



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 03:09 PM EDT

PDB ID : 3R4X
Title : Crystal structure of bovine lactoperoxidase complexed with pyrazine-2-carboxamide at 2 Å resolution
Authors : Pandey, N.; Singh, R.P.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2011-03-18
Resolution : 2.01 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

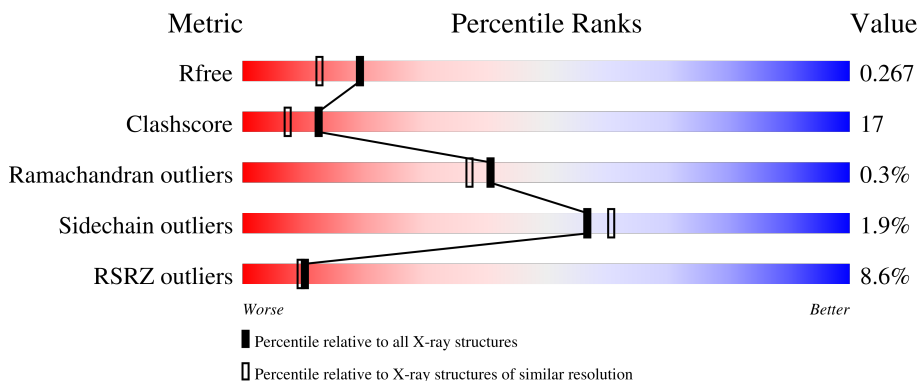
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



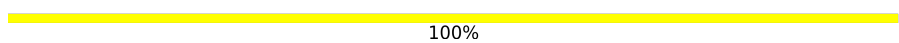
The reported resolution of this entry is 2.01 Å.

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	595	
2	B	2	
2	C	2	

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
11	GOL	A	621	-	X	X	-
2	NAG	B	2	-	-	-	X
6	IOD	A	612	-	-	X	-
9	PZA	A	597	-	-	X	X
9	PZA	A	598	-	-	X	-

2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 5468 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Lactoperoxidase.

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

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



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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

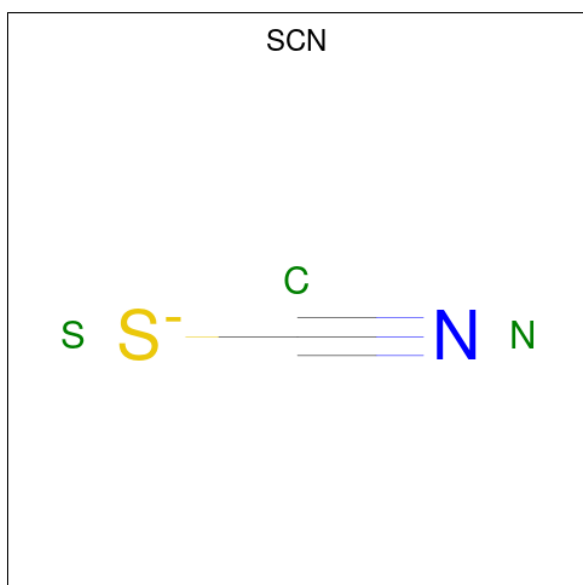
- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	11	Total I 11 11	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

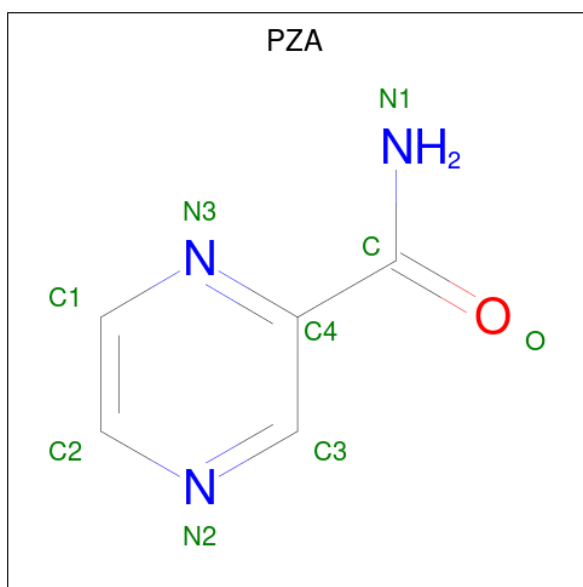
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Zn 1 1	0	0

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



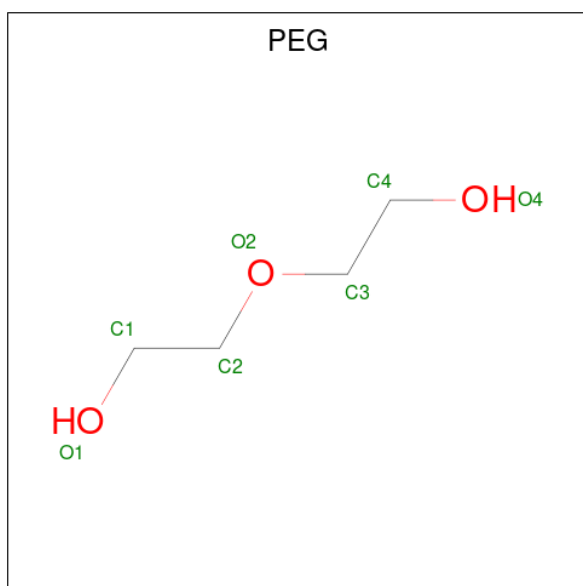
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N S 3 1 1 1	0	0

- Molecule 9 is PYRAZINE-2-CARBOXAMIDE (three-letter code: PZA) (formula: C₅H₅N₃O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			9	5	3	1		
9	A	1	Total	C	N	O	0	0
			9	5	3	1		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



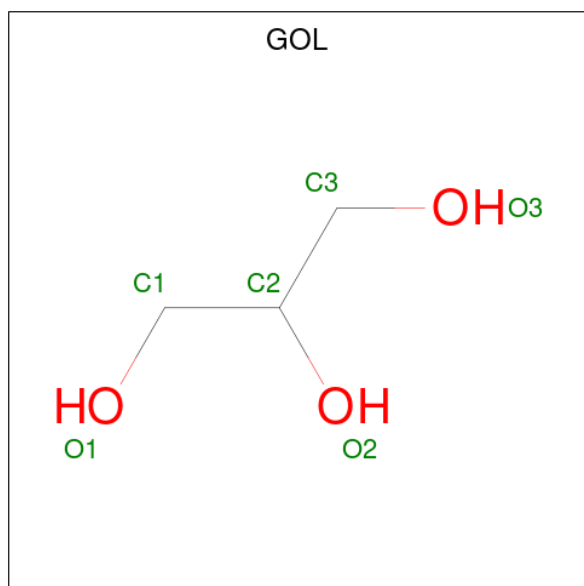
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

