

# Full wwPDB X-ray Structure Validation Report (i)

### Aug 21, 2020 – 12:30 AM BST

PDB ID : 1D7C

Title : CYTOCHROME DOMAIN OF CELLOBIOSE DEHYDROGENASE, PH 4.6

Authors: Hallberg, B.M.; Bergfors, T.; Backbro, K.; Divne, C.

Deposited on : 1999-10-16

Resolution : 1.90 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 following versions of software and data (see references (1)) 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 : 2.13.1

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)

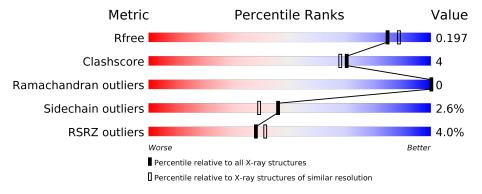
Validation Pipeline (wwPDB-VP) : 2.13.1

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar  resolution} \\ (\#{\rm Entries,  resolution  range(\AA)}) \end{array}$
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	190	3%	89%	11%
1	В	190	5%	89%	10% •
2	С	3	33%	67%	
2	D	3	33%	67%	

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 crite-



### ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BMA	С	3	-	-	-	X
2	BMA	D	3	-	-	-	X



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3406 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 CELLOBIOSE DEHYDROGENASE.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	1 A	190	Total	С	N	О	S	0	0	0
			1440	914	233	290	3	U		
1	D	В 190	Total	С	N	Ο	S	0	0	0
1			1440	914	233	290	3	0		

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



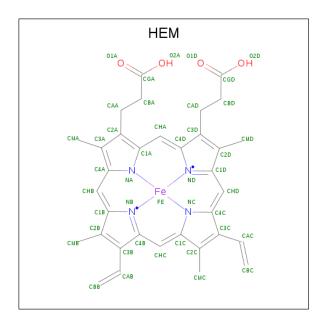
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	С	3	Total C 39 22	N 2 2		0	0	0
2	D	3	Total C 39 22	N 2 2	O 15	0	0	0

• Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mo	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
3		В	1	Total Cd 1 1	0	0
3		A	4	$\begin{array}{ccc} \text{Total} & \text{Cd} \\ & 4 & 4 \end{array}$	0	0

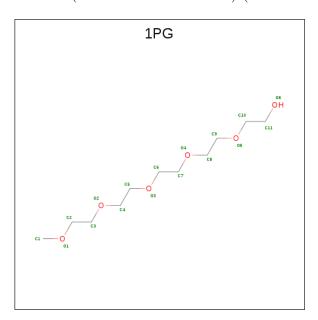
• Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf				
1	1 Λ	Λ 1	Total	С	Fe	N	О	0	0			
4 A	1	43	34	1	4	4	0	U				
1	4 B	D	D	B	1	Total	С	Fe	N	О	0	0
4		1	43	34	1	4	4	0	U			

• Molecule 5 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ET HANOL (three-letter code: 1PG) (formula:  $C_{11}H_{24}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	В	1	Total 17	C 11	O 6	0	0



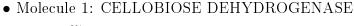
### • Molecule 6 is water.

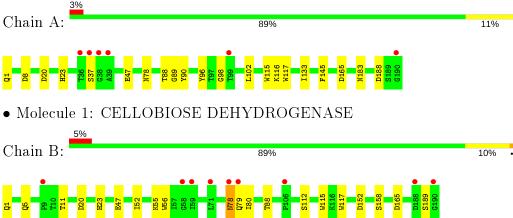
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	179	Total O 179 179	0	0
6	В	161	Total O 161 161	0	0



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

Chain C: 33% 67%

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

Chain D: 33% 67%





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants	$139.40 ext{Å}$ $139.40 ext{Å}$ $53.94 ext{Å}$	Domositon
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	25.00 - 1.90	Depositor
Resolution (A)	24.64 - 1.90	EDS
% Data completeness	97.4 (25.00-1.90)	Depositor
(in resolution range)	97.5 (24.64-1.90)	EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	7.25 (at 1.90Å)	Xtriage
Refinement program	CNS, SHELXL-97	Depositor
D D.	0.187 , 0.220	Depositor
$R, R_{free}$	0.166 , $0.197$	DCC
$R_{free}$ test set	2017  reflections  (4.37%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.9	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.38 , 60.6	EDS
L-test for twinning <sup>2</sup>	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3406	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: BMA, NAG, 1PG, CD, HEM, PCA

