

wwPDB X-ray Structure Validation Summary Report (i)

Feb 21, 2022 – 05:03 pm GMT

PDB ID : 7NI3

Title : CRYSTAL STRUCTURE OF NATIVE HUMAN MYELOPEROXIDASE IN

COMPLEX WITH CPD 3

Authors : Sjogren, T.; Inghardt, T.

Deposited on : 2021-02-11

Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul: 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.26

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0267$

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

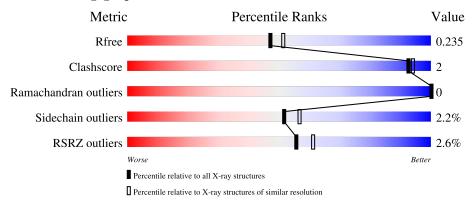
Validation Pipeline (wwPDB-VP) : 2.26

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 2.10 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	
			5%		
1	A	105		92%	8%
			2%		
1	В	105		91%	7% •
			2%		
2	С	466		92%	7%
			3%		
2	D	466		94%	5%
3	Е	4	25%	75%	

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Mol	Chain	Length	Quality	of chain
3	F	4	50%	50%



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10213 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.

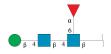
• Molecule 1 is a protein called Myeloperoxidase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	105	Total 842	C 532		O 156	S 5	0	0	0
1	В	103	Total 832	C 526		O 154	S 5	0	0	0

• Molecule 2 is a protein called Myeloperoxidase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	С	464	Total 3720	C 2343	N 685	O 665	S 27	0	0	0
2	D	464	Total 3720	C 2343	N 685	O 665	S 27	0	0	0

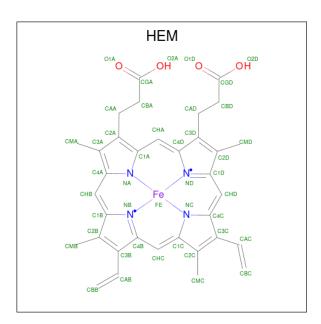
• Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



\mathbf{M}	ol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
3		E	4	Total 49	C 28		0	0	0
3		F	4	Total 49	C 28	O 19	0	0	0

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





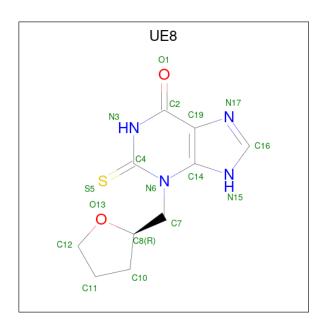
Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	
4	Λ	1	Total	С	Fe	N	О	0	0	
4	Α	1	43	34	1	4	4	0	U	
1	D	1	Total	С	Fe	N	О	0	0	
4	Б	1	43	34	1	4	4	0		

• Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	В	2	Total Cl 2 2	0	0
5	С	2	Total Cl 2 2	0	0

• Molecule 6 is 2-sulfanylidene-3-[(2R)-tetrahydro-2-furanylmethyl]-1,2,3,7-tetrahydro-6H-pur in-6-one (three-letter code: UE8) (formula: $C_{10}H_{12}N_4O_2S$) (labeled as "Ligand of Interest" by depositor).





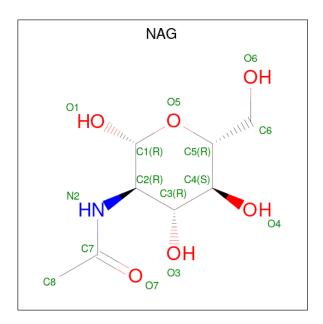
Mol	Chain	Residues		Ato	$\mathbf{m}\mathbf{s}$			ZeroOcc	AltConf
6	C	1	Total	С	N	О	S	0	0
0		1	17	10	4	2	1	0	
6	D	1	Total	С	N	О	S	0	0
ρ	Ъ	1	17	10	4	2	1		

• Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

\mathbf{N}	/Iol	Chain	Residues	Atoms	ZeroOcc	AltConf
	7	С	1	Total Ca 1 1	0	0
	7	D	1	Total Ca 1 1	0	0