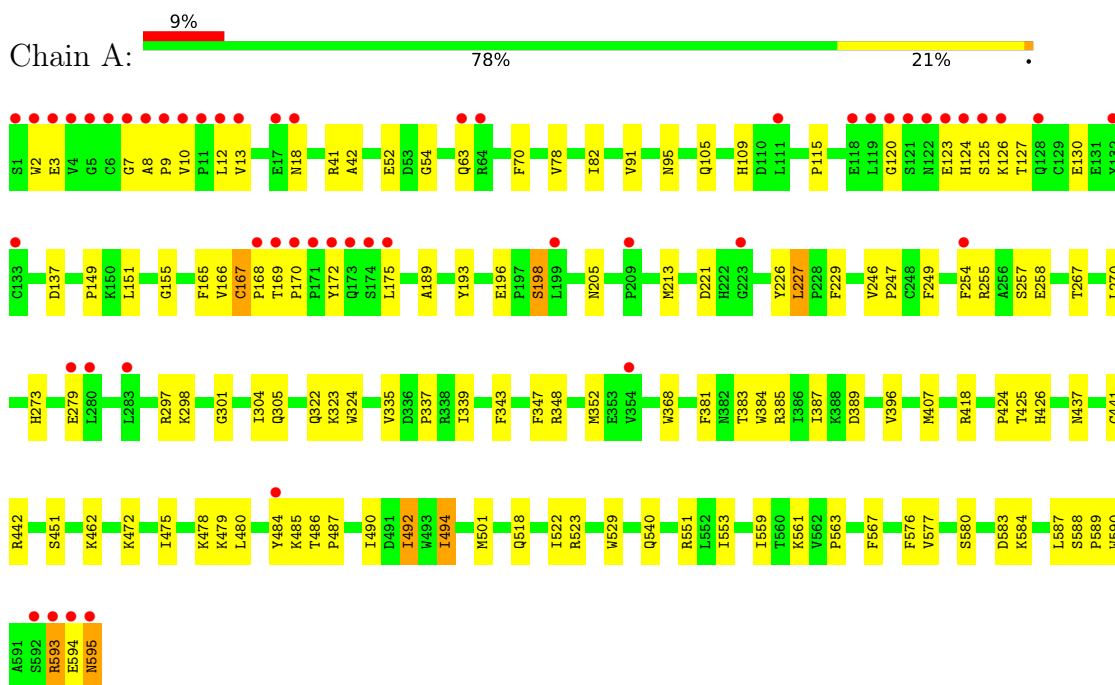
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	499	Total O 499 499	0	0

3 Residue-property plots

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

Chain B: 



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

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.92Å 79.72Å 77.00Å 90.00° 102.22° 90.00°	Depositor
Resolution (Å)	75.26 – 2.01 43.96 – 2.01	Depositor EDS
% Data completeness (in resolution range)	97.8 (75.26-2.01) 97.8 (43.96-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 2.01Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.210 , 0.256 0.228 , 0.267	Depositor DCC
R_{free} test set	2106 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtrriage
Anisotropy	0.908	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5468	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.74	0/4891	0.85	2/6634 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	227	LEU	CA-CB-CG	5.15	127.14	115.30

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	4774	0	4687	150	0
2	B	28	0	25	0	0
2	C	28	0	25	1	0
3	A	1	0	0	0	0
4	A	43	0	30	7	0
5	A	28	0	26	4	0
6	A	11	0	0	4	0
7	A	1	0	0	0	0
8	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	18	0	10	18	0
10	A	14	0	20	4	0
11	A	12	0	14	6	0
12	A	8	0	12	1	0
13	A	499	0	0	21	0
All	All	5468	0	4849	165	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 17.

