



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:52 PM BST

PDB ID : 3S4F  
Title : Crystal structure of the complex of bovine lactoperoxidase with 1H-pyrazolo[4,3-c] pyridine at 1.99 Å resolution  
Authors : Singh, A.; Singh, A.K.; Singh, R.P.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2011-05-19  
Resolution : 2.00 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](mailto: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.

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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 : 2.13.1  
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

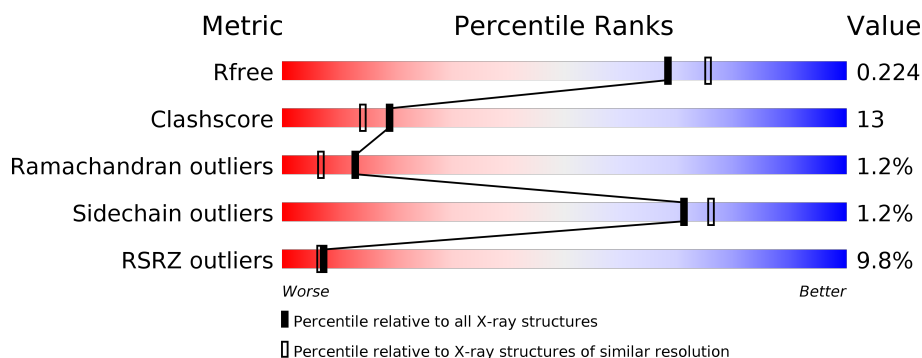
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	<div> <div>10%</div> <div>79%</div> <div>19%</div> </div>
2	B	2	<div> <div>50%</div> <div>50%</div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>

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
6	PZR	A	608	-	-	X	-
9	PEG	A	621	-	-	X	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5410 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4774	3037	847	863	1	26			

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



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

- Molecule 3 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
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

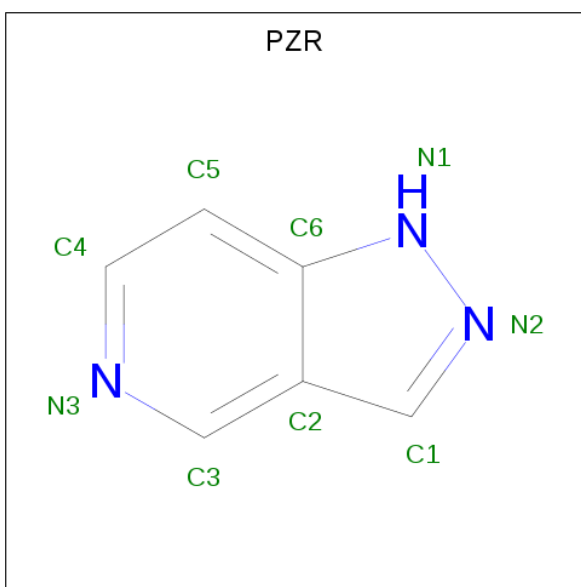
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total I 10 10	0	0

- Molecule 6 is 1H-pyrazolo[4,3-c]pyridine (three-letter code: PZR) (formula:  $C_6H_5N_3$ ).



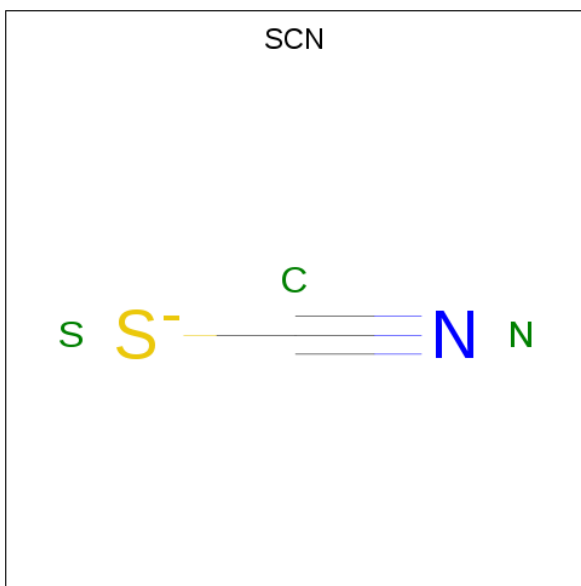
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			9	6	3		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



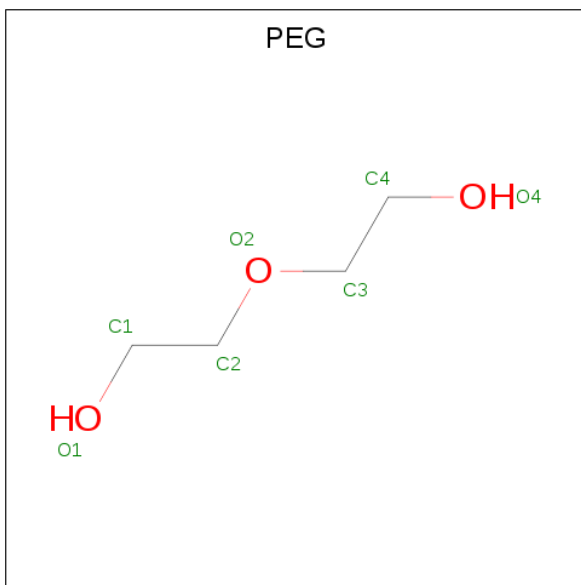
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



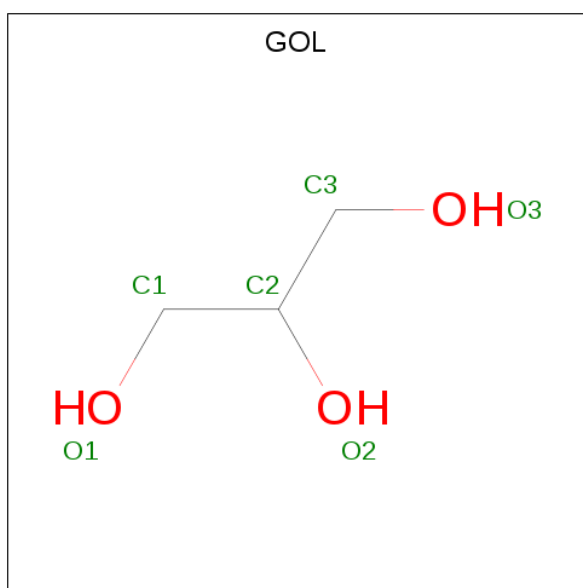
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is water.