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	0.38	0/1477	0.94	$2/2030 \ (0.1\%)$	
1	В	0.38	0/1477	0.93	3/2030 (0.1%)	
All	All	0.38	0/2954	0.94	5/4060 (0.1%)	

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
1	A	115	TRP	CA-CB-CG	6.44	125.94	113.70
1	A	145	PHE	CB-CG-CD1	6.15	125.10	120.80
1	В	56	TRP	CA-CB-CG	5.57	124.28	113.70
1	В	88	THR	CA-C-N	5.48	127.15	116.20
1	В	115	TRP	CA-CB-CG	5.10	123.40	113.70

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	A	1440	0	1317	8	1
1	В	1440	0	1317	12	0
2	С	39	0	34	1	0
2	D	39	0	34	0	0

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$\circ$	110116	picolous	puyc

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	0	0	0
3	В	1	0	0	0	0
4	A	43	0	30	0	0
4	В	43	0	30	0	0
5	В	17	0	23	1	0
6	A	179	0	0	1	0
6	В	161	0	0	3	1
All	All	3406	0	2785	21	1

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 4.

All (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 4 1	A 4 O	Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	overlap (Å)
1:B:78:ASN:HD22	1:B:78:ASN:H	1.32	0.78
1:B:78:ASN:H	1:B:78:ASN:ND2	1.97	0.63
1:B:52:ILE:HD13	1:B:112:SER:O	2.00	0.61
1:B:78:ASN:N	1:B:78:ASN:HD22	2.01	0.56
2:C:2:NAG:H4	2:C:3:BMA:O2	2.05	0.56
1:A:23:HIS:HE1	1:A:165:ASP:OD2	1.90	0.53
1:B:23:HIS:HD2	6:B:2618:HOH:O	1.91	0.53
1:A:1:PCA:N	5:B:402:1PG:H102	2.23	0.52
1:B:23:HIS:HE1	1:B:165:ASP:OD2	1.93	0.52
1:A:23:HIS:HD2	6:A:1618:HOH:O	1.93	0.51
1:B:55:LYS:HE2	6:B:2757:HOH:O	2.11	0.50
1:A:8:ASP:OD2	1:A:116:LYS:NZ	2.41	0.49
1:B:80:ILE:HG21	1:B:117:TRP:CD1	2.47	0.48
1:B:5:GLN:HG3	6:B:2751:HOH:O	2.14	0.48
1:A:89:GLY:O	1:A:90:TYR:HB2	2.14	0.47
1:A:96:TYR:CZ	1:A:98:GLY:HA3	2.50	0.47
1:A:47:GLU:HA	1:A:117:TRP:O	2.19	0.43
1:B:152:ASP:O	1:B:158:SER:HB2	2.20	0.41
1:B:11:THR:O	1:B:189:SER:HB3	2.20	0.41
1:A:183:ASN:HB3	1:A:188:ASP:HB2	2.02	0.41
1:B:47:GLU:HA	1:B:117:TRP:O	2.21	0.40

All (1) 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	$egin{array}{c}  ext{Interatomic} \  ext{distance } ( ext{Å}) \end{array}$	Clash overlap (Å)
1:A:88:THR:OG1	6:B:2706:HOH:O[5_555]	2.01	0.19

# 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	${f naly} {f sed} \qquad {f Favoured} \qquad {f Allowed}$		Outliers	Perce	ntiles
1	A	188/190 (99%)	183 (97%)	5 (3%)	0	100	100
1	В	188/190 (99%)	183 (97%)	5 (3%)	0	100	100
All	All	376/380 (99%)	366 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric   Outliers		Percentiles		
1	A	$152/152 \; (100\%)$	147 (97%)	5 (3%)	38 29		
1	В	$152/152 \; (100\%)$	149 (98%)	3 (2%)	55 51		
All	All	304/304 (100%)	296 (97%)	8 (3%)	46 39		

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	37	SER
1	A	78	ASN

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Mol	Chain	Res	Type
1	A	102	LEU
1	A	133	ILE
1	В	20	ASP
1	В	78	ASN
1	В	79	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	${f Res}$	Type
1	A	23	HIS
1	A	78	ASN
1	В	23	HIS
1	В	78	ASN
1	В	182	GLN
1	В	186	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)

