



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 08:55 AM BST

PDB ID : 4NJB
Title : Crystal structure of the complex of lactoperoxidase from bovine with 3,3-oxydipyridine at 2.31 Å resolution
Authors : Yamini, S.; Sirohi, H.V.; Sinha, M.; Bhushan, A.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2013-11-09
Resolution : 2.31 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 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

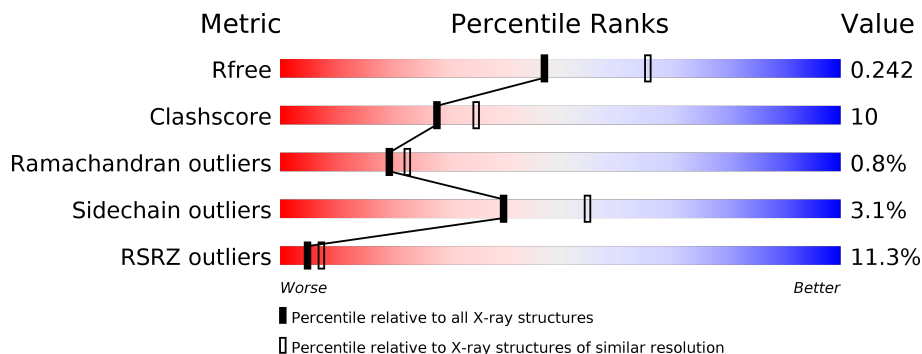
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 11% 80% 18%
2	B	2	 100%
2	C	2	 100%

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
1	SEP	A	198	-	X	-	-
2	NAG	B	2	-	-	-	X
5	NAG	A	603	-	-	-	X
6	IOD	A	614	-	-	X	-

2 Entry composition [i](#)

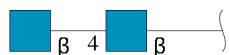
There are 10 unique types of molecules in this entry. The entry contains 5371 atoms, of which 0 are hydrogens and 0 are deuteriums.

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).

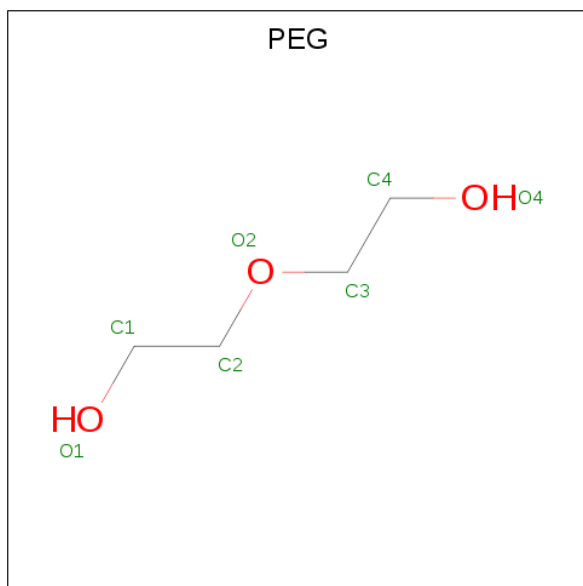
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

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

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

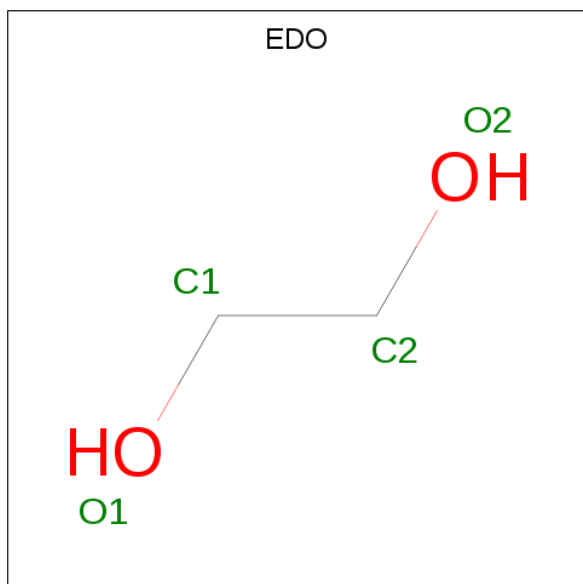
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	11	Total I 11 11	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