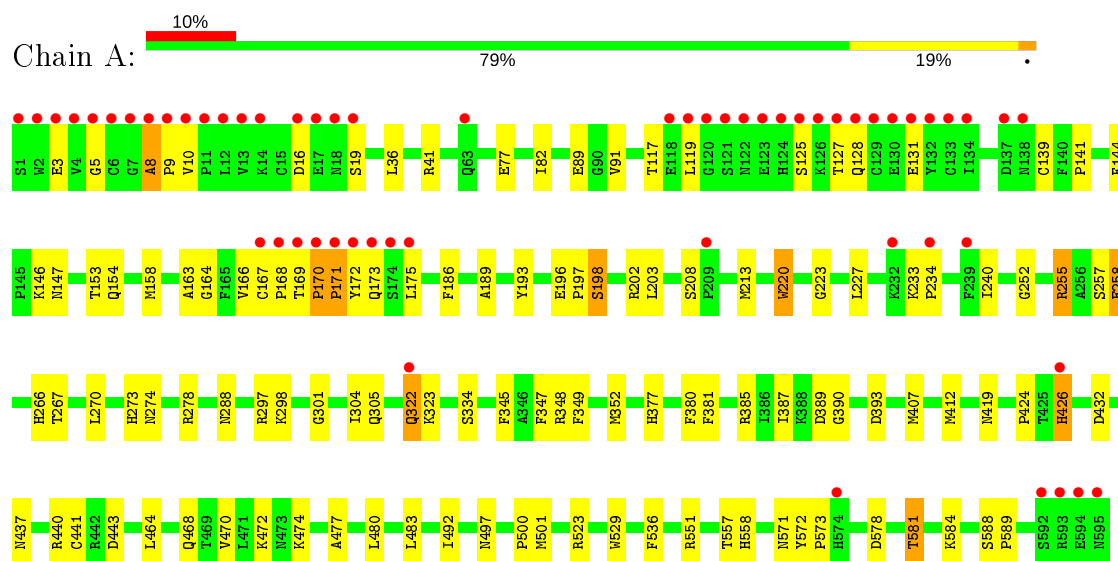
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	431	Total	O	0	0
			431	431		



### 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



- 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, $\alpha$ , $\beta$ , $\gamma$	53.35Å 80.33Å 73.39Å 90.00° 103.94° 90.00°	Depositor
Resolution (Å)	43.50 – 2.00 43.52 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (43.50-2.00) 96.5 (43.52-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.40 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.196 , 0.225 0.193 , 0.224	Depositor DCC
$R_{free}$ test set	1975 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5410	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SCN, NAG, SEP, CA, PZR, HEM, PEG, IOD

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	0.68	4/4891 (0.1%)	0.77	5/6634 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	ARG	CD-NE	-8.37	1.32	1.46
1	A	571	ASN	C-N	-5.74	1.20	1.34
1	A	186	PHE	CD1-CE1	-5.62	1.28	1.39
1	A	477	ALA	C-N	-5.38	1.21	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	HIS	CB-CA-C	5.60	121.60	110.40
1	A	258	GLU	CA-CB-CG	-5.50	101.30	113.40
1	A	166	VAL	N-CA-C	5.36	125.48	111.00
1	A	390	GLY	N-CA-C	5.26	126.24	113.10
1	A	255	ARG	CG-CD-NE	5.20	122.72	111.80

There are no chirality outliers.

There are no planarity outliers.

### 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	4774	0	4684	127	0
2	B	28	0	25	0	0
2	C	28	0	25	2	0
3	A	43	0	30	8	0
4	A	1	0	0	0	0
5	A	10	0	0	0	0
6	A	9	0	5	8	0
7	A	28	0	26	2	0
8	A	3	0	0	0	0
9	A	49	0	70	18	0
10	A	6	0	8	3	0
11	A	431	0	0	12	0
All	All	5410	0	4873	128	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 13.