2 non-standard protein/DNA/RNA residues 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	Dag	T in le	B	ond leng	$_{ m gths}$	В	ond ang	gles
MIOI	Mol Type Chain Re	Res	$\mathbf{s} \mid \mathbf{Link} \mid$	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
1	PCA	В	1	1	7,8,9	1.09	0	9,10,12	1.09	1 (11%)
1	PCA	A	1	1	7,8,9	1.12	0	9,10,12	1.08	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
1	PCA	В	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
1	В	1	PCA	O-C-CA	-2.03	119.47	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	PCA	1	0

# 5.5 Carbohydrates (i)

6 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		Bo	nd leng	ths	Bond angles				
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	С	1	1,2	14,14,15	0.57	0	17,19,21	0.58	0
2	NAG	С	2	2	14,14,15	0.52	0	17,19,21	0.69	0
2	BMA	С	3	2	11,11,12	0.50	0	15,15,17	0.36	0
2	NAG	D	1	1,2	14,14,15	0.45	0	17,19,21	0.60	0
2	NAG	D	2	2	14,14,15	0.89	1 (7%)	17,19,21	1.31	3 (17%)
2	BMA	D	3	2	11,11,12	0.63	0	15,15,17	0.99	1 (6%)

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	С	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	С	2	2	-	2/6/23/26	0/1/1/1
2	BMA	С	3	2	-	2/2/19/22	0/1/1/1
2	NAG	D	1	1,2	1	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1

### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	${ m Observed}({ m \AA})$	Ideal(A)
2	D	2	NAG	C1-C2	2.48	1.56	1.52

### All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
2	D	3	BMA	C1-C2-C3	3.19	113.59	109.67
2	D	2	NAG	C4-C3-C2	-3.11	106.46	111.02
2	D	2	NAG	O4-C4-C3	2.34	115.75	110.35
2	D	2	NAG	C3-C4-C5	-2.05	106.59	110.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	BMA	C4-C5-C6-O6
2	С	2	NAG	C4-C5-C6-O6
2	С	3	BMA	O5-C5-C6-O6
2	С	2	NAG	O5-C5-C6-O6
2	D	3	BMA	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	С	3	BMA	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

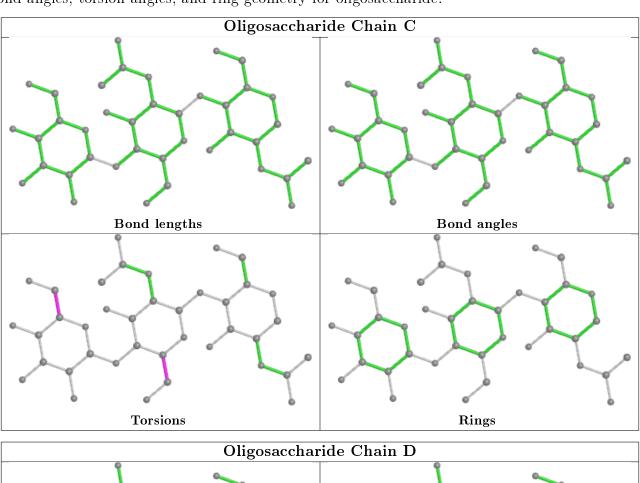
There are no ring outliers.