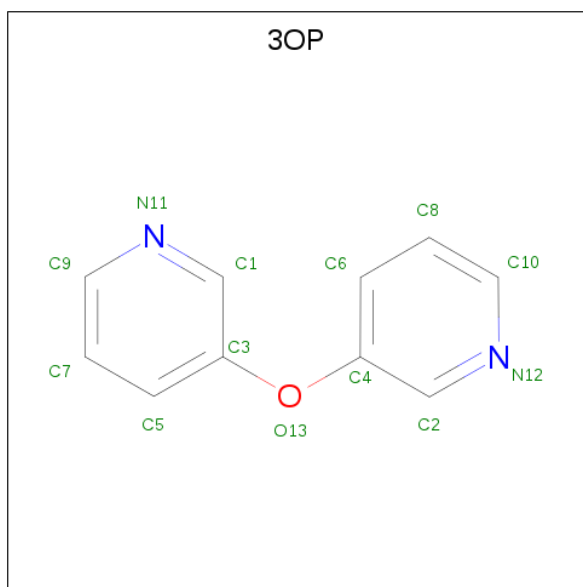
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 9 is 3,3'-oxydipyridine (three-letter code: 3OP) (formula: C₁₀H₈N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			13	10	2	1		

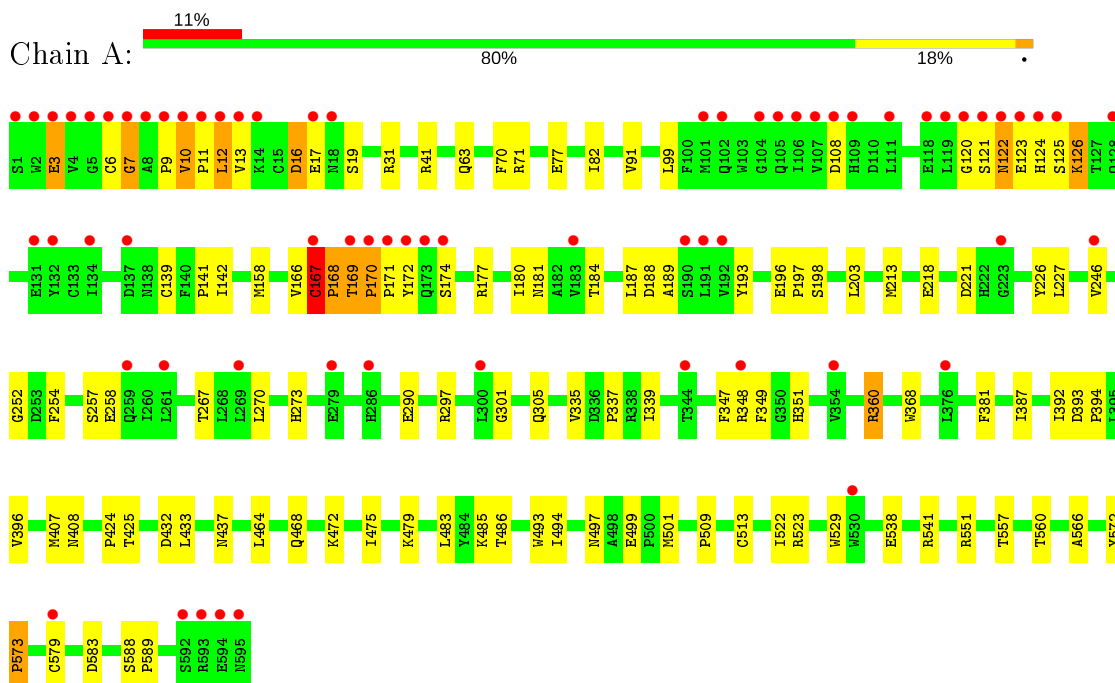
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	430	Total	O	0	0
			430	430		