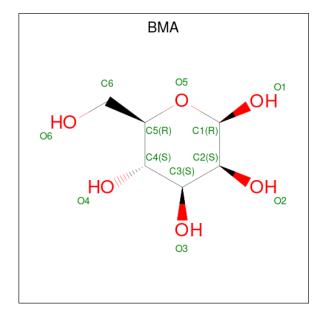
 \bullet Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\rm C_8H_{15}NO_6).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
8	С	1	Total C N O	0	0	
		_	14 8 1 5	Ŭ	Ŭ.	
Q	C	1	Total C N O	0	0	
0		1	14 8 1 5	0		
Q	D	1	Total C N O	0	0	
0	D	1	14 8 1 5	0		
Q	D	1	Total C N O	0	0	
0	D	1	14 8 1 5	0		

 \bullet Molecule 9 is beta-D-mann opyranose (three-letter code: BMA) (formula: $\rm C_6H_{12}O_6).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	С	1	Total C O 11 6 5	0	0
9	D	1	Total C O 11 6 5	0	0

$\bullet\,$ Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	84	Total O 84 84	0	0
10	В	75	Total O 75 75	0	0
10	С	342	Total O 342 342	0	0
10	D	295	Total O 295 295	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: Myeloperoxidase Chain A: • Molecule 1: Myeloperoxidase Chain B: 91% • Molecule 2: Myeloperoxidase Chain C: 92% 7% • Molecule 2: Myeloperoxidase Chain D: 94% 5%

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alp ha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



Chain E: 25% 75% • Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alp $ha-L-fucopyranose-(1-6)] \\ 2-acetamido-2-deoxy-beta-D-glucopyranose$ Chain F: 50% 50%





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	92.66Å 63.64Å 111.03Å	Depositor	
a, b, c, α , β , γ	90.00° 97.15° 90.00°	Depositor	
Resolution (Å)	30.61 - 2.10	Depositor	
rtesolution (A)	30.61 - 2.10	EDS	
% Data completeness	75.0 (30.61-2.10)	Depositor	
(in resolution range)	75.0 (30.61-2.10)	EDS	
R_{merge}	0.10	Depositor	
R_{sym}	0.10	Depositor	
$< I/\sigma(I) > 1$	2.70 (at 2.10Å)	Xtriage	
Refinement program	BUSTER 2.11.7	Depositor	
P. P.	0.175 , 0.224	Depositor	
R, R_{free}	0.182 , 0.235	DCC	
R_{free} test set	2737 reflections (4.84%)	wwPDB-VP	
Wilson B-factor (Å ²)	12.2	Xtriage	
Anisotropy	0.222	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS	
L-test for twinning ²	$ < L > = 0.47, < L^2 > = 0.29$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.93	EDS	
Total number of atoms	10213	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 5.38% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: UE8, BMA, CA, HEM, NAG, FUC, CSO, 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	Bond	Bond lengths		Bond angles	
IVIOI	Wioi Chain		# Z > 5	RMSZ	# Z > 5	
1	A	0.51	0/867	0.70	0/1181	
1	В	0.49	0/857	0.69	0/1167	
2	С	0.51	0/3798	0.64	0/5151	
2	D	0.50	0/3798	0.64	0/5151	
All	All	0.51	0/9320	0.65	0/12650	

There are no bond length outliers.

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	842	0	803	6	0
1	В	832	0	793	5	0
2	С	3720	0	3711	14	0
2	D	3720	0	3711	11	0
3	Е	49	0	43	0	0
3	F	49	0	43	0	0
4	A	43	0	30	0	0
4	В	43	0	30	1	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	В	2	0	0	0	0
5	С	2	0	0	0	0
6	С	17	0	0	0	0
6	D	17	0	0	0	0
7	С	1	0	0	0	0
7	D	1	0	0	0	0
8	С	28	0	26	0	0
8	D	28	0	26	0	0
9	С	11	0	10	0	0
9	D	11	0	10	0	0
10	A	84	0	0	0	0
10	В	75	0	0	0	0
10	С	342	0	0	0	0
10	D	295	0	0	0	0
All	All	10213	0	9236	28	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 2.