All (128) 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:19:SER:HB2	11:A:885:HOH:O	1.36	1.20
1:A:322:GLN:HE21	1:A:322:GLN:CA	1.54	1.18
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.14	1.12
1:A:258:GLU:OE2	3:A:605:HEM:HMB3	1.57	1.04
1:A:322:GLN:HA	1:A:322:GLN:NE2	1.48	1.04
1:A:170:PRO:CB	1:A:171:PRO:HD3	1.96	0.94
1:A:472:LYS:NZ	9:A:621:PEG:H32	1.89	0.87
1:A:202:ARG:HH11	10:A:622:GOL:H11	1.37	0.87
1:A:348:ARG:CG	3:A:605:HEM:HMD3	2.05	0.86
1:A:322:GLN:HE21	1:A:322:GLN:HA	0.72	0.85
1:A:170:PRO:HB2	1:A:171:PRO:CD	2.04	0.84
1:A:163:ALA:HB2	1:A:440:ARG:NH1	1.93	0.82
1:A:258:GLU:OE2	3:A:605:HEM:CMB	2.33	0.77
1:A:470:VAL:HG22	9:A:620:PEG:H11	1.68	0.76
1:A:227:LEU:HD21	1:A:267:THR:HA	1.68	0.76
1:A:348:ARG:HG3	3:A:605:HEM:HMD3	1.67	0.75
1:A:202:ARG:NH1	10:A:622:GOL:H11	2.02	0.74
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.68	0.74
1:A:348:ARG:HG2	3:A:605:HEM:HMD3	1.68	0.73
1:A:407:MET:HB3	1:A:501:MET:CE	2.19	0.72
1:A:163:ALA:HB2	1:A:440:ARG:HH11	1.52	0.71
1:A:258:GLU:HG3	6:A:608:PZR:H3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:TRP:HB3	9:A:618:PEG:H31	1.75	0.66
1:A:172:TYR:HE2	1:A:175:LEU:H	1.43	0.66
1:A:197:PRO:HB3	9:A:619:PEG:H41	1.77	0.66
1:A:258:GLU:HG3	6:A:608:PZR:C3	2.26	0.66
1:A:197:PRO:CB	9:A:619:PEG:H41	2.27	0.65
1:A:407:MET:HB3	1:A:501:MET:HE1	1.81	0.63
3:A:605:HEM:HBD2	11:A:1019:HOH:O	1.99	0.62
1:A:227:LEU:HD13	1:A:270:LEU:HD22	1.82	0.62
1:A:393:ASP:OD2	1:A:558:HIS:HB2	2.00	0.61
1:A:258:GLU:HG3	6:A:608:PZR:C1	2.31	0.60
1:A:170:PRO:CB	1:A:171:PRO:CD	2.70	0.60
1:A:258:GLU:CG	6:A:608:PZR:H3	2.31	0.60
1:A:117:THR:HG22	1:A:164:GLY:HA2	1.84	0.59
1:A:500:PRO:HB2	9:A:621:PEG:H22	1.85	0.59
1:A:10:VAL:HB	1:A:41:ARG:NH2	2.18	0.58
1:A:352:MET:SD	1:A:407:MET:SD	3.01	0.58
1:A:472:LYS:HZ2	9:A:621:PEG:H32	1.68	0.58
1:A:8:ALA:H	1:A:9:PRO:CD	2.16	0.58
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.41	0.56
1:A:202:ARG:HD2	10:A:622:GOL:H32	1.87	0.55
1:A:258:GLU:CD	3:A:605:HEM:HMB3	2.25	0.55
1:A:258:GLU:HG3	6:A:608:PZR:C2	2.37	0.55
1:A:572:TYR:CD1	1:A:573:PRO:HA	2.42	0.54
1:A:501:MET:O	9:A:621:PEG:H21	2.07	0.54
1:A:472:LYS:HZ1	9:A:621:PEG:H32	1.67	0.54
1:A:227:LEU:HD23	11:A:728:HOH:O	2.07	0.54
1:A:470:VAL:CG2	9:A:620:PEG:H11	2.37	0.54
1:A:348:ARG:HG2	3:A:605:HEM:CMD	2.36	0.54
1:A:240:ILE:HD12	11:A:757:HOH:O	2.08	0.54
1:A:578:ASP:O	1:A:581:THR:HB	2.08	0.54
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.43	0.53
1:A:258:GLU:HG3	6:A:608:PZR:H1	1.90	0.53
1:A:158:MET:HE1	1:A:432:ASP:H	1.73	0.53
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.07	0.53
1:A:208:SER:HB3	2:C:1:NAG:H62	1.91	0.53
1:A:197:PRO:HB3	9:A:619:PEG:C4	2.39	0.53
1:A:119:LEU:HD13	1:A:170:PRO:HG3	1.90	0.53
1:A:472:LYS:CE	9:A:621:PEG:H32	2.38	0.53
1:A:8:ALA:N	1:A:9:PRO:CD	2.72	0.52
1:A:153:THR:HG22	1:A:154:GLN:HG3	1.92	0.52
1:A:257:SER:O	1:A:381:PHE:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:H	1:A:9:PRO:HD3	1.75	0.51
1:A:407:MET:HB3	1:A:501:MET:HE3	1.91	0.51
1:A:16:ASP:OD1	1:A:19:SER:HB3	2.10	0.51
1:A:441:CYS:SG	1:A:492:ILE:HG22	2.51	0.50
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.94	0.50
1:A:208:SER:CB	2:C:1:NAG:H62	2.42	0.50
1:A:193:TYR:CE1	1:A:297:ARG:HG3	2.46	0.50
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.75	0.50
1:A:127:THR:O	1:A:131:GLU:N	2.36	0.50
1:A:419:ASN:HD21	9:A:615:PEG:H32	1.77	0.50
1:A:322:GLN:CA	1:A:322:GLN:NE2	2.28	0.50
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.94	0.49
1:A:322:GLN:HG2	11:A:963:HOH:O	2.12	0.49
1:A:464:LEU:O	1:A:468:GLN:HG3	2.12	0.49
1:A:227:LEU:HD12	11:A:738:HOH:O	2.11	0.49
1:A:440:ARG:NH1	1:A:443:ASP:OD2	2.46	0.49
1:A:158:MET:CE	1:A:432:ASP:H	2.25	0.49
1:A:266:HIS:HE1	11:A:670:HOH:O	1.96	0.49
1:A:220:TRP:CE3	9:A:618:PEG:H32	2.48	0.48
1:A:220:TRP:HE3	9:A:618:PEG:H32	1.78	0.48
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.48	0.48
1:A:393:ASP:OD1	1:A:557:THR:HB	2.14	0.48
1:A:172:TYR:OH	1:A:175:LEU:HB2	2.14	0.48
1:A:227:LEU:HD21	1:A:267:THR:CA	2.42	0.48
1:A:223:GLY:HA3	11:A:1034:HOH:O	2.14	0.48
1:A:298:LYS:HG2	1:A:536:PHE:CZ	2.49	0.47
1:A:117:THR:CG2	1:A:164:GLY:HA2	2.44	0.47
1:A:146:LYS:O	1:A:147:ASN:HB2	2.15	0.47
1:A:255:ARG:HD2	6:A:608:PZR:C4	2.45	0.47
1:A:255:ARG:HD2	6:A:608:PZR:C5	2.46	0.46
1:A:440:ARG:HD2	11:A:666:HOH:O	2.16	0.46
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.28	0.46
1:A:227:LEU:CD2	1:A:267:THR:HA	2.42	0.45
1:A:36:LEU:CD2	9:A:616:PEG:H42	2.46	0.45
1:A:91:VAL:O	1:A:91:VAL:HG22	2.17	0.45
1:A:220:TRP:CD1	1:A:220:TRP:C	2.89	0.45
1:A:82:ILE:HD13	1:A:480:LEU:CD2	2.47	0.45
1:A:278:ARG:HD2	11:A:905:HOH:O	2.17	0.44
1:A:77:GLU:HG2	1:A:483:LEU:HD21	1.99	0.44
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.43	0.44
1:A:345:PHE:CE2	1:A:440:ARG:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD11	1:A:252:GLY:HA2	1.99	0.44
1:A:323:LYS:HD2	11:A:977:HOH:O	2.17	0.43
1:A:144:PHE:CE2	1:A:158:MET:HG3	2.53	0.43
1:A:163:ALA:N	1:A:440:ARG:HH12	2.16	0.43
1:A:301:GLY:O	1:A:305:GLN:HG3	2.18	0.43
1:A:584:LYS:NZ	1:A:584:LYS:HB3	2.33	0.43
1:A:36:LEU:HD21	9:A:616:PEG:H42	2.01	0.43
1:A:468:GLN:CD	1:A:474:LYS:HG2	2.39	0.42
1:A:233:LYS:HA	1:A:234:PRO:C	2.39	0.42
1:A:385:ARG:O	1:A:389:ASP:HB3	2.19	0.42
1:A:3:GLU:O	1:A:3:GLU:HG2	2.18	0.42
1:A:426:HIS:HA	11:A:922:HOH:O	2.20	0.42
1:A:189:ALA:HB2	1:A:304:ILE:HD12	2.02	0.41
1:A:334:SER:HB2	7:A:613:NAG:H5	2.01	0.41
1:A:387:ILE:CG2	9:A:617:PEG:H21	2.50	0.41
1:A:125:SER:HA	1:A:128:GLN:HB3	2.01	0.41
1:A:274:ASN:O	1:A:278:ARG:HG3	2.21	0.41
1:A:139:CYS:SG	1:A:141:PRO:HG3	2.60	0.41
1:A:196:GLU:HB3	1:A:198:SEP:OG	2.21	0.41
1:A:82:ILE:HD11	1:A:483:LEU:HD12	2.03	0.40
1:A:322:GLN:HE21	1:A:322:GLN:N	2.09	0.40
1:A:407:MET:HE3	1:A:412:MET:HG2	2.03	0.40
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.67	0.40
1:A:334:SER:CB	7:A:613:NAG:H5	2.51	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	592/595 (100%)	560 (95%)	25 (4%)	7 (1%)	<b>13</b> <b>7</b>

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	PRO
1	A	173	GLN
1	A	424	PRO
1	A	169	THR
1	A	5	GLY
1	A	8	ALA
1	A	171	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	517/517 (100%)	511 (99%)	6 (1%)	71	76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLU
1	A	220	TRP
1	A	288	ASN
1	A	322	GLN
1	A	347	PHE
1	A	581	THR

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

Mol	Chain	Res	Type
1	A	18	ASN
1	A	266	HIS
1	A	288	ASN
1	A	322	GLN
1	A	437	ASN
1	A	497	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	SEP	A	198	1	8,9,10	1.00	0	8,12,14	2.28	4 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	198	1	-	5/5/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O3P-P-OG	3.14	115.08	106.73
1	A	198	SEP	O2P-P-OG	3.09	114.95	106.73
1	A	198	SEP	O3P-P-O1P	-2.78	99.80	110.68
1	A	198	SEP	OG-CB-CA	2.64	110.71	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