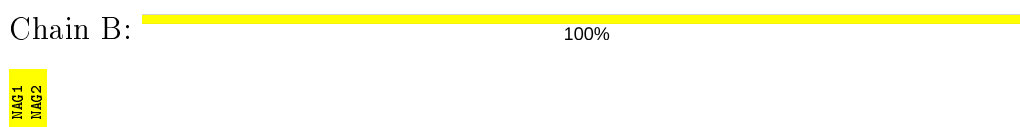
3 Residue-property plots [i](#)

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.

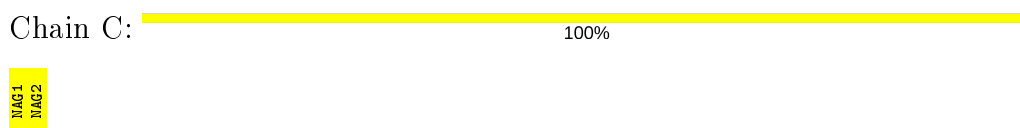
- Molecule 1: Lactoperoxidase



- 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, α , β , γ	54.36Å 80.40Å 76.28Å 90.00° 103.37° 90.00°	Depositor
Resolution (Å)	39.02 – 2.31 39.02 – 2.31	Depositor EDS
% Data completeness (in resolution range)	95.6 (39.02-2.31) 95.6 (39.02-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.09 (at 2.31Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.227 0.201 , 0.242	Depositor DCC
R_{free} test set	1331 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtrriage
Anisotropy	0.767	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5371	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: PEG, NAG, SEP, CA, EDO, 3OP, HEM, 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	0.40	0/4891	0.74	3/6634 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	PRO	N-CA-C	-7.51	92.56	112.10
1	A	167	CYS	CA-CB-SG	-6.27	102.71	114.00
1	A	3	GLU	N-CA-C	5.63	126.20	111.00

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	92	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
3	A	1	0	0	0	0
4	A	43	0	30	7	0
5	A	28	0	26	0	0
6	A	11	0	0	4	0
7	A	7	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	8	0	12	0	0
9	A	13	0	8	4	0
10	A	430	0	0	9	0
All	All	5371	0	4822	97	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 10.