The worst 5 of 28 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
2:D:336:HIS:HD1	2:D:421:ASN:HD21	1.22	0.85
2:C:336:HIS:HD1	2:C:421:ASN:HD21	1.21	0.83
2:C:137:ILE:HG12	2:C:413:ILE:HD11	1.90	0.53
1:A:83:SER:HB3	2:C:554:SER:O	2.09	0.52
4:B:202:HEM:HMC2	4:B:202:HEM:HBC2	1.92	0.49

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	103/105~(98%)	100 (97%)	3 (3%)	0	100 100
1	В	$101/105\ (96\%)$	99 (98%)	2 (2%)	0	100 100
2	С	$461/466\ (99\%)$	450 (98%)	11 (2%)	0	100 100
2	D	461/466~(99%)	450 (98%)	11 (2%)	0	100 100
All	All	$1126/1142\ (99\%)$	1099 (98%)	27 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2Protein 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	Percei	ntiles
1	A	90/90~(100%)	89 (99%)	1 (1%)	73	79
1	В	90/90 (100%)	89 (99%)	1 (1%)	73	79
2	\mathbf{C}	409/410~(100%)	398 (97%)	11 (3%)	44	48
2	D	409/410 (100%)	400 (98%)	9 (2%)	52	57
All	All	998/1000 (100%)	976 (98%)	22 (2%)	52	57

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	175	MET
2	D	348	ASN
2	D	318	ASP
2	D	393	ARG
2	С	254	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	С	523	GLN
2	D	348	ASN
2	D	523	GLN

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Mol	Chain	Res	Type
2	D	467	GLN
2	С	467	GLN

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	Trino	Chain	Res Link		В	ond leng	$_{ m gths}$	Е	Sond angles	
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	CSO	С	150	2	3,6,7	0.76	0	0,6,8	-	-
2	CSO	D	150	2	3,6,7	0.83	0	0,6,8	-	-

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	С	150	2	-	0/1/5/7	-
2	CSO	D	150	2	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



5.5 Carbohydrates (i)

8 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	Вс	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	Е	1	3,2	14,14,15	0.28	0	17,19,21	1.07	1 (5%)
3	NAG	Е	2	3	14,14,15	0.29	0	17,19,21	1.12	2 (11%)
3	BMA	Е	3	3	11,11,12	0.29	0	15,15,17	0.88	1 (6%)
3	FUC	Е	4	3	10,10,11	0.48	0	14,14,16	0.62	0
3	NAG	F	1	3,2	14,14,15	0.39	0	17,19,21	0.94	1 (5%)
3	NAG	F	2	3	14,14,15	0.25	0	17,19,21	0.89	1 (5%)
3	BMA	F	3	3	11,11,12	0.37	0	15,15,17	0.74	0
3	FUC	F	4	3	10,10,11	0.52	0	14,14,16	0.61	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
3	NAG	Е	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	Е	2	3	-	0/6/23/26	0/1/1/1
3	BMA	Е	3	3	-	0/2/19/22	0/1/1/1
3	FUC	Е	4	3	-	-	0/1/1/1
3	NAG	F	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	FUC	F	4	3	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
3	Е	2	NAG	C1-O5-C5	3.43	116.84	112.19
3	Е	1	NAG	O5-C1-C2	-3.09	106.41	111.29

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
3	Ε	3	BMA	C1-O5-C5	3.07	116.35	112.19
3	F	1	NAG	O5-C1-C2	-2.72	106.99	111.29
3	F	2	NAG	C1-O5-C5	2.40	115.44	112.19

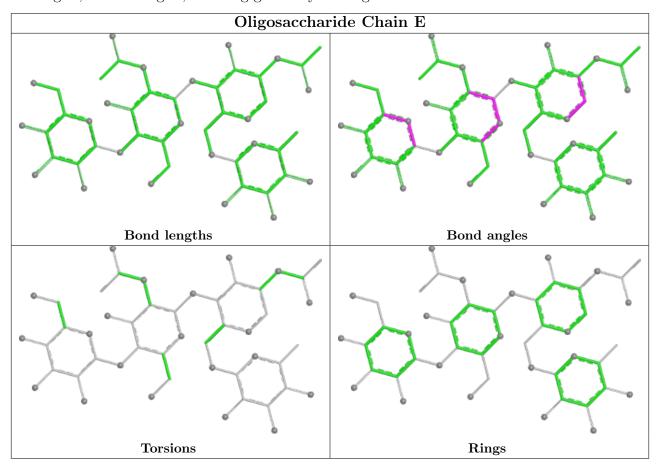
There are no chirality outliers.