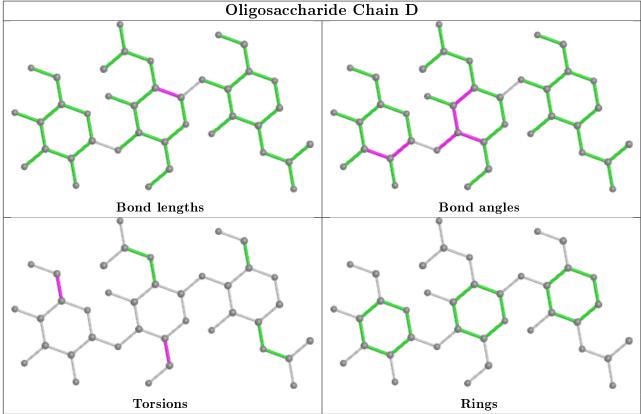
2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	2	NAG	1	0
2	С	3	BMA	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	Tuno	Chain	Des	Link	В	ond leng	$\operatorname{gths}$	Bond angles		
MIOI	Type	Chain	m Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	HEM	A	401	1,3	27,50,50	2.05	8 (29%)	17,82,82	1.67	4 (23%)
4	HEM	В	401	1,3	27,50,50	2.09	10 (37%)	17,82,82	1.62	4 (23%)
5	1PG	В	402	-	16,16,16	1.32	1 (6%)	15,15,15	0.32	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	${ m Res}$	Link	Chirals	${f Torsions}$	Rings
4	HEM	A	401	1,3	-	0/6/54/54	-
4	HEM	В	401	1,3	-	0/6/54/54	-
5	1PG	В	402	-	-	5/14/14/14	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	${ m Observed}( m \AA)$	Ideal(Å)
4	A	401	HEM	C3C-CAC	4.23	1.56	1.47
4	В	401	HEM	C3C-CAC	4.05	1.56	1.47
4	В	401	HEM	C3B-CAB	4.00	1.56	1.47
4	A	401	HEM	C3B-CAB	3.71	1.55	1.47
4	В	401	HEM	CBB-CAB	3.64	1.53	1.29
4	A	401	HEM	CBB-CAB	3.63	1.53	1.29
4	A	401	HEM	CBC-CAC	3.62	1.53	1.29
4	В	401	HEM	CBC-CAC	3.54	1.52	1.29
4	A	401	HEM	C3C-C2C	-3.07	1.36	1.40
4	В	401	HEM	C3C-C2C	-2.93	1.36	1.40
4	В	401	HEM	CAA-C2A	2.78	1.56	1.52
4	A	401	HEM	CAA-C2A	2.67	1.56	1.52
5	В	402	1PG	O1-C1	2.51	1.54	1.42

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(\mathbf{\mathring{A}})$	Ideal(Å)
4	A	401	HEM	C1C-C2C	2.49	1.48	1.42
4	В	401	HEM	C1D-ND	2.44	1.41	1.36
4	В	401	HEM	CMC-C2C	2.31	1.57	1.51
4	В	401	HEM	C1C-C2C	2.27	1.47	1.42
4	A	401	HEM	C3B-C2B	-2.24	1.37	1.40
4	В	401	HEM	C3B-C2B	-2.06	1.37	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
4	A	401	HEM	CMB-C2B-C3B	3.74	131.68	124.68
4	A	401	HEM	CMD-C2D-C1D	-3.35	123.31	128.46
4	В	401	HEM	CMD-C2D-C1D	-3.12	123.66	128.46
4	В	401	HEM	CMA-C3A-C4A	-2.96	123.91	128.46
4	A	401	HEM	CMC-C2C-C3C	2.93	130.15	124.68
4	В	401	HEM	CMB-C2B-C3B	2.91	130.12	124.68
4	В	401	HEM	CMC-C2C-C3C	2.32	129.02	124.68
4	A	401	HEM	CMD-C2D-C3D	2.10	128.89	124.94

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	402	1PG	O2-C4-C5-O3
5	В	402	1PG	O5-C10-C11-O6
5	В	402	1PG	O4-C8-C9-O5
5	В	402	1PG	C6-C7-O4-C8
5	В	402	1PG	C8-C9-O5-C10

There are no ring outliers.

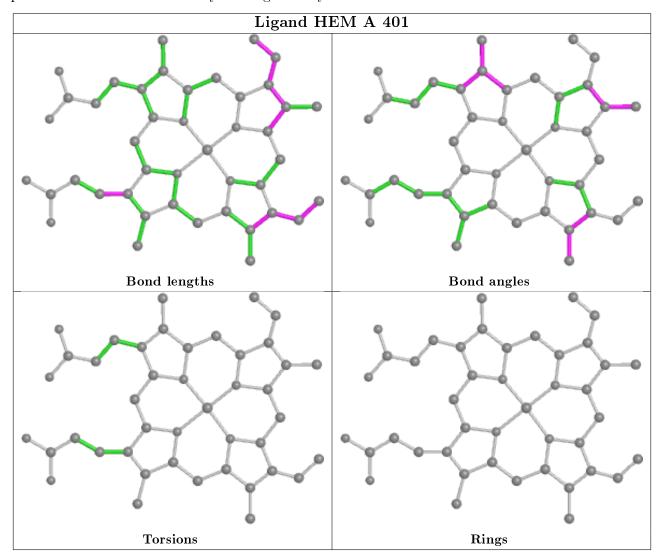
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	В	402	1PG	1	0