All (165) 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:12:LEU:HD23	1:A:13:VAL:N	1.40	1.36
1:A:10:VAL:HG11	1:A:41:ARG:CZ	1.65	1.26
5:A:596:NAG:O7	11:A:621:GOL:H11	1.39	1.20
1:A:424:PRO:O	1:A:425:THR:HG22	1.37	1.19
1:A:593:ARG:HH11	1:A:593:ARG:HG2	0.96	1.11
1:A:123:GLU:HG3	1:A:125:SER:H	1.00	1.08
1:A:167:CYS:CB	1:A:168:PRO:CD	2.31	1.08
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.28	1.07
1:A:105:GLN:HE21	9:A:597:PZA:H2	1.02	1.02
1:A:167:CYS:HB3	1:A:168:PRO:CD	1.91	1.00
1:A:167:CYS:HB3	1:A:168:PRO:HD3	1.46	0.97
1:A:167:CYS:CB	1:A:168:PRO:HD2	1.92	0.96
1:A:169:THR:HB	1:A:170:PRO:HD3	1.48	0.95
1:A:593:ARG:HG2	1:A:593:ARG:NH1	1.71	0.93
1:A:123:GLU:HG3	1:A:125:SER:N	1.83	0.93
1:A:196:GLU:HB3	1:A:198:SEP:O3P	1.70	0.90
9:A:597:PZA:H5	9:A:598:PZA:C	2.02	0.90
1:A:10:VAL:CG1	1:A:41:ARG:CZ	2.52	0.87
1:A:593:ARG:HH11	1:A:593:ARG:CG	1.85	0.87
1:A:168:PRO:HG3	1:A:172:TYR:HD1	1.38	0.86
1:A:54:GLY:HA2	13:A:936:HOH:O	1.74	0.85
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.57	0.85
1:A:12:LEU:HD23	1:A:13:VAL:H	1.41	0.85
1:A:279:GLU:HG2	1:A:587:LEU:HD12	1.57	0.85
1:A:12:LEU:CD2	1:A:13:VAL:N	2.34	0.84
1:A:255:ARG:HA	9:A:598:PZA:N2	1.94	0.82
1:A:9:PRO:CD	1:A:167:CYS:HA	2.10	0.81
1:A:12:LEU:HD23	1:A:12:LEU:C	2.00	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:PRO:O	1:A:425:THR:CG2	2.28	0.79
1:A:462:LYS:HD2	13:A:974:HOH:O	1.83	0.78
1:A:10:VAL:HG11	1:A:41:ARG:NH2	2.00	0.77
1:A:105:GLN:NE2	9:A:597:PZA:H2	1.82	0.75
1:A:124:HIS:HB2	1:A:127:THR:HB	1.68	0.75
1:A:10:VAL:CG1	1:A:41:ARG:NH2	2.50	0.74
1:A:168:PRO:HG3	1:A:172:TYR:CD1	2.21	0.74
1:A:339:ILE:HD13	1:A:522:ILE:HD11	1.71	0.72
1:A:9:PRO:HG2	1:A:167:CYS:O	1.92	0.70
1:A:95:ASN:HD22	11:A:621:GOL:H12	1.57	0.69
1:A:109:HIS:NE2	9:A:597:PZA:C	2.56	0.69
1:A:396:VAL:HG11	1:A:553:ILE:HD12	1.74	0.69
1:A:105:GLN:HG3	9:A:597:PZA:N1	2.08	0.68
1:A:12:LEU:HD23	1:A:13:VAL:CA	2.23	0.68
1:A:9:PRO:HG2	1:A:167:CYS:CA	2.24	0.68
1:A:10:VAL:HG11	1:A:41:ARG:NH1	2.08	0.67
1:A:494:ILE:HD13	1:A:494:ILE:O	1.94	0.67
1:A:127:THR:HA	13:A:1122:HOH:O	1.95	0.67
1:A:227:LEU:HD22	1:A:270:LEU:HD22	1.75	0.67
1:A:105:GLN:HG3	9:A:597:PZA:H1	1.62	0.65
1:A:258:GLU:HB2	9:A:598:PZA:H4	1.77	0.65
1:A:12:LEU:CD2	1:A:12:LEU:C	2.66	0.64
6:A:614:IOD:I	13:A:1014:HOH:O	2.85	0.64
1:A:418:ARG:HH22	10:A:603:PEG:C4	2.11	0.64
1:A:105:GLN:NE2	9:A:597:PZA:H4	2.13	0.63
1:A:475:ILE:HG22	1:A:479:LYS:HE3	1.81	0.62
1:A:9:PRO:HD2	1:A:167:CYS:HA	1.81	0.62
1:A:78:VAL:HG21	1:A:484:TYR:OH	2.00	0.61
1:A:82:ILE:HD13	1:A:480:LEU:HD23	1.83	0.61
1:A:169:THR:N	1:A:170:PRO:CD	2.63	0.61
9:A:597:PZA:H5	9:A:598:PZA:N1	2.16	0.60
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.36	0.60
1:A:165:PHE:CZ	1:A:169:THR:O	2.54	0.60
1:A:559:ILE:HG23	6:A:607:IOD:I	2.73	0.59
1:A:63:GLN:H	1:A:63:GLN:CD	2.06	0.58
1:A:105:GLN:HE21	9:A:597:PZA:H4	1.69	0.58
1:A:407:MET:HB3	1:A:501:MET:HE3	1.86	0.57
1:A:492:ILE:O	1:A:492:ILE:HD13	2.05	0.57
1:A:168:PRO:HB2	1:A:170:PRO:O	2.06	0.56
1:A:18:ASN:ND2	13:A:1008:HOH:O	2.37	0.56
1:A:594:GLU:O	1:A:595:ASN:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:PHE:CG	1:A:247:PRO:HG2	2.41	0.55
1:A:10:VAL:HG12	1:A:41:ARG:NH2	2.21	0.55
1:A:105:GLN:CG	9:A:597:PZA:N1	2.70	0.55
1:A:580:SER:HA	11:A:622:GOL:O2	2.07	0.55
1:A:339:ILE:CD1	1:A:522:ILE:HD11	2.35	0.54
1:A:9:PRO:CG	1:A:167:CYS:HA	2.36	0.54
1:A:82:ILE:HD13	1:A:480:LEU:CD2	2.38	0.54
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.43	0.54
1:A:492:ILE:HD13	1:A:492:ILE:C	2.28	0.54
1:A:472:LYS:HE3	12:A:624:EDO:H21	1.89	0.53
5:A:596:NAG:O7	11:A:621:GOL:C1	2.33	0.53
1:A:169:THR:HB	1:A:170:PRO:CD	2.31	0.53
4:A:605:HEM:HMC2	4:A:605:HEM:HBC2	1.91	0.53
1:A:551:ARG:HD3	1:A:583:ASP:O	2.09	0.53
1:A:149:PRO:HB2	10:A:603:PEG:H22	1.91	0.52
1:A:518:GLN:O	1:A:522:ILE:HG12	2.10	0.52
1:A:383:THR:HG22	1:A:387:ILE:HD12	1.91	0.52
1:A:169:THR:N	1:A:170:PRO:HD2	2.24	0.52
1:A:258:GLU:HG3	9:A:598:PZA:N1	2.25	0.52
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.45	0.52
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.57	0.51
4:A:605:HEM:NC	9:A:597:PZA:N1	2.58	0.51
1:A:451:SER:HA	13:A:1042:HOH:O	2.08	0.51
1:A:426:HIS:HE1	13:A:1057:HOH:O	1.92	0.51
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.07	0.51
1:A:323:LYS:HD3	1:A:324:TRP:CE2	2.46	0.51
1:A:227:LEU:HD21	1:A:267:THR:HA	1.92	0.51
6:A:612:IOD:I	13:A:1072:HOH:O	2.88	0.51
1:A:9:PRO:HG2	1:A:167:CYS:C	2.32	0.50
1:A:109:HIS:NE2	9:A:597:PZA:C4	2.74	0.50
4:A:605:HEM:HBD2	13:A:886:HOH:O	2.10	0.50
1:A:42:ALA:HB2	1:A:166:VAL:HG11	1.93	0.50
1:A:384:TRP:CZ2	2:C:1:NAG:H2	2.45	0.50
1:A:584:LYS:HE3	11:A:622:GOL:H11	1.93	0.49
1:A:407:MET:HB3	1:A:501:MET:CE	2.42	0.49
1:A:63:GLN:CD	1:A:63:GLN:N	2.66	0.49
1:A:70:PHE:CG	1:A:485:LYS:HB2	2.48	0.49
1:A:82:ILE:CD1	1:A:480:LEU:HD23	2.42	0.48
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.94	0.48
1:A:249:PHE:CE1	1:A:383:THR:HG23	2.49	0.48
1:A:301:GLY:O	1:A:305:GLN:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLU:HG2	13:A:981:HOH:O	2.14	0.47
1:A:487:PRO:HA	1:A:490:ILE:HD12	1.96	0.47
10:A:619:PEG:H41	13:A:900:HOH:O	2.14	0.47
1:A:123:GLU:HG2	1:A:125:SER:HB3	1.97	0.47
5:A:596:NAG:H4	13:A:1056:HOH:O	2.15	0.46
1:A:63:GLN:NE2	13:A:1019:HOH:O	2.47	0.46
1:A:368:TRP:O	1:A:368:TRP:CE3	2.69	0.46
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.51	0.46
1:A:385:ARG:O	1:A:389:ASP:HB3	2.15	0.46
5:A:596:NAG:H2	11:A:621:GOL:H31	1.97	0.46
1:A:494:ILE:HD13	1:A:494:ILE:C	2.36	0.46
1:A:9:PRO:CG	1:A:167:CYS:O	2.61	0.45
1:A:205:ASN:HA	13:A:1068:HOH:O	2.16	0.45
1:A:540:GLN:HG2	1:A:590:TRP:CE2	2.51	0.45
1:A:561:LYS:HA	1:A:577:VAL:O	2.17	0.44
1:A:246:VAL:HG11	1:A:387:ILE:HD12	1.99	0.44
1:A:249:PHE:CZ	1:A:383:THR:HG23	2.52	0.44
1:A:8:ALA:N	1:A:9:PRO:CD	2.80	0.44
1:A:257:SER:O	1:A:381:PHE:HA	2.18	0.44
1:A:123:GLU:HG2	1:A:125:SER:CB	2.48	0.44
1:A:279:GLU:CG	1:A:587:LEU:HD12	2.38	0.44
1:A:418:ARG:HH22	10:A:603:PEG:H42	1.82	0.44
4:A:605:HEM:CMB	4:A:605:HEM:HBB2	2.48	0.43
1:A:298:LYS:HG3	13:A:1061:HOH:O	2.18	0.43
4:A:605:HEM:C1A	9:A:597:PZA:N3	2.87	0.43
1:A:123:GLU:CG	1:A:125:SER:CB	2.96	0.43
1:A:175:LEU:HD12	13:A:1106:HOH:O	2.18	0.43
1:A:227:LEU:CD2	1:A:270:LEU:HD22	2.45	0.43
1:A:254:PHE:CE2	9:A:598:PZA:C1	3.02	0.43
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.54	0.43
1:A:424:PRO:C	1:A:425:THR:HG22	2.22	0.43
1:A:563:PRO:HD3	1:A:576:PHE:CE2	2.54	0.43
1:A:567:PHE:HB2	6:A:612:IOD:I	2.89	0.43
1:A:335:VAL:O	1:A:337:PRO:HD3	2.19	0.42
1:A:396:VAL:CG1	1:A:553:ILE:HD12	2.46	0.42
1:A:9:PRO:CG	1:A:167:CYS:CA	2.94	0.42
1:A:193:TYR:OH	1:A:297:ARG:HA	2.20	0.42
1:A:540:GLN:HG2	1:A:590:TRP:CZ2	2.54	0.42
1:A:120:GLY:HA3	1:A:126:LYS:HG3	2.02	0.42
4:A:605:HEM:ND	9:A:597:PZA:O	2.53	0.42
1:A:368:TRP:O	1:A:368:TRP:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLU:CG	1:A:125:SER:HB3	2.50	0.41
1:A:2:TRP:HA	13:A:773:HOH:O	2.20	0.41
1:A:478:LYS:HE2	13:A:978:HOH:O	2.21	0.41
1:A:130:GLU:OE1	1:A:426:HIS:ND1	2.51	0.41
1:A:151:LEU:HD12	1:A:155:GLY:O	2.21	0.41
1:A:189:ALA:HB2	1:A:304:ILE:HD12	2.02	0.41
1:A:322:GLN:HG2	13:A:687:HOH:O	2.20	0.41
1:A:352:MET:CB	1:A:407:MET:HG2	2.51	0.41
1:A:487:PRO:HA	1:A:490:ILE:CD1	2.50	0.41
1:A:78:VAL:HG13	1:A:82:ILE:HD12	2.03	0.40
1:A:229:PHE:HZ	1:A:387:ILE:HD13	1.86	0.40
1:A:115:PRO:HG2	13:A:1037:HOH:O	2.21	0.40
1:A:105:GLN:HG3	4:A:605:HEM:C1C	2.56	0.40
1:A:130:GLU:HB2	13:A:1057:HOH:O	2.22	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%)	569 (96%)	21 (4%)	2 (0%)	41 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	7	GLY