There are no torsion outliers.

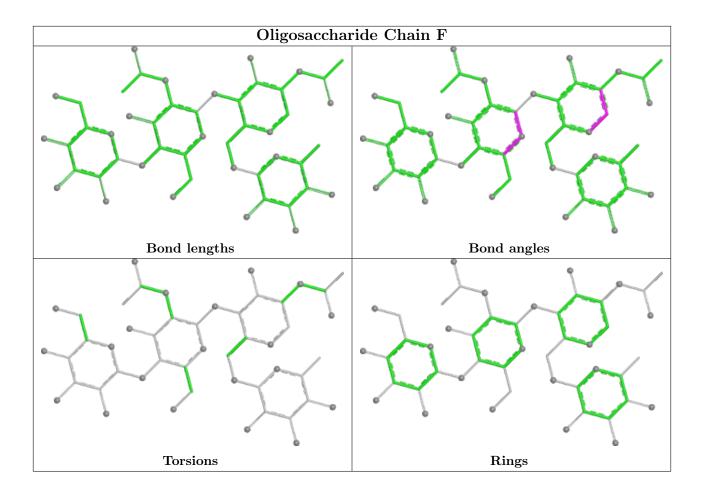
There are no ring outliers.

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 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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	Bo	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	D	2203	2	14,14,15	0.31	0	17,19,21	0.78	1 (5%)
4	HEM	A	201	1,2,10	27,50,50	1.16	2 (7%)	17,82,82	2.23	7 (41%)
4	HEM	В	202	1,2	27,50,50	1.23	3 (11%)	17,82,82	2.43	6 (35%)
6	UE8	D	2201	_	12,19,19	1.73	2 (16%)	13,27,27	4.82	5 (38%)
6	UE8	С	602	-	12,19,19	1.66	2 (16%)	13,27,27	5.01	5 (38%)
8	NAG	D	2204	2	14,14,15	0.28	0	17,19,21	0.70	1 (5%)



Mol	Trme	Chain	Dag	Link Bond lengths			Bond angles			
MIOI	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
9	BMA	D	2202	-	11,11,12	0.36	0	15,15,17	0.85	1 (6%)
8	NAG	С	605	2	14,14,15	0.31	0	17,19,21	0.72	1 (5%)
9	BMA	С	607	-	11,11,12	0.36	0	15,15,17	0.94	2 (13%)
8	NAG	С	606	2	14,14,15	0.36	0	17,19,21	0.64	1 (5%)

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
8	NAG	D	2203	2	-	0/6/23/26	0/1/1/1
4	HEM	A	201	1,2,10	-	0/6/54/54	-
4	HEM	В	202	1,2	-	0/6/54/54	-
6	UE8	D	2201	-	-	0/4/11/11	0/3/3/3
6	UE8	С	602	-	-	0/4/11/11	0/3/3/3
8	NAG	D	2204	2	-	0/6/23/26	0/1/1/1
9	BMA	D	2202	-	-	2/2/19/22	0/1/1/1
8	NAG	С	605	2	-	0/6/23/26	0/1/1/1
9	BMA	С	607	_	-	2/2/19/22	0/1/1/1
8	NAG	С	606	2	-	0/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}({ ext{A}})$
6	С	602	UE8	C2-N3	4.73	1.41	1.33
6	D	2201	UE8	C2-N3	4.72	1.41	1.33
4	В	202	HEM	C3D-C4D	3.10	1.49	1.42
6	D	2201	UE8	C7-N6	-2.98	1.45	1.48
4	В	202	HEM	C3C-CAC	2.61	1.53	1.47

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
6	С	602	UE8	C2-N3-C4	13.78	130.02	115.93
6	D	2201	UE8	C2-N3-C4	13.16	129.39	115.93
6	С	602	UE8	C19-C2-N3	-9.76	110.08	123.43
6	D	2201	UE8	C19-C2-N3	-9.25	110.78	123.43
4	A	201	HEM	CBA-CAA-C2A	-5.28	102.74	112.49

There are no chirality outliers.