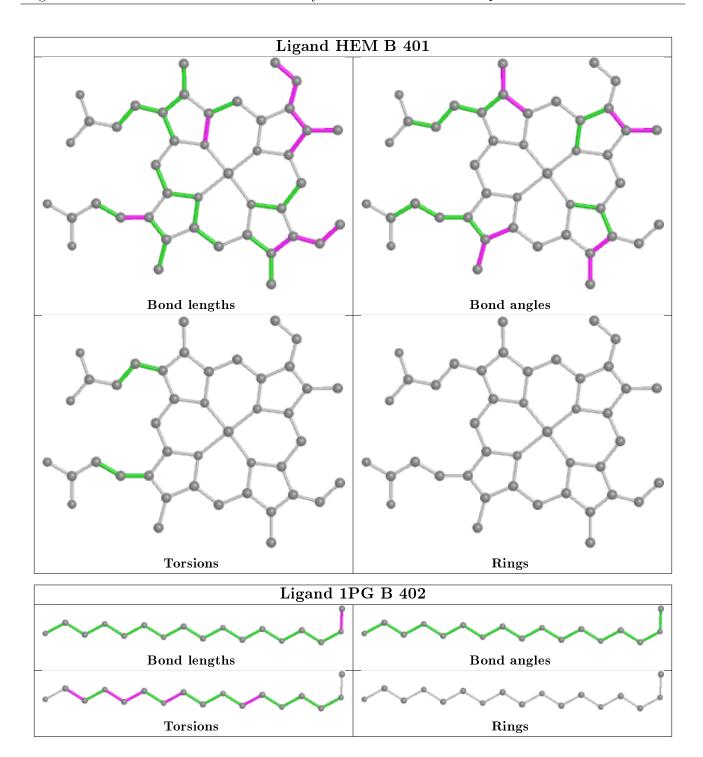
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	189/190 (99%)	-0.04	6 (3%) 47 50	11, 17, 35, 68	0
1	В	189/190 (99%)	0.04	9 (4%) 30 33	12, 18, 34, 68	0
All	All	378/380 (99%)	-0.00	15 (3%) 38 41	11, 18, 35, 68	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	SER	5.8
1	A	190	GLY	4.6
1	A	36	THR	4.3
1	A	38	GLY	3.7
1	В	59	ILE	3.3
1	В	188	ASP	3.2
1	В	9	PRO	2.9
1	В	190	GLY	2.9
1	В	79	GLN	2.6
1	В	71	LEU	2.3
1	В	106	PRO	2.2
1	В	58	GLY	2.2
1	A	39	ALA	2.1
1	В	78	ASN	2.1
1	A	99	THR	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains (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.



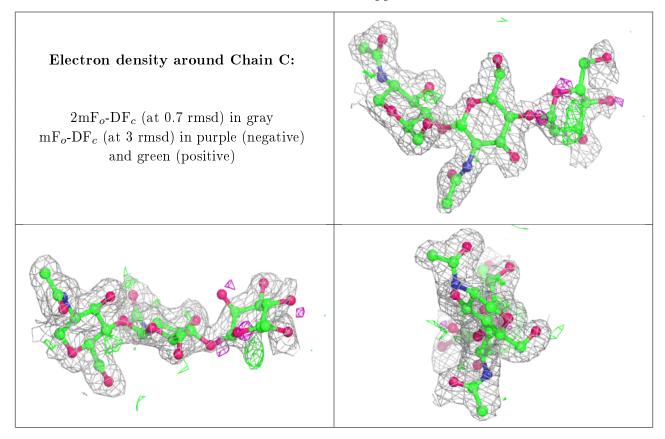
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f A}^2)$	Q<0.9
1	PCA	В	1	8/9	0.96	0.08	12,14,17,18	0
1	PCA	A	1	8/9	0.98	0.09	13,15,16,18	0