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%)	507 (98%)	10 (2%)	57 61

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	91	VAL
1	A	137	ASP
1	A	347	PHE
1	A	441	CYS
1	A	486	THR
1	A	492	ILE
1	A	494	ILE
1	A	593	ARG
1	A	595	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	105	GLN
1	A	259	GLN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	570	ASN
1	A	571	ASN
1	A	574	HIS
1	A	595	ASN

5.3.3 RNA [i](#)

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	1.60	1 (12%)	8,12,14	1.26	1 (12%)

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	-	4/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O1P	3.41	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-CB-CA	2.36	110.44	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	CB-OG-P-O1P
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	0.49	0	17,19,21	0.82	0
2	NAG	B	2	2	14,14,15	1.07	1 (7%)	17,19,21	1.47	4 (23%)
2	NAG	C	1	1,2	14,14,15	0.66	0	17,19,21	0.77	0
2	NAG	C	2	2	14,14,15	0.44	0	17,19,21	2.19	4 (23%)

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	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C8-C7	2.56	1.55	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	6.87	121.50	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C4-C3-C2	3.27	115.81	111.02
2	C	2	NAG	C4-C3-C2	-2.89	106.79	111.02
2	B	2	NAG	C1-O5-C5	-2.61	108.65	112.19
2	C	2	NAG	O5-C5-C4	2.52	116.96	110.83
2	C	2	NAG	C1-C2-N2	2.32	114.44	110.49
2	B	2	NAG	C2-N2-C7	2.06	125.84	122.90
2	B	2	NAG	O5-C5-C6	2.00	110.35	107.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

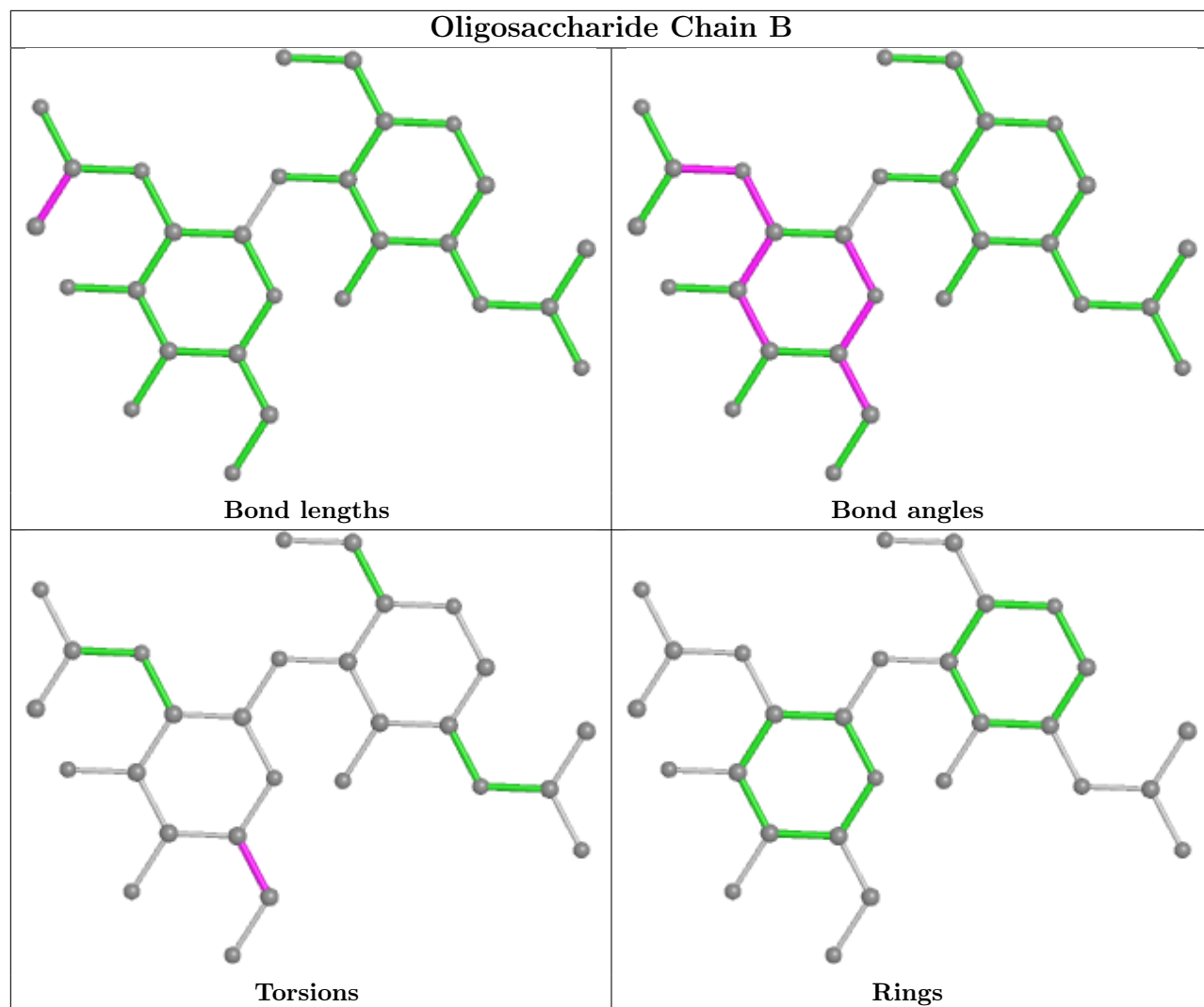
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6