All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	С	607	BMA	C4-C5-C6-O6
9	D	2202	BMA	C4-C5-C6-O6
9	D	2202	BMA	O5-C5-C6-O6
9	С	607	BMA	O5-C5-C6-O6

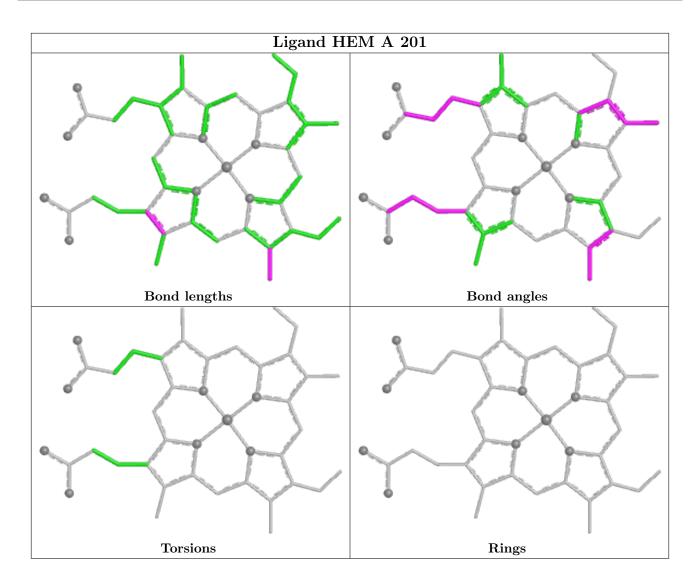
There are no ring outliers.

1 monomer is involved in 1 short contact:

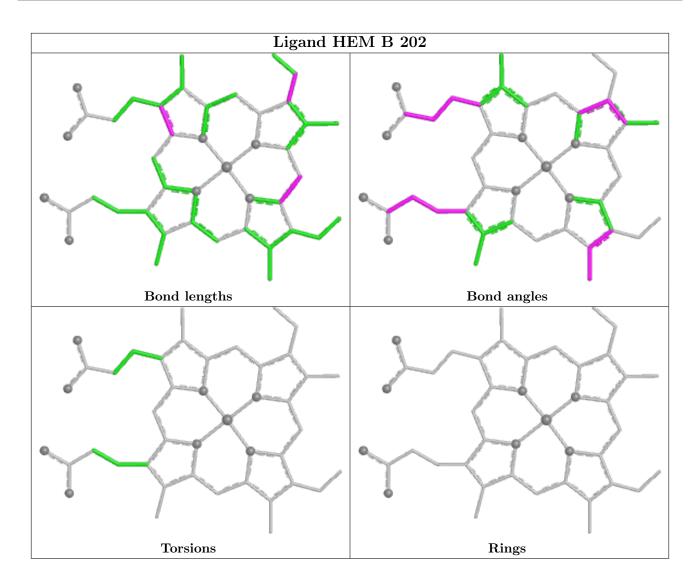
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	202	HEM	1	0

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.