## 5.5 Carbohydrates [i](#)

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	1	1,2	14,14,15	0.26	0	17,19,21	1.02	1 (5%)
2	NAG	B	2	2	14,14,15	0.58	0	17,19,21	0.66	0
2	NAG	C	1	1,2	14,14,15	1.22	2 (14%)	17,19,21	1.88	3 (17%)
2	NAG	C	2	2	14,14,15	0.73	0	17,19,21	2.32	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	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	-2.53	1.39	1.43
2	C	1	NAG	O7-C7	-2.39	1.17	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C2-N2-C7	-6.99	112.95	122.90
2	C	1	NAG	C1-C2-N2	-5.57	100.97	110.49
2	C	1	NAG	O5-C1-C2	-3.35	106.00	111.29
2	C	2	NAG	O6-C6-C5	-3.27	100.06	111.29
2	B	1	NAG	C1-C2-N2	-3.23	104.96	110.49
2	C	2	NAG	C1-C2-N2	-3.23	104.97	110.49
2	C	1	NAG	C1-O5-C5	2.47	115.53	112.19
2	C	2	NAG	O5-C1-C2	-2.23	107.77	111.29
2	C	2	NAG	O5-C5-C4	2.08	115.89	110.83
2	C	2	NAG	C3-C4-C5	2.07	113.93	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

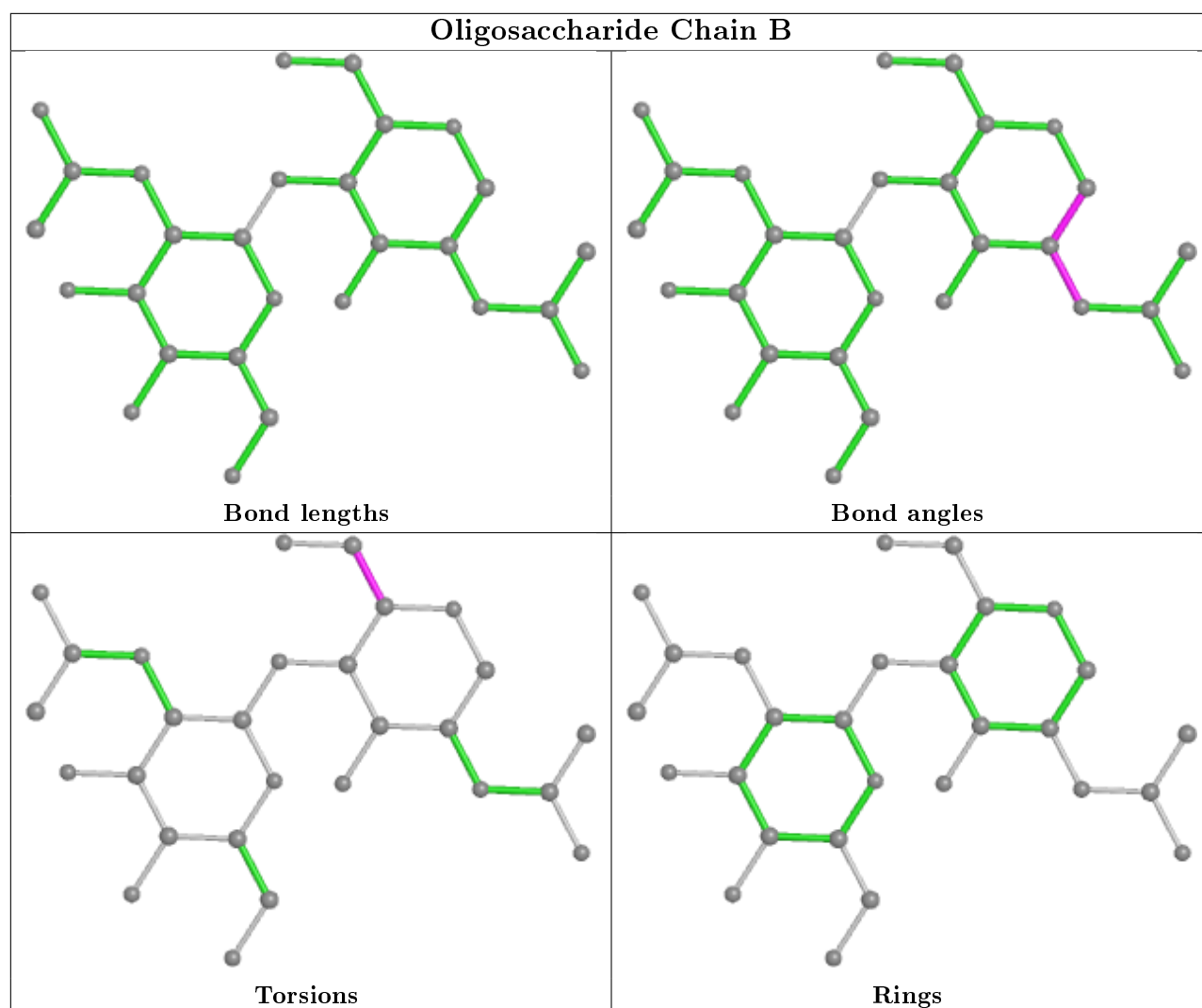
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

