C3-C2-C1	-2.02	103.84	111.70

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	А	405	GOL	O1-C1-C2-C3
8	А	405	GOL	O1-C1-C2-O2
4	А	401	HEM	C2B-C3B-CAB-CBB
4	А	401	HEM	C4B-C3B-CAB-CBB
4	А	401	HEM	CAA-CBA-CGA-O1A
4	А	401	HEM	CAA-CBA-CGA-O2A

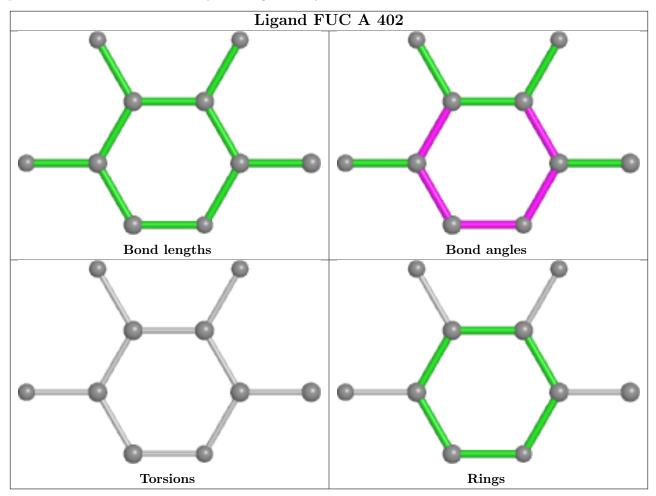


There are no ring outliers.

2 monomers are involved in 3 short contacts:

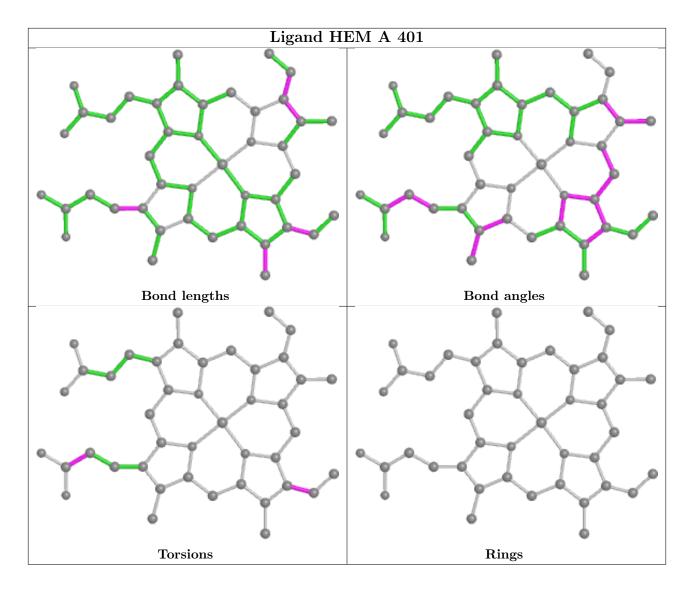
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	402	FUC	1	0
4	А	401	HEM	2	0

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.









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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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> #RSRZ>2		$OWAB(Å^2)$	Q<0.9	
1	А	302/337~(89%)	-0.09	4 (1%)	77	77	7, 13, 26, 42	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res		RSRZ
1	А	10	PRO	5.0
1	А	61	GLY	2.9
1	А	79	GLN	2.8
1	А	11	VAL	2.1

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

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

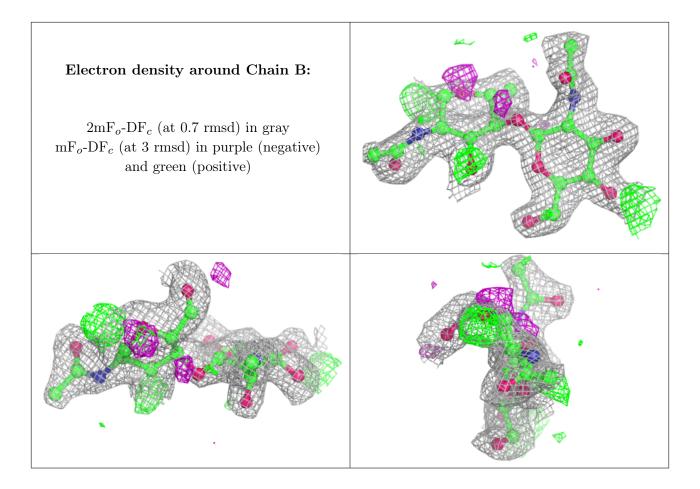
6.3 Carbohydrates (i)

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, 95^{th} 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.