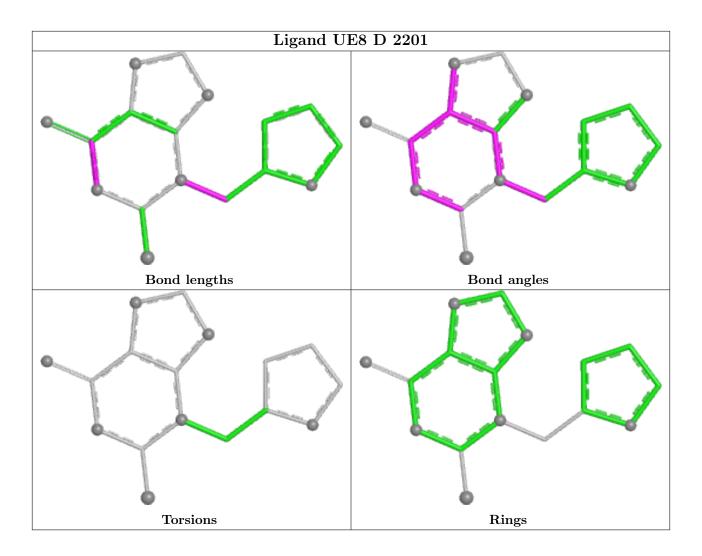




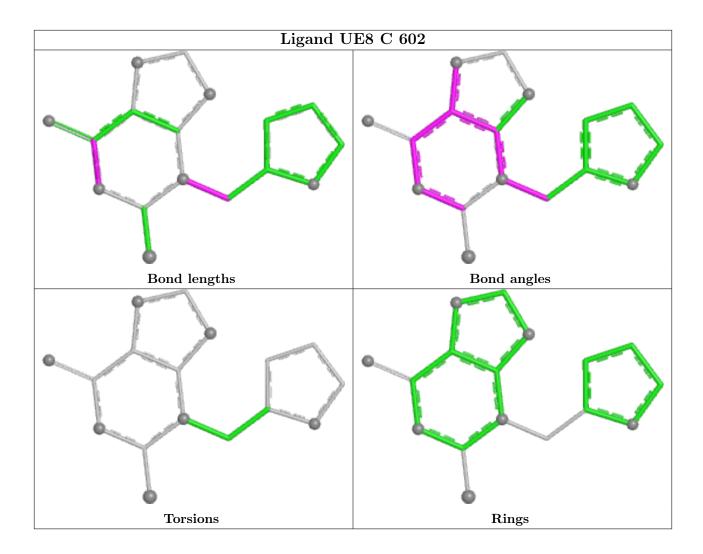












5.7 Other polymers (i)

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></rsrz>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	$105/105\ (100\%)$	-0.03	5 (4%) 30 36	4, 10, 36, 57	0
1	В	103/105~(98%)	-0.10	2 (1%) 66 71	6, 13, 28, 44	0
2	С	463/466~(99%)	-0.08	10 (2%) 62 66	4, 13, 33, 52	0
2	D	463/466 (99%)	0.05	13 (2%) 53 59	5, 16, 35, 56	0
All	All	$1134/1142 \ (99\%)$	-0.03	30 (2%) 56 61	4, 14, 35, 57	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	355	PRO	6.5
2	С	355	PRO	5.7
1	A	3	GLU	5.6
2	С	217	HIS	5.0
2	D	217	HIS	4.3

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	CSO	D	150	7/8	0.95	0.10	13,15,25,26	0
2	CSO	С	150	7/8	0.98	0.07	6,12,15,15	0