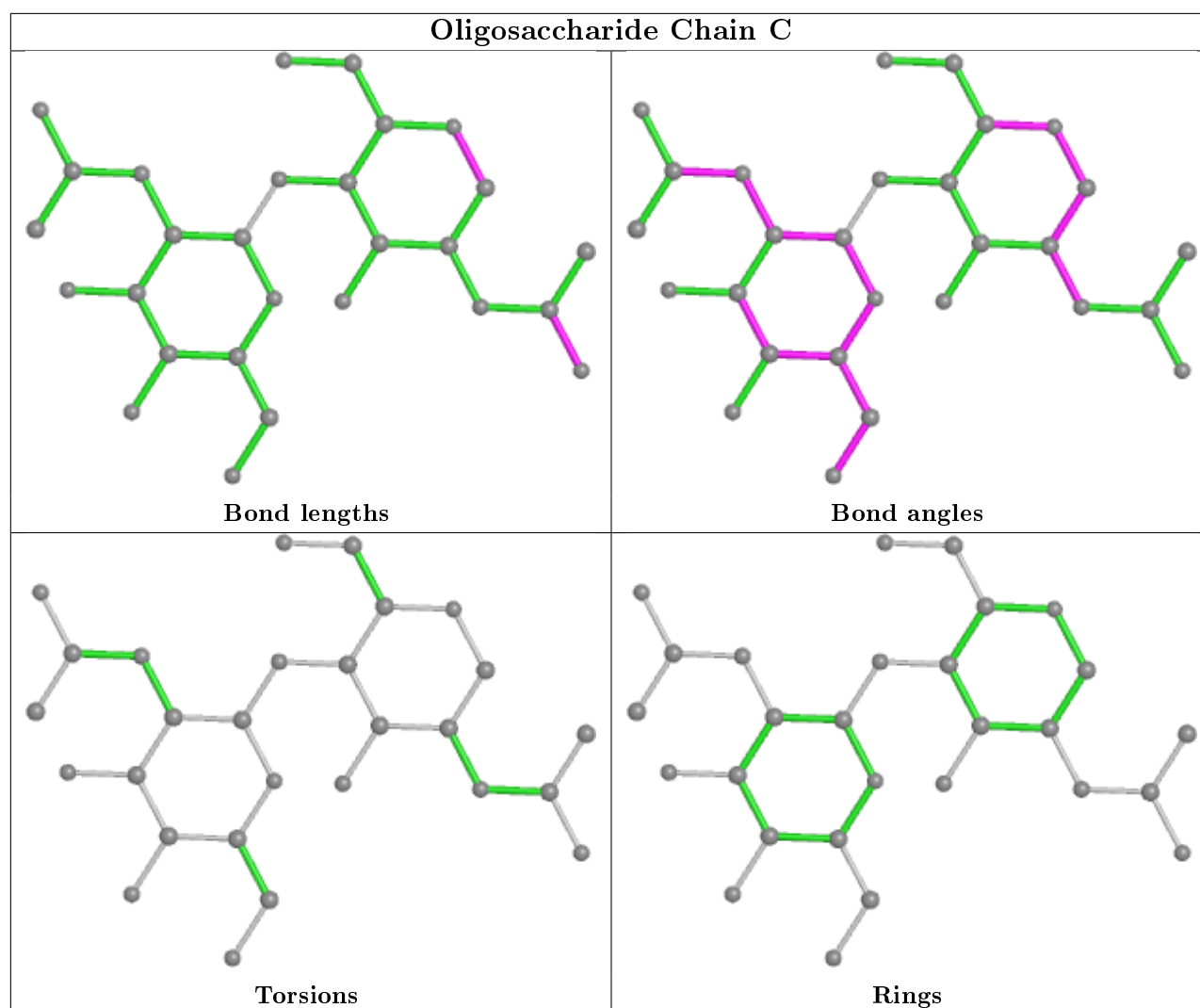
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	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 oligosaccharide.





## 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 11 are monoatomic - leaving 13 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	$\# Z  > 2$
6	PZR	A	608	-	8,10,10	1.44	2 (25%)	8,13,13	1.63	1 (12%)
9	PEG	A	618	-	6,6,6	1.10	0	5,5,5	2.45	2 (40%)
9	PEG	A	620	-	6,6,6	0.93	0	5,5,5	1.27	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SCN	A	6788	-	1,2,2	0.08	0	0,1,1	0.00	-
7	NAG	A	614	1	14,14,15	0.76	0	17,19,21	1.41	3 (17%)
9	PEG	A	617	-	6,6,6	0.77	0	5,5,5	2.17	1 (20%)
10	GOL	A	622	-	5,5,5	0.34	0	5,5,5	2.55	1 (20%)
3	HEM	A	605	1,11	27,50,50	2.46	10 (37%)	17,82,82	4.68	11 (64%)
7	NAG	A	613	1	14,14,15	0.67	0	17,19,21	1.87	5 (29%)
9	PEG	A	616	-	6,6,6	1.14	0	5,5,5	2.36	2 (40%)
9	PEG	A	621	-	6,6,6	0.85	0	5,5,5	2.35	2 (40%)
9	PEG	A	619	-	6,6,6	0.98	0	5,5,5	2.61	2 (40%)
9	PEG	A	615	-	6,6,6	0.82	0	5,5,5	2.22	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 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
6	PZR	A	608	-	-	-	0/2/2/2
9	PEG	A	618	-	-	2/4/4/4	-
9	PEG	A	620	-	-	1/4/4/4	-
7	NAG	A	614	1	-	2/6/23/26	0/1/1/1
9	PEG	A	617	-	-	2/4/4/4	-
10	GOL	A	622	-	-	3/4/4/4	-
3	HEM	A	605	1,11	-	0/6/54/54	-
7	NAG	A	613	1	-	0/6/23/26	0/1/1/1
9	PEG	A	616	-	-	2/4/4/4	-
9	PEG	A	621	-	-	1/4/4/4	-
9	PEG	A	619	-	-	2/4/4/4	-
9	PEG	A	615	-	-	1/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	HEM	C4D-C3D	5.09	1.54	1.42
3	A	605	HEM	C1D-CHD	4.99	1.54	1.41
3	A	605	HEM	C3D-C2D	4.30	1.50	1.37
3	A	605	HEM	C1D-ND	-4.14	1.27	1.36
3	A	605	HEM	C3B-CAB	3.58	1.55	1.47
3	A	605	HEM	C1A-NA	-3.58	1.28	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	HEM	C2A-C3A	3.20	1.47	1.37
3	A	605	HEM	C1A-CHA	3.17	1.49	1.41
6	A	608	PZR	C1-C2	2.72	1.46	1.40
6	A	608	PZR	C5-C6	-2.51	1.37	1.41
3	A	605	HEM	C3C-CAC	2.48	1.52	1.47
3	A	605	HEM	C3B-C2B	-2.44	1.37	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	605	HEM	CAD-CBD-CGD	-9.01	97.55	112.67
3	A	605	HEM	CBD-CAD-C3D	6.93	125.25	112.48
3	A	605	HEM	C1D-C2D-C3D	-6.91	102.19	107.00
3	A	605	HEM	CMD-C2D-C1D	-6.50	118.47	128.46
3	A	605	HEM	CMC-C2C-C3C	6.23	136.33	124.68
3	A	605	HEM	CBA-CAA-C2A	-6.10	101.23	112.49
10	A	622	GOL	O2-C2-C3	-5.67	84.14	109.12
3	A	605	HEM	CMD-C2D-C3D	-4.96	115.59	124.94
9	A	619	PEG	O2-C3-C4	-4.67	89.53	110.07
7	A	613	NAG	C1-C2-N2	-4.63	102.58	110.49
9	A	618	PEG	O2-C3-C4	-4.43	90.60	110.07
9	A	616	PEG	O2-C3-C4	-4.40	90.74	110.07
9	A	615	PEG	O2-C3-C4	-4.37	90.88	110.07
9	A	617	PEG	O2-C3-C4	-4.19	91.68	110.07
9	A	621	PEG	O2-C3-C4	-3.64	94.08	110.07
9	A	621	PEG	C3-O2-C2	3.63	129.00	113.29
6	A	608	PZR	C5-C6-N1	3.53	135.94	130.19
3	A	605	HEM	C4A-C3A-C2A	-3.46	104.59	107.00
7	A	613	NAG	O5-C1-C2	-3.19	106.26	111.29
3	A	605	HEM	CAD-C3D-C2D	-3.15	118.21	127.25
7	A	614	NAG	C1-O5-C5	-2.96	108.19	112.19
3	A	605	HEM	C4C-C3C-C2C	2.91	108.93	106.90
9	A	619	PEG	C3-O2-C2	2.90	125.87	113.29
3	A	605	HEM	C3B-C4B-NB	2.72	112.72	109.21
7	A	614	NAG	O6-C6-C5	-2.60	102.38	111.29
7	A	613	NAG	O5-C5-C6	2.54	111.18	107.20
7	A	613	NAG	O5-C5-C4	-2.51	104.72	110.83
7	A	614	NAG	C2-N2-C7	-2.50	119.35	122.90
9	A	618	PEG	C3-O2-C2	2.46	123.93	113.29
7	A	613	NAG	O4-C4-C3	-2.43	104.74	110.35
9	A	620	PEG	O2-C3-C4	-2.37	99.67	110.07
9	A	616	PEG	C3-O2-C2	2.29	123.21	113.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	619	PEG	C1-C2-O2-C3
10	A	622	GOL	O1-C1-C2-O2
9	A	615	PEG	O1-C1-C2-O2
9	A	617	PEG	O1-C1-C2-O2
9	A	616	PEG	O1-C1-C2-O2
10	A	622	GOL	O1-C1-C2-C3
7	A	614	NAG	C4-C5-C6-O6
7	A	614	NAG	O5-C5-C6-O6
9	A	621	PEG	O1-C1-C2-O2
9	A	618	PEG	O1-C1-C2-O2
9	A	620	PEG	O1-C1-C2-O2
9	A	619	PEG	O1-C1-C2-O2
10	A	622	GOL	C1-C2-C3-O3
9	A	616	PEG	C1-C2-O2-C3
9	A	617	PEG	C1-C2-O2-C3
9	A	618	PEG	C1-C2-O2-C3