All (97) 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:108:ASP:OD1	4:A:602:HEM:HMD1	1.40	1.20
1:A:258:GLU:HG3	9:A:623:3OP:H1	1.15	1.08
1:A:424:PRO:O	1:A:425:THR:HG22	1.56	1.05
1:A:258:GLU:CG	9:A:623:3OP:H1	1.89	1.01
1:A:258:GLU:HG3	9:A:623:3OP:C5	2.07	0.80
1:A:169:THR:H	1:A:170:PRO:CD	1.95	0.79
1:A:408:ASN:HB2	10:A:843:HOH:O	1.82	0.78
1:A:108:ASP:OD1	4:A:602:HEM:CMD	2.28	0.77
1:A:258:GLU:OE1	4:A:602:HEM:HMB3	1.84	0.77
1:A:246:VAL:HG11	1:A:387:ILE:HD12	1.70	0.73
1:A:63:GLN:CD	1:A:63:GLN:H	1.94	0.71
1:A:258:GLU:OE1	4:A:602:HEM:CMB	2.40	0.70
1:A:485:LYS:N	10:A:1127:HOH:O	2.27	0.67
6:A:614:IOD:I	10:A:1100:HOH:O	2.83	0.67
1:A:538:GLU:HG2	1:A:541:ARG:NH2	2.11	0.66
1:A:120:GLY:HA3	1:A:126:LYS:HD2	1.79	0.64
1:A:227:LEU:HD22	1:A:270:LEU:HD22	1.79	0.64
6:A:618:IOD:I	10:A:1105:HOH:O	2.86	0.62
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.35	0.62
1:A:171:PRO:HG2	10:A:1056:HOH:O	2.01	0.60
1:A:168:PRO:HG3	1:A:172:TYR:HB2	1.85	0.59
1:A:475:ILE:HG22	1:A:479:LYS:HE3	1.83	0.59
1:A:572:TYR:CD1	1:A:573:PRO:HA	2.39	0.58
1:A:254:PHE:HB2	10:A:970:HOH:O	2.05	0.56
1:A:169:THR:N	1:A:170:PRO:CD	2.65	0.56
1:A:551:ARG:HD3	1:A:583:ASP:O	2.06	0.56
1:A:424:PRO:O	1:A:425:THR:CG2	2.43	0.55
1:A:71:ARG:NH1	1:A:71:ARG:HG2	2.22	0.55
1:A:227:LEU:HD21	1:A:267:THR:HA	1.87	0.55
1:A:560:THR:HA	1:A:579:CYS:SG	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:PRO:HG3	1:A:172:TYR:CD1	2.42	0.54
1:A:169:THR:H	1:A:170:PRO:HD3	1.72	0.54
1:A:123:GLU:HG3	1:A:125:SER:H	1.72	0.53
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.43	0.53
1:A:12:LEU:HD23	1:A:13:VAL:H	1.74	0.53
1:A:468:GLN:O	1:A:472:LYS:N	2.42	0.53
1:A:572:TYR:CE2	1:A:573:PRO:HB3	2.44	0.53
1:A:139:CYS:SG	1:A:141:PRO:HD3	2.49	0.52
1:A:63:GLN:CD	1:A:63:GLN:N	2.62	0.52
6:A:614:IOD:I	10:A:1075:HOH:O	2.89	0.52
1:A:167:CYS:CB	1:A:168:PRO:CD	2.89	0.51
1:A:121:SER:O	1:A:122:ASN:ND2	2.44	0.51
1:A:6:CYS:SG	1:A:7:GLY:N	2.84	0.50
1:A:257:SER:O	1:A:381:PHE:HA	2.12	0.50
1:A:407:MET:HB3	1:A:501:MET:CE	2.42	0.49
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.47	0.49
1:A:71:ARG:HH11	1:A:71:ARG:HG2	1.76	0.48
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.94	0.48
1:A:180:ILE:HG22	1:A:181:ASN:N	2.30	0.47
1:A:158:MET:CE	1:A:432:ASP:H	2.27	0.47
1:A:464:LEU:O	1:A:468:GLN:HG3	2.15	0.47
1:A:348:ARG:NH2	4:A:602:HEM:HAD1	2.30	0.47
1:A:99:LEU:HD23	1:A:566:ALA:HB1	1.95	0.47
1:A:122:ASN:C	1:A:122:ASN:HD22	2.17	0.46
4:A:602:HEM:HMB1	4:A:602:HEM:HBB2	1.96	0.46
1:A:572:TYR:CZ	1:A:573:PRO:HB3	2.50	0.46
1:A:70:PHE:CD2	1:A:485:LYS:HG3	2.51	0.45
1:A:177:ARG:HB2	10:A:915:HOH:O	2.16	0.45
1:A:16:ASP:OD2	1:A:19:SER:HB2	2.15	0.45
1:A:301:GLY:O	1:A:305:GLN:HG3	2.16	0.45
1:A:16:ASP:OD1	1:A:16:ASP:C	2.55	0.45
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.14	0.44
1:A:493:TRP:O	1:A:497:ASN:OD1	2.36	0.44
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.83	0.44
1:A:17:GLU:O	1:A:31:ARG:NH2	2.51	0.44
1:A:142:ILE:HG23	10:A:977:HOH:