# 6.3 Carbohydrates (i)

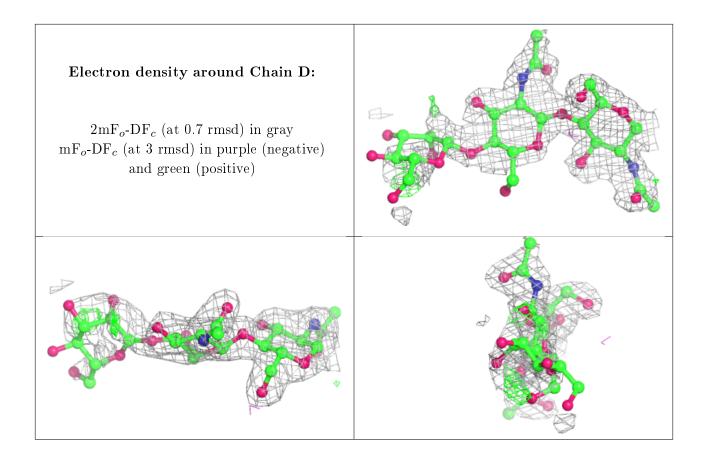
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	BMA	D	3	11/12	0.53	0.47	72,104,114,114	0
2	BMA	С	3	11/12	0.77	0.45	34,61,78,80	0
2	NAG	С	2	14/15	0.87	0.22	30,37,51,55	0
2	NAG	D	2	14/15	0.90	0.27	32,46,75,81	0
2	NAG	D	1	14/15	0.90	0.17	32,37,62,65	0
2	NAG	С	1	14/15	0.94	0.08	14,20,27,31	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.







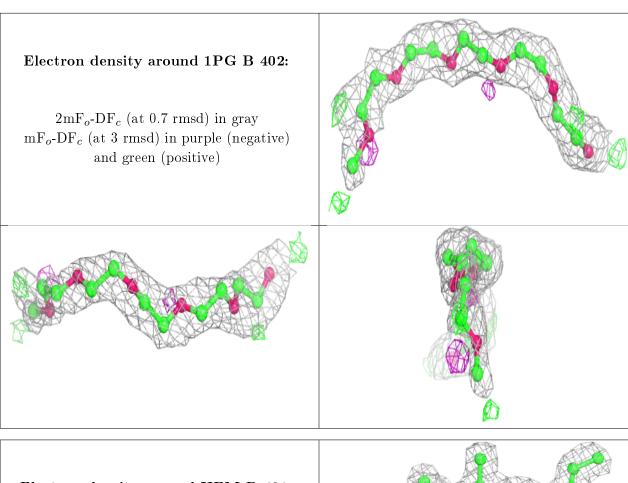
# 6.4 Ligands (i)

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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
3	CD	A	503	1/1	0.76	0.36	81,81,81,81	0
5	1PG	В	402	17/17	0.85	0.16	34,43,59,64	0
3	CD	A	504	1/1	0.92	0.18	68,68,68,68	0
4	HEM	В	401	43/43	0.97	0.09	7,14,18,22	0
4	HEM	A	401	43/43	0.97	0.10	7,13,20,22	0
3	CD	A	501	1/1	0.99	0.05	17,17,17,17	0
3	CD	В	502	1/1	1.00	0.04	18,18,18,18	0
3	CD	A	502	1/1	1.00	0.04	16,16,16,16	0

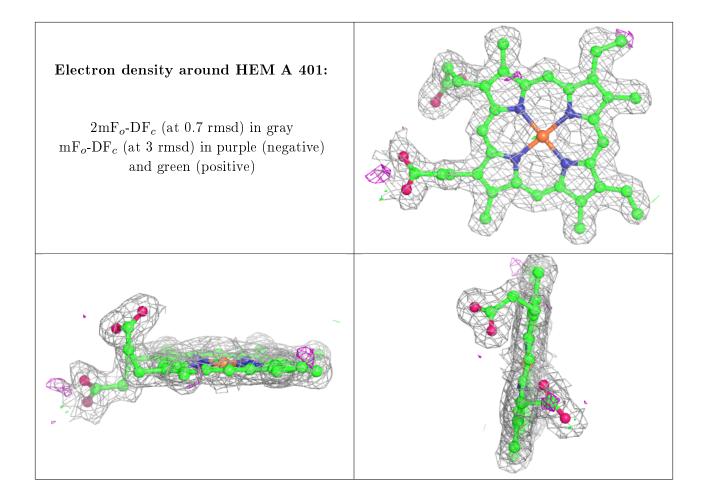
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





# Electron density around HEM B 401: 2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative) and green (positive)





# 6.5 Other polymers (i)

There are no such residues in this entry.