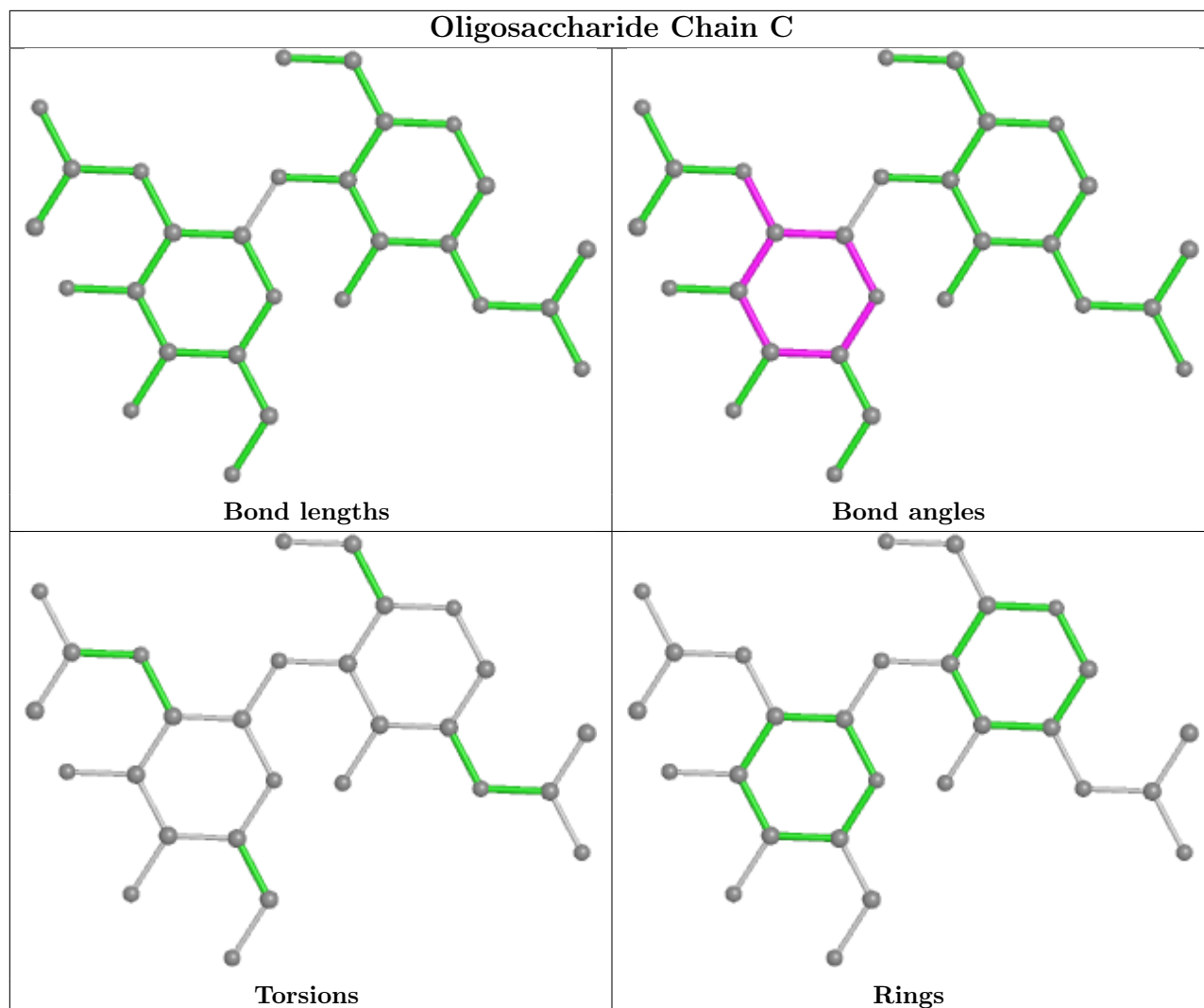
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 13 are monoatomic - leaving 12 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$
11	GOL	A	621	-	5,5,5	3.38	2 (40%)	5,5,5	2.49	4 (80%)
5	NAG	A	604	1	14,14,15	0.45	0	17,19,21	0.83	0
9	PZA	A	598	-	9,9,9	0.40	0	11,11,11	1.86	3 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	A	605	1,9	41,50,50	2.22	12 (29%)	45,82,82	2.46	15 (33%)
12	EDO	A	623	-	3,3,3	0.93	0	2,2,2	0.85	0
9	PZA	A	597	4	9,9,9	0.53	0	11,11,11	1.91	5 (45%)
12	EDO	A	624	-	3,3,3	0.44	0	2,2,2	0.42	0
5	NAG	A	596	1	14,14,15	0.77	1 (7%)	17,19,21	1.66	3 (17%)
10	PEG	A	603	-	6,6,6	1.60	1 (16%)	5,5,5	0.99	0
10	PEG	A	619	-	6,6,6	1.45	1 (16%)	5,5,5	0.94	0
11	GOL	A	622	-	5,5,5	1.04	0	5,5,5	1.15	1 (20%)
8	SCN	A	620	-	1,2,2	1.24	0	0,1,1	-	-

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
11	GOL	A	621	-	-	2/4/4/4	-
5	NAG	A	604	1	-	0/6/23/26	0/1/1/1
9	PZA	A	598	-	-	4/4/4/4	0/1/1/1
4	HEM	A	605	1,9	-	4/12/54/54	-
12	EDO	A	623	-	-	0/1/1/1	-
9	PZA	A	597	4	-	4/4/4/4	0/1/1/1
12	EDO	A	624	-	-	0/1/1/1	-
5	NAG	A	596	1	-	0/6/23/26	0/1/1/1
10	PEG	A	603	-	-	1/4/4/4	-
10	PEG	A	619	-	-	4/4/4/4	-
11	GOL	A	622	-	-	2/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	HEM	C3D-C2D	7.01	1.51	1.36
11	A	621	GOL	O2-C2	-6.98	1.22	1.43
4	A	605	HEM	C4D-ND	-5.39	1.31	1.40
4	A	605	HEM	CAB-C3B	4.17	1.58	1.47
4	A	605	HEM	C3C-CAC	3.67	1.55	1.47
4	A	605	HEM	C1B-NB	-3.25	1.34	1.40
10	A	603	PEG	C2-C1	-3.23	1.32	1.49
4	A	605	HEM	FE-NB	3.03	2.11	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	HEM	CMC-C2C	2.96	1.58	1.51
10	A	619	PEG	C2-C1	-2.70	1.35	1.49
11	A	621	GOL	O1-C1	2.45	1.52	1.42
5	A	596	NAG	C8-C7	2.32	1.55	1.50
4	A	605	HEM	C1A-CHA	-2.27	1.34	1.41
4	A	605	HEM	CHC-C4B	-2.22	1.34	1.41
4	A	605	HEM	CHB-C1B	2.21	1.40	1.35
4	A	605	HEM	FE-ND	2.12	2.07	1.96
4	A	605	HEM	CBD-CGD	-2.11	1.45	1.50