There are no ring outliers.

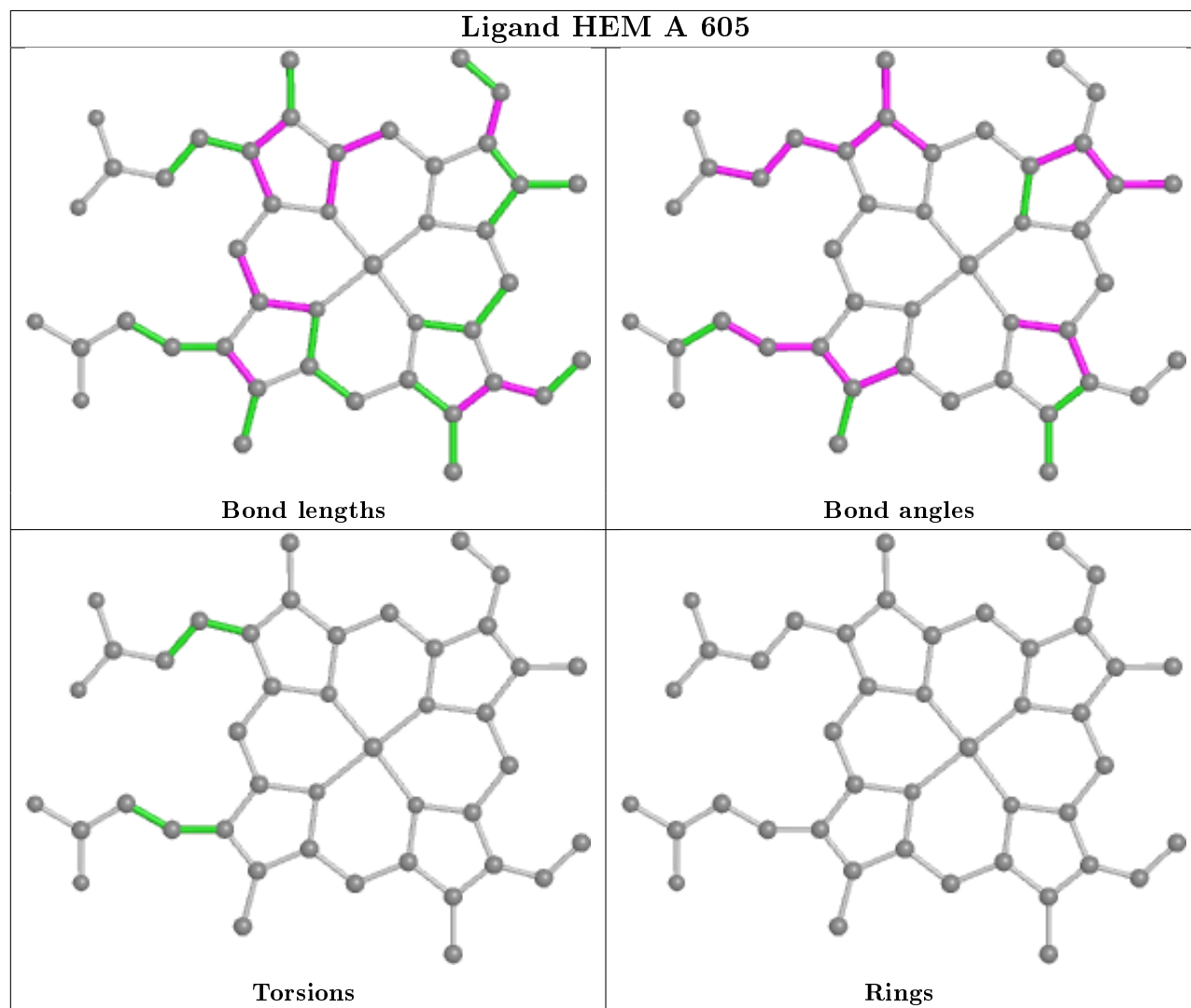
11 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	608	PZR	8	0
9	A	618	PEG	3	0
9	A	620	PEG	2	0
9	A	617	PEG	1	0
10	A	622	GOL	3	0
3	A	605	HEM	8	0
7	A	613	NAG	2	0
9	A	616	PEG	2	0
9	A	621	PEG	6	0
9	A	619	PEG	3	0
9	A	615	PEG	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 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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	594/595 (99%)	0.55	58 (9%) 7 7	12, 23, 76, 115	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	20.1
1	A	121	SER	18.6
1	A	172	TYR	15.6
1	A	13	VAL	15.4
1	A	173	GLN	13.4
1	A	119	LEU	12.6
1	A	5	GLY	11.9
1	A	6	CYS	11.8
1	A	122	ASN	11.3
1	A	7	GLY	11.1
1	A	120	GLY	11.0
1	A	124	HIS	10.6
1	A	3	GLU	9.2
1	A	595	ASN	8.7
1	A	8	ALA	8.4
1	A	132	TYR	7.4
1	A	11	PRO	7.1
1	A	10	VAL	7.1
1	A	128	GLN	6.9
1	A	118	GLU	6.8
1	A	12	LEU	6.4
1	A	171	PRO	6.3
1	A	127	THR	6.2
1	A	1	SER	6.2
1	A	125	SER	6.1
1	A	129	CYS	6.0
1	A	123	GLU	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	169	THR	6.0
1	A	234	PRO	5.9
1	A	4	VAL	5.8
1	A	170	PRO	5.1
1	A	594	GLU	5.0
1	A	19	SER	4.5
1	A	126	LYS	4.4
1	A	168	PRO	4.3
1	A	134	ILE	4.2
1	A	18	ASN	3.8
1	A	593	ARG	3.7
1	A	167	CYS	3.7
1	A	174	SER	3.5
1	A	14	LYS	3.4
1	A	131	GLU	3.3
1	A	175	LEU	3.2
1	A	16	ASP	3.1
1	A	9	PRO	3.1
1	A	138	ASN	3.1
1	A	17	GLU	2.9
1	A	426	HIS	2.7
1	A	63	GLN	2.7
1	A	137	ASP	2.5
1	A	130	GLU	2.4
1	A	574	HIS	2.3
1	A	133	CYS	2.2
1	A	209	PRO	2.2
1	A	232	LYS	2.2
1	A	322	GLN	2.1
1	A	239	PHE	2.0
1	A	592	SER	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<sup>th</sup> 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.