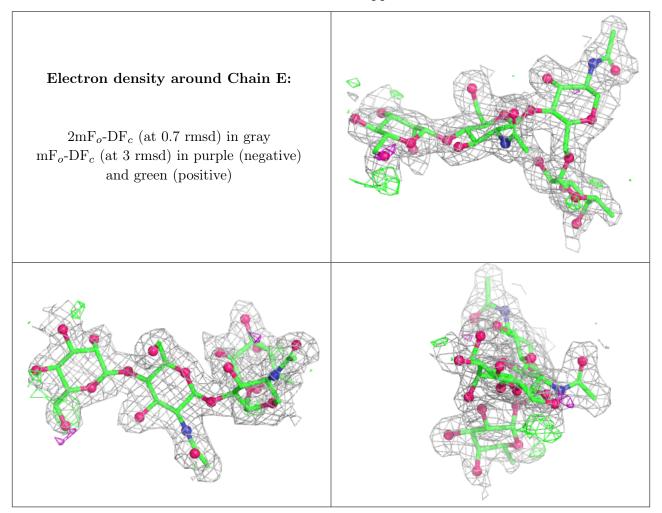


6.3 Carbohydrates (i)

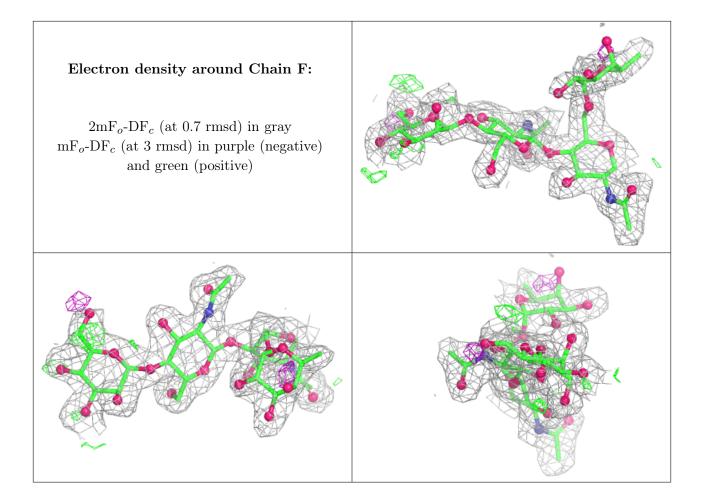
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
3	FUC	F	4	10/11	0.75	0.30	35,38,41,45	0
3	BMA	F	3	11/12	0.82	0.19	28,35,36,36	0
3	BMA	Е	3	11/12	0.87	0.18	31,35,38,40	0
3	FUC	Е	4	10/11	0.90	0.18	22,27,28,30	0
3	NAG	F	1	14/15	0.93	0.14	14,18,21,28	0
3	NAG	F	2	14/15	0.96	0.11	10,16,19,25	0
3	NAG	Е	1	14/15	0.98	0.08	6,10,22,24	0
3	NAG	Е	2	14/15	0.98	0.09	9,10,14,23	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	$oxed{ \mathbf{B\text{-}factors}(\mathbf{\mathring{A}}^2) }$	Q < 0.9
9	BMA	D	2202	11/12	0.56	0.29	68,70,72,73	0
9	BMA	С	607	11/12	0.81	0.16	30,36,39,40	0
6	UE8	D	2201	17/17	0.83	0.20	30,40,50,50	0
8	NAG	D	2204	14/15	0.85	0.25	38,42,47,48	0
8	NAG	С	606	14/15	0.89	0.22	31,35,37,38	0
6	UE8	С	602	17/17	0.90	0.17	12,31,43,44	0
8	NAG	D	2203	14/15	0.92	0.15	13,22,27,29	0
8	NAG	С	605	14/15	0.94	0.18	18,23,27,28	0
5	CL	С	604	1/1	0.97	0.07	31,31,31,31	0
4	HEM	A	201	43/43	0.97	0.12	7,8,11,17	0
4	HEM	В	202	43/43	0.97	0.14	11,12,15,19	0
5	CL	A	202	1/1	0.99	0.05	23,23,23,23	0

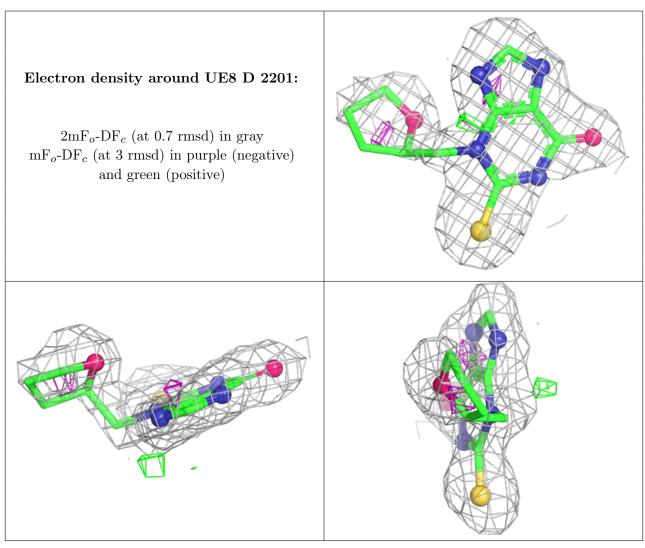
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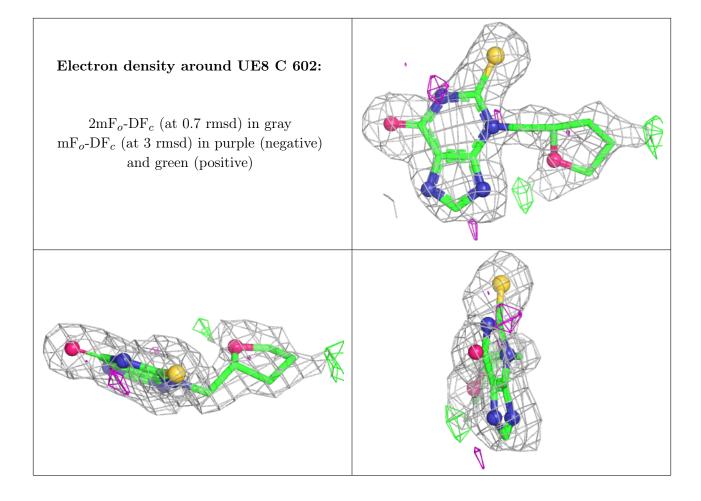
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q < 0.9
5	CL	В	201	1/1	0.99	0.11	11,11,11,11	0
5	CL	В	203	1/1	0.99	0.04	25,25,25,25	0
5	CL	С	601	1/1	1.00	0.09	6,6,6,6	0
7	CA	С	603	1/1	1.00	0.08	3,3,3,3	0
7	CA	D	2205	1/1	1.00	0.14	3,3,3,3	1