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	HEM	CMD-C2D-C1D	7.95	137.15	125.04
4	A	605	HEM	CAD-C3D-C4D	5.80	134.80	124.66
4	A	605	HEM	C2C-C3C-C4C	-5.03	103.38	106.90
4	A	605	HEM	C4B-CHC-C1C	4.75	128.82	122.56
5	A	596	NAG	C1-O5-C5	4.16	117.83	112.19
5	A	596	NAG	O5-C1-C2	-3.49	105.78	111.29
9	A	598	PZA	C4-C-N1	3.37	119.58	116.25
4	A	605	HEM	C4D-C3D-C2D	-3.28	102.12	106.90
4	A	605	HEM	C3D-C4D-ND	3.24	113.77	110.17
9	A	597	PZA	C4-C-N1	3.24	119.45	116.25
4	A	605	HEM	C1D-C2D-C3D	-3.23	103.56	106.96
4	A	605	HEM	C4D-ND-C1D	3.11	108.28	105.07
11	A	621	GOL	O2-C2-C1	2.99	122.30	109.12
5	A	596	NAG	C1-C2-N2	2.87	115.39	110.49
11	A	621	GOL	O2-C2-C3	2.86	121.70	109.12
9	A	597	PZA	C4-C3-N2	-2.83	118.53	122.05
4	A	605	HEM	CAD-C3D-C2D	-2.72	122.81	127.88
4	A	605	HEM	CMB-C2B-C1B	2.70	129.15	125.04
11	A	621	GOL	C3-C2-C1	-2.68	101.28	111.70
9	A	598	PZA	C1-N3-C4	2.61	120.32	116.93
9	A	597	PZA	C1-N3-C4	2.56	120.25	116.93
4	A	605	HEM	C4C-CHD-C1D	2.55	125.92	122.56
4	A	605	HEM	CBA-CAA-C2A	-2.54	108.28	112.62
4	A	605	HEM	CMD-C2D-C3D	-2.51	119.30	126.12
9	A	597	PZA	C2-N2-C3	2.43	121.05	116.85
11	A	622	GOL	O2-C2-C3	-2.34	98.81	109.12
4	A	605	HEM	CHD-C1D-C2D	-2.29	121.40	124.98
9	A	597	PZA	C2-C1-N3	-2.25	118.94	122.17
9	A	598	PZA	C2-N2-C3	2.22	120.68	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	621	GOL	O1-C1-C2	-2.17	99.81	110.20
4	A	605	HEM	O1D-CGD-CBD	-2.03	116.56	123.08

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	597	PZA	O-C-C4-N3
9	A	598	PZA	N1-C-C4-C3
9	A	598	PZA	N1-C-C4-N3
9	A	598	PZA	O-C-C4-C3
9	A	598	PZA	O-C-C4-N3
11	A	622	GOL	C1-C2-C3-O3
9	A	597	PZA	N1-C-C4-N3
9	A	597	PZA	N1-C-C4-C3
9	A	597	PZA	O-C-C4-C3
10	A	619	PEG	O1-C1-C2-O2
10	A	603	PEG	O2-C3-C4-O4
11	A	622	GOL	O2-C2-C3-O3
11	A	621	GOL	O1-C1-C2-O2
11	A	621	GOL	O2-C2-C3-O3
10	A	619	PEG	O2-C3-C4-O4
10	A	619	PEG	C4-C3-O2-C2
4	A	605	HEM	CAD-CBD-CGD-O2D
4	A	605	HEM	CAA-CBA-CGA-O1A
4	A	605	HEM	CAA-CBA-CGA-O2A
4	A	605	HEM	CAD-CBD-CGD-O1D
10	A	619	PEG	C1-C2-O2-C3

There are no ring outliers.

9 monomers are involved in 34 short contacts:

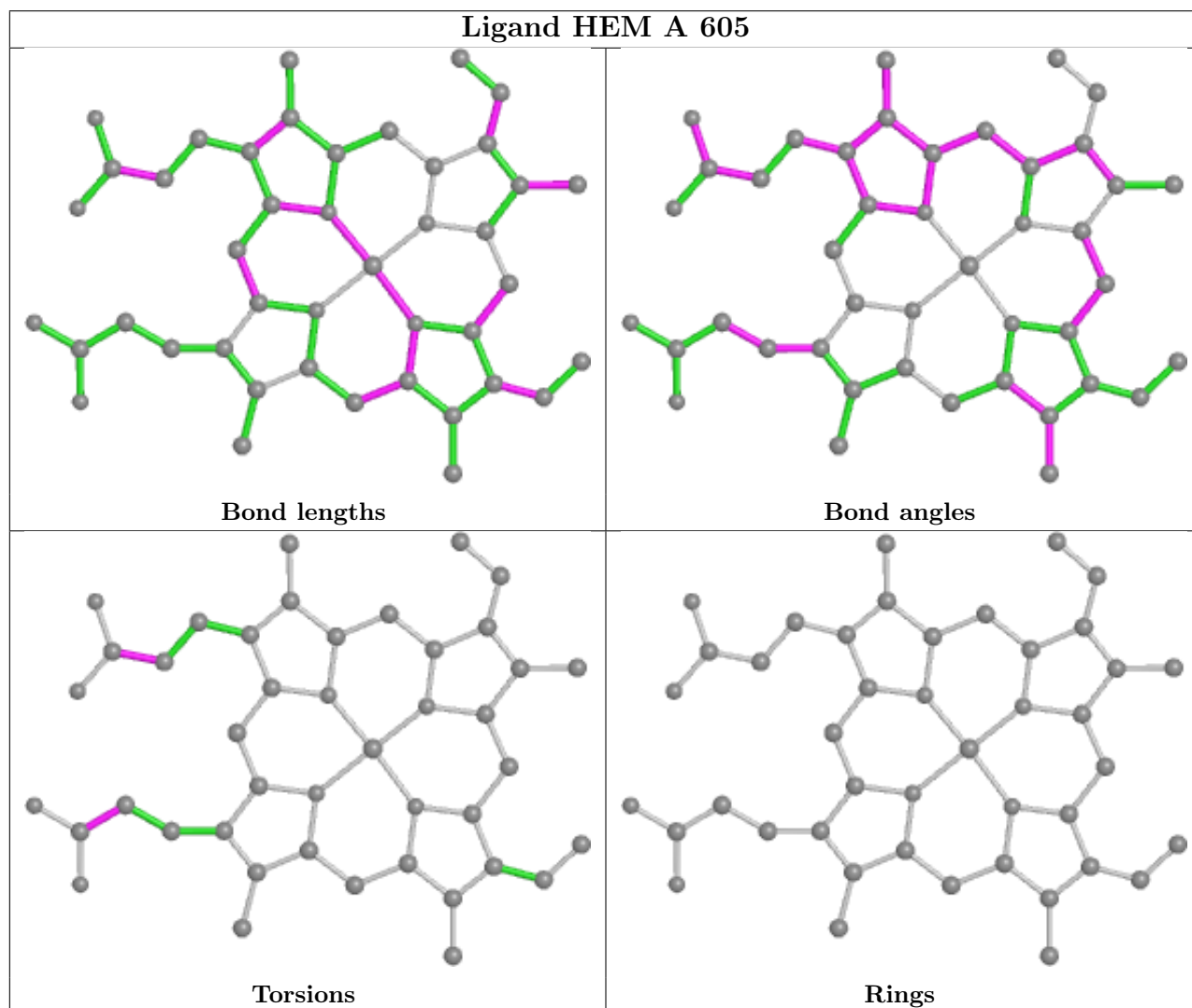
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	621	GOL	4	0
9	A	598	PZA	6	0
4	A	605	HEM	7	0
9	A	597	PZA	14	0
12	A	624	EDO	1	0
5	A	596	NAG	4	0
10	A	603	PEG	3	0
10	A	619	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	622	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	594/595 (99%)	0.49	51 (8%) 10 9	15, 31, 57, 94	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	14.7
1	A	172	TYR	10.8
1	A	121	SER	9.7
1	A	12	LEU	9.6
1	A	171	PRO	8.8
1	A	119	LEU	8.5
1	A	11	PRO	8.2
1	A	173	GLN	7.6
1	A	120	GLY	7.5
1	A	13	VAL	7.1
1	A	7	GLY	6.7
1	A	4	VAL	6.6
1	A	122	ASN	6.3
1	A	10	VAL	6.0
1	A	6	CYS	5.8
1	A	170	PRO	5.6
1	A	283	LEU	5.6
1	A	1	SER	5.6
1	A	8	ALA	5.4
1	A	124	HIS	5.4
1	A	123	GLU	5.2
1	A	593	ARG	4.8
1	A	595	ASN	4.7
1	A	174	SER	4.7
1	A	169	THR	4.2
1	A	3	GLU	3.7
1	A	128	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	132	TYR	3.6
1	A	133	CYS	3.5
1	A	18	ASN	3.4
1	A	594	GLU	3.4
1	A	5	GLY	3.3
1	A	223	GLY	2.9
1	A	64	ARG	2.9
1	A	279	GLU	2.9
1	A	175	LEU	2.7
1	A	592	SER	2.5
1	A	63	GLN	2.5
1	A	17	GLU	2.5
1	A	125	SER	2.5
1	A	9	PRO	2.5
1	A	280	LEU	2.3
1	A	254	PHE	2.3
1	A	168	PRO	2.3
1	A	199	LEU	2.2
1	A	118	GLU	2.2
1	A	111	LEU	2.1
1	A	484	TYR	2.1
1	A	354	VAL	2.1
1	A	209	PRO	2.1
1	A	126	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