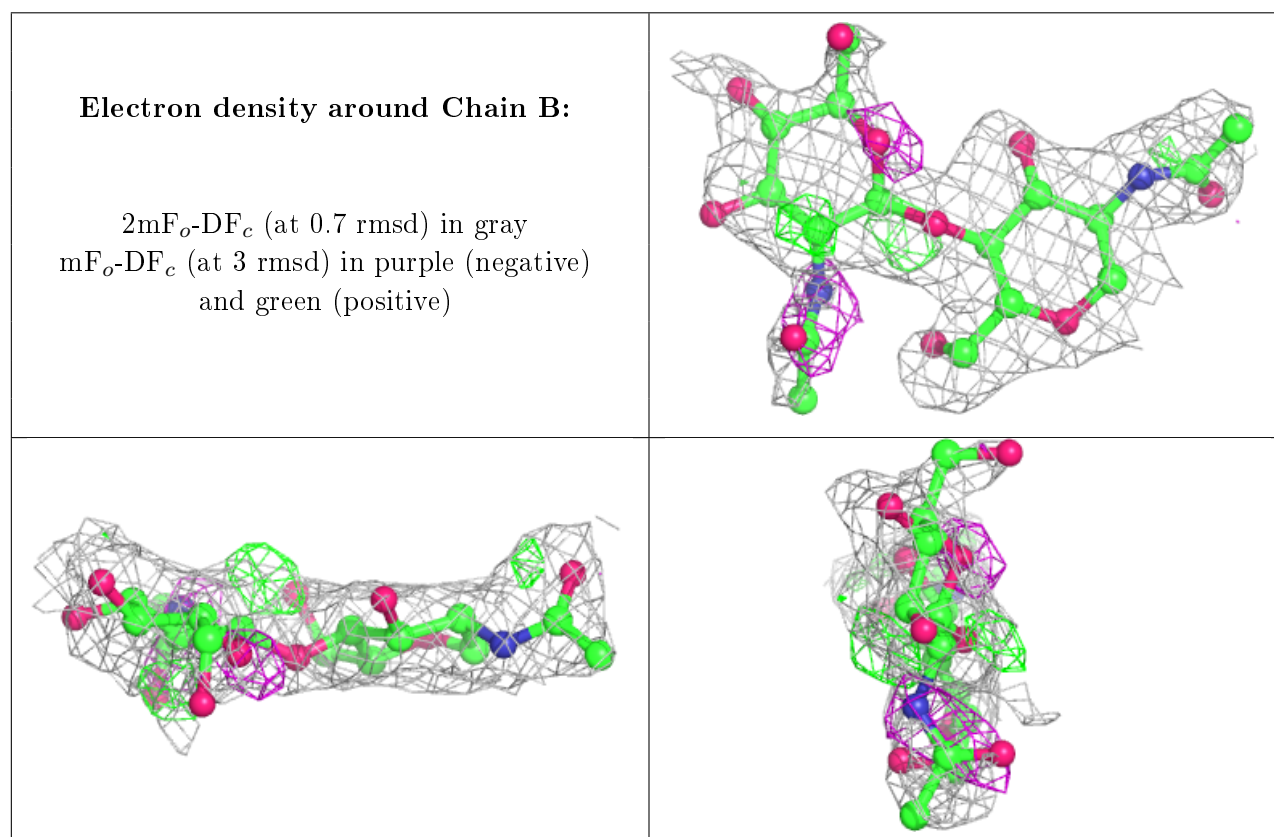
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	SEP	A	198	10/11	0.72	0.25	34,38,44,45	0

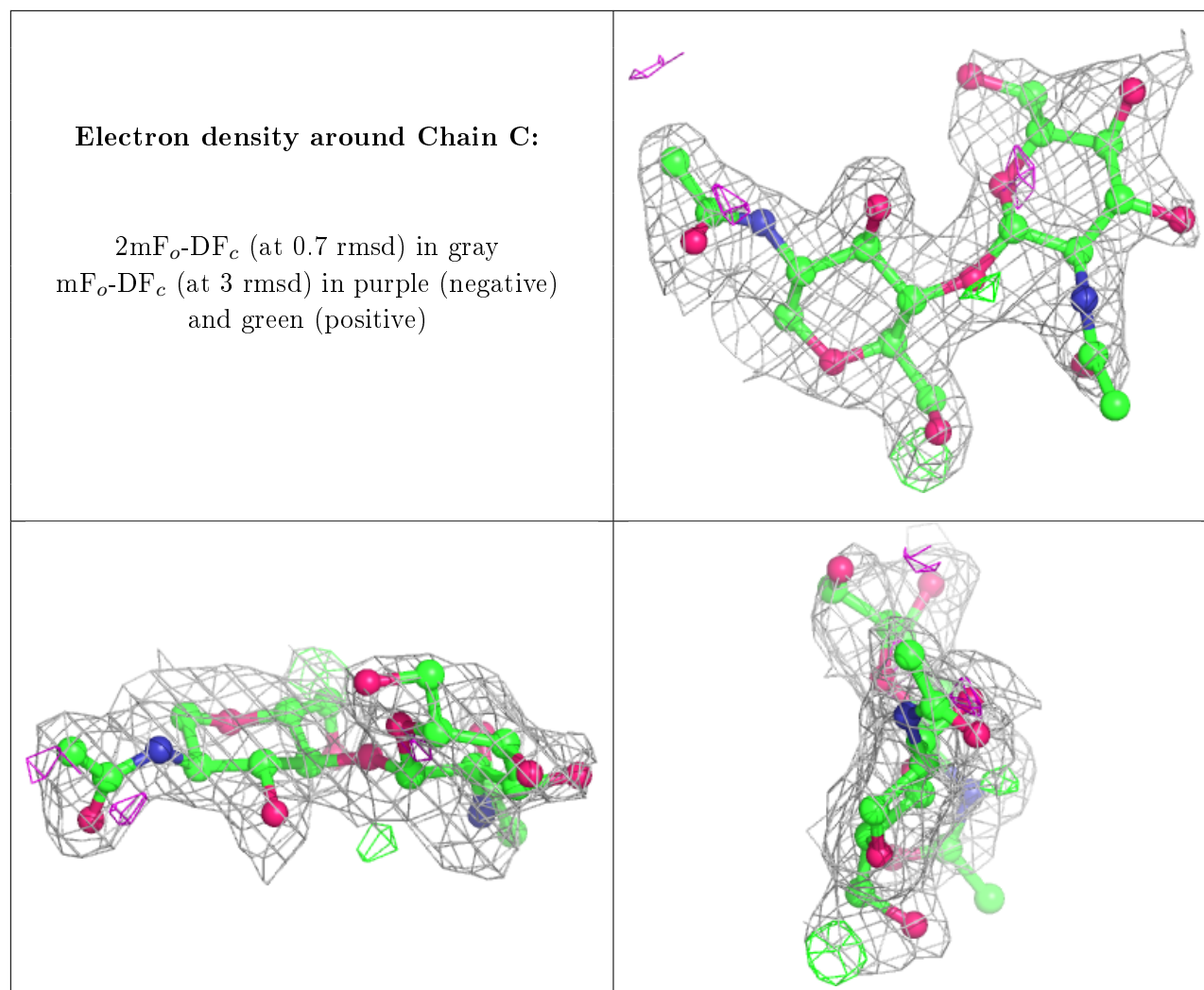
### 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	2	14/15	0.59	0.36	40,43,46,48	0
2	NAG	C	2	14/15	0.79	0.30	42,45,46,48	0
2	NAG	B	1	14/15	0.82	0.17	34,40,42,42	0
2	NAG	C	1	14/15	0.89	0.12	28,39,42,43	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 ⓘ