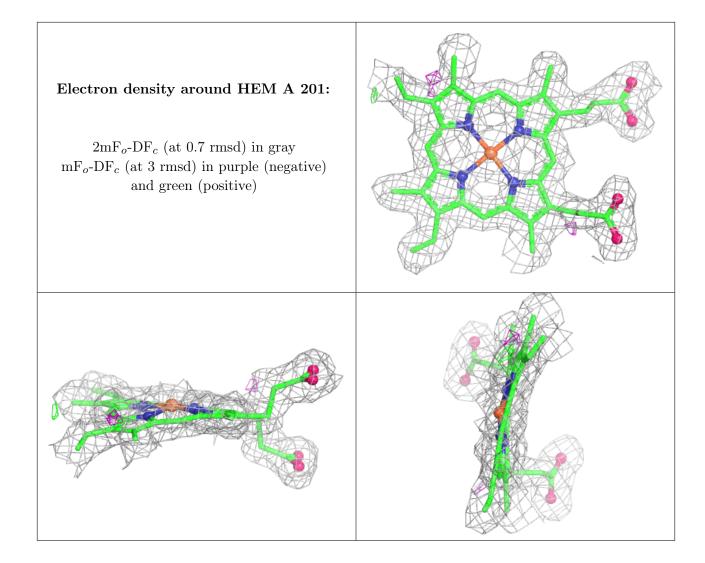
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



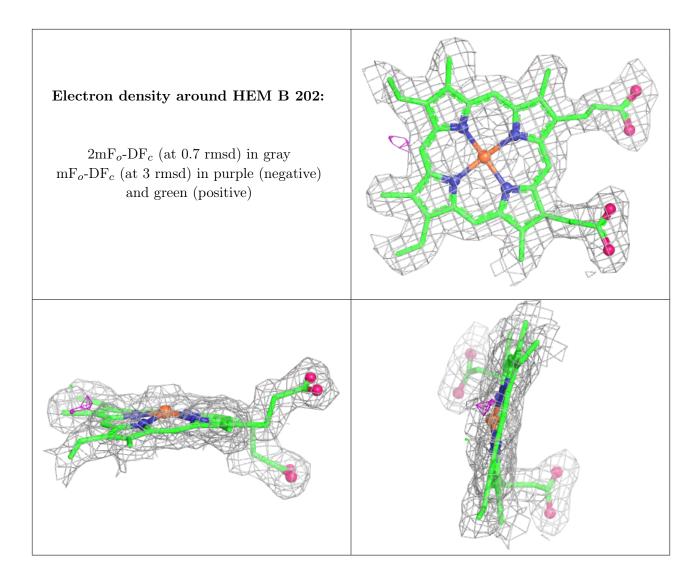












6.5 Other polymers (i)

There are no such residues in this entry.