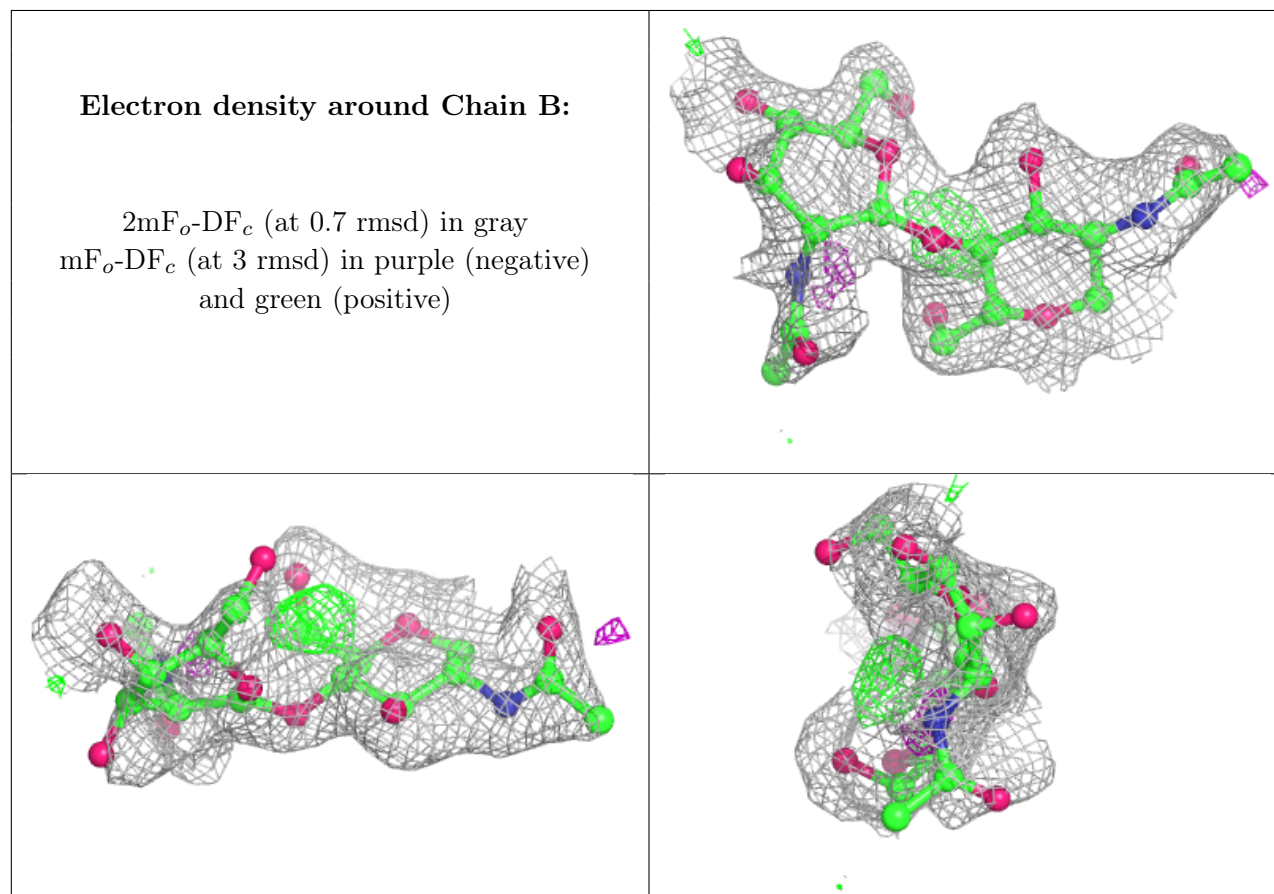
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	A	198	10/11	0.85	0.24	39,40,41,41	0

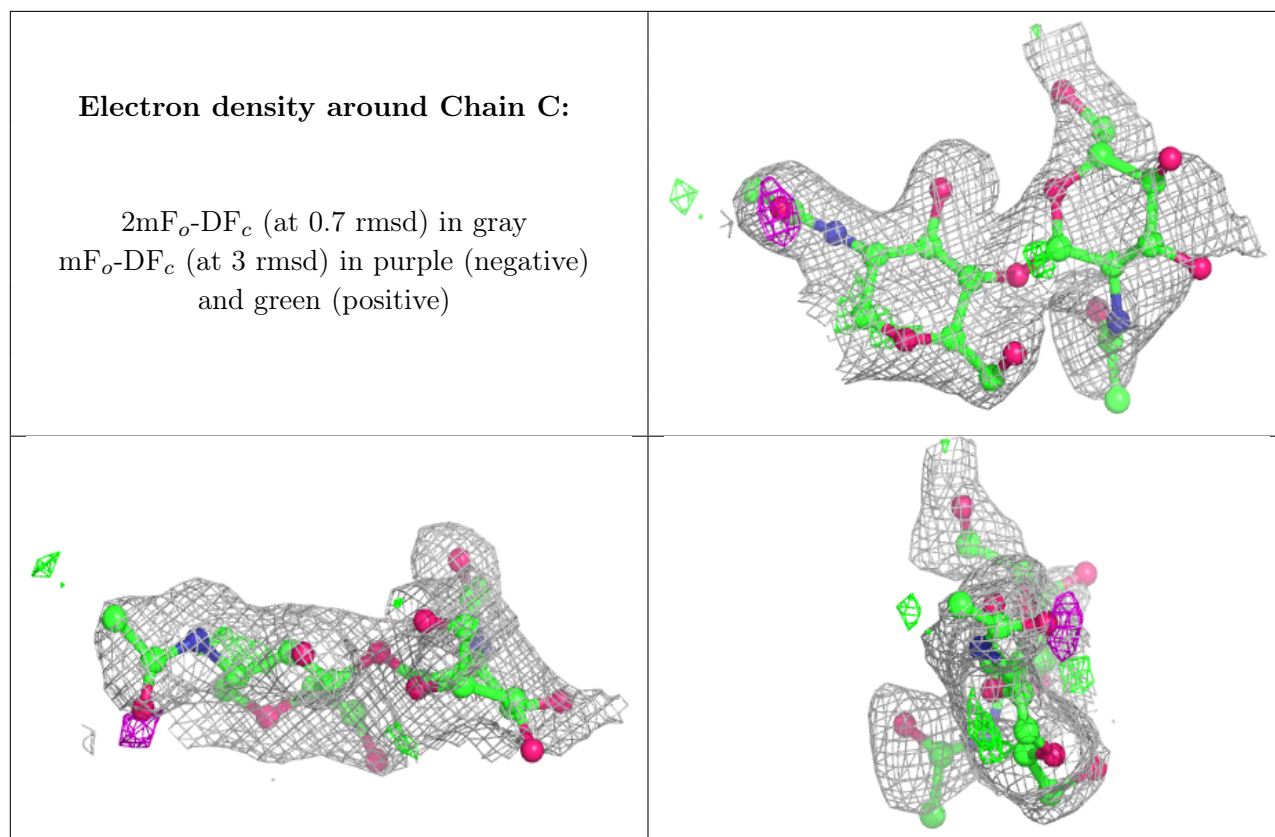
6.3 Carbohydrates [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	B	2	14/15	0.71	0.41	54,57,58,58	0
2	NAG	C	2	14/15	0.73	0.24	51,55,56,56	0
2	NAG	C	1	14/15	0.77	0.17	38,40,43,47	0
2	NAG	B	1	14/15	0.84	0.15	39,44,46,50	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