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<sup>th</sup> 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.

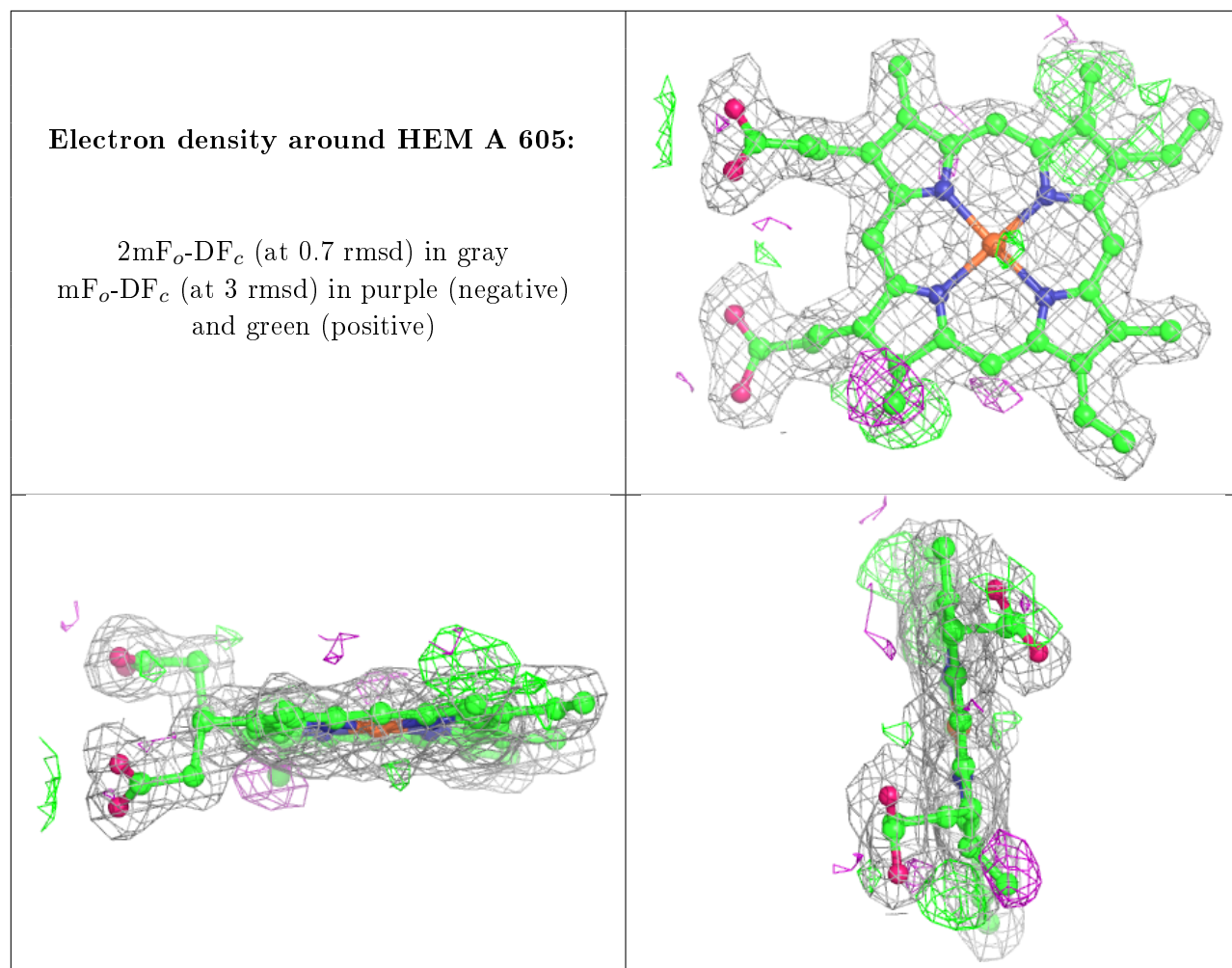
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	GOL	A	622	6/6	0.67	0.28	20,21,22,23	0
9	PEG	A	620	7/7	0.70	0.25	49,50,51,51	0
9	PEG	A	618	7/7	0.74	0.20	52,52,52,53	0
9	PEG	A	616	7/7	0.75	0.20	46,48,50,51	0
9	PEG	A	621	7/7	0.77	0.24	50,51,51,51	0
9	PEG	A	617	7/7	0.80	0.15	53,53,53,53	0
8	SCN	A	6788	3/3	0.81	0.15	24,24,25,30	0
6	PZR	A	608	9/9	0.81	0.39	28,30,32,32	0
7	NAG	A	613	14/15	0.84	0.26	36,40,44,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	A	614	14/15	0.84	0.29	30,35,39,44	0
9	PEG	A	619	7/7	0.87	0.16	37,40,44,45	0
9	PEG	A	615	7/7	0.89	0.19	26,26,28,29	0
5	IOD	A	602	1/1	0.94	0.08	54,54,54,54	1
3	HEM	A	605	43/43	0.95	0.17	12,13,17,18	0
5	IOD	A	603	1/1	0.96	0.07	85,85,85,85	0
5	IOD	A	597	1/1	0.97	0.07	61,61,61,61	1
5	IOD	A	599	1/1	0.98	0.09	14,14,14,14	1
4	CA	A	606	1/1	0.98	0.13	18,18,18,18	0
5	IOD	A	598	1/1	0.99	0.15	17,17,17,17	1
5	IOD	A	607	1/1	0.99	0.23	50,50,50,50	0
5	IOD	A	604	1/1	0.99	0.05	44,44,44,44	0
5	IOD	A	596	1/1	0.99	0.09	24,24,24,24	1
5	IOD	A	600	1/1	1.00	0.14	14,14,14,14	1
5	IOD	A	601	1/1	1.00	0.17	8,8,8,8	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 ⓘ

There are no such residues in this entry.