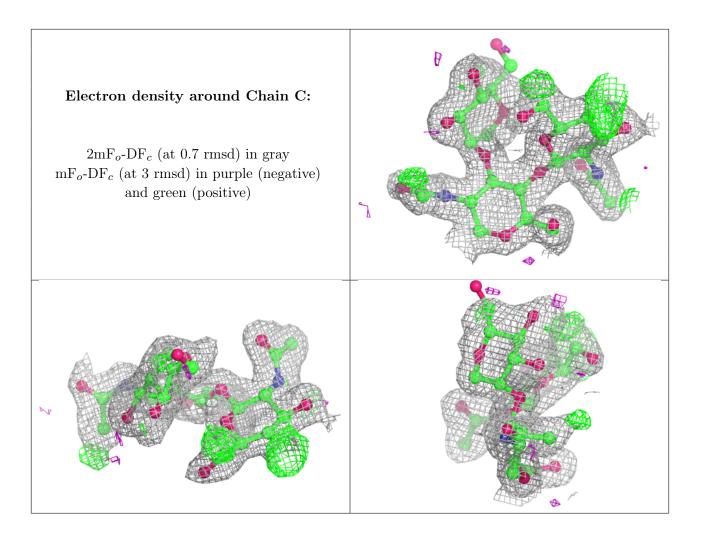
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
2	NAG	В	1	14/15	0.79	0.19	$22,\!30,\!36,\!37$	0
2	NAG	В	2	14/15	0.80	0.18	$36,\!47,\!54,\!54$	0
3	MAN	С	2	10/12	0.87	0.19	$19,\!30,\!56,\!62$	0
3	NAG	С	3	13/15	0.88	0.13	21,23,28,30	0
3	NAG	С	1	14/15	0.92	0.12	15,18,23,41	0

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)

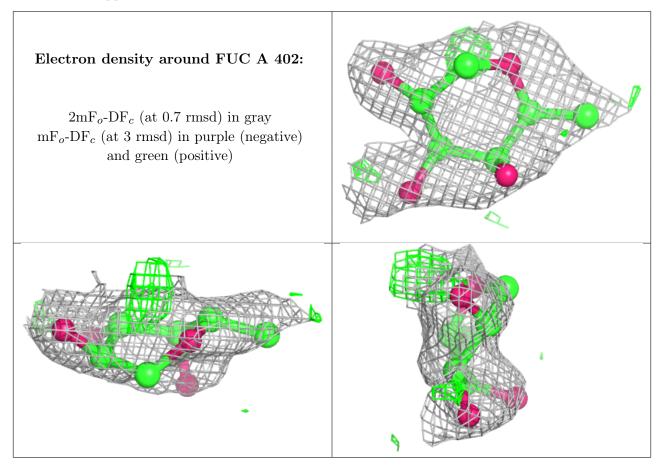
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
8	GOL	А	405	6/6	0.66	0.22	$27,\!34,\!38,\!44$	0
5	FUC	А	402	10/11	0.78	0.22	41,46,50,51	0
9	CL	А	408	1/1	0.87	0.15	31,31,31,31	1
9	CL	А	407	1/1	0.90	0.07	39,39,39,39	0
4	HEM	А	401	43/43	0.97	0.10	6,9,12,15	0
9	CL	А	406	1/1	0.98	0.06	17,17,17,17	0
7	NA	А	404	1/1	0.99	0.07	9,9,9,9	0
6	CA	А	403	1/1	1.00	0.07	10,10,10,10	0

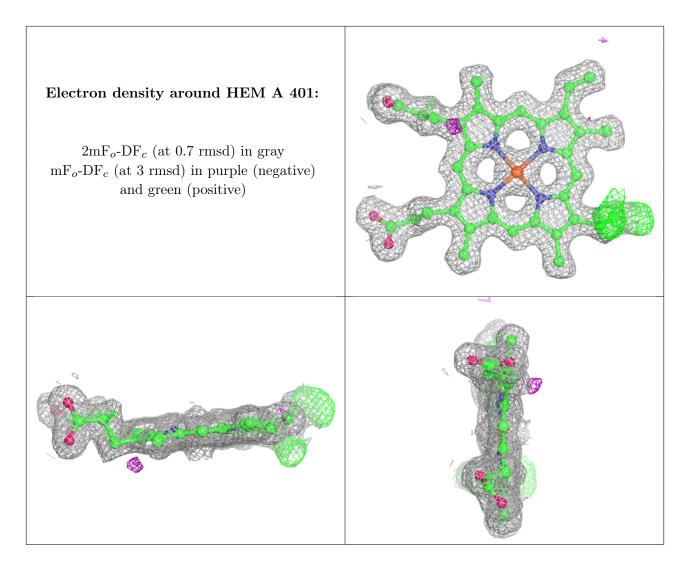
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers



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.