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

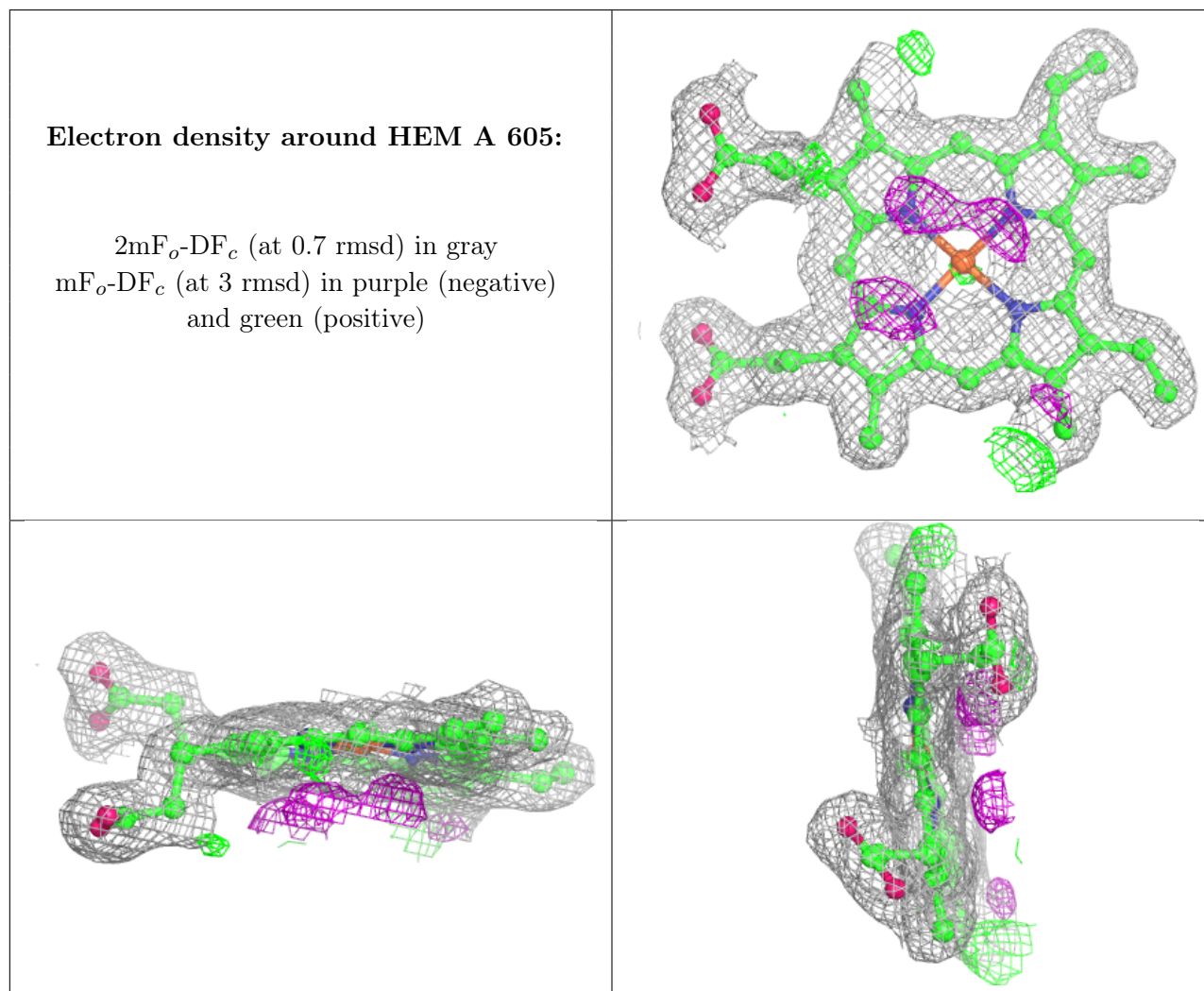
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	604	14/15	0.62	0.30	39,39,40,40	0
9	PZA	A	597	9/9	0.64	0.42	28,29,30,31	0
5	NAG	A	596	14/15	0.69	0.32	47,50,52,52	0
11	GOL	A	622	6/6	0.70	0.18	58,58,59,60	0
9	PZA	A	598	9/9	0.74	0.39	27,27,27,28	9
10	PEG	A	619	7/7	0.78	0.14	50,51,51,51	0
10	PEG	A	603	7/7	0.81	0.19	33,35,36,37	0
11	GOL	A	621	6/6	0.83	0.26	45,46,47,49	0
8	SCN	A	620	3/3	0.83	0.19	30,30,30,30	0
12	EDO	A	624	4/4	0.87	0.13	30,31,32,34	0
6	IOD	A	614	1/1	0.94	0.06	55,55,55,55	1
12	EDO	A	623	4/4	0.95	0.17	41,42,42,43	0
6	IOD	A	607	1/1	0.95	0.05	51,51,51,51	0
6	IOD	A	612	1/1	0.96	0.05	52,52,52,52	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	HEM	A	605	43/43	0.97	0.16	14,18,22,24	0
6	IOD	A	613	1/1	0.97	0.07	64,64,64,64	1
6	IOD	A	609	1/1	0.97	0.03	57,57,57,57	0
7	ZN	A	618	1/1	0.98	0.04	44,44,44,44	0
6	IOD	A	611	1/1	0.98	0.09	63,63,63,63	0
3	CA	A	606	1/1	0.99	0.11	22,22,22,22	0
6	IOD	A	610	1/1	0.99	0.04	58,58,58,58	0
6	IOD	A	608	1/1	0.99	0.03	40,40,40,40	0
6	IOD	A	616	1/1	0.99	0.07	36,36,36,36	0
6	IOD	A	617	1/1	0.99	0.07	53,53,53,53	0
6	IOD	A	615	1/1	1.00	0.04	26,26,26,26	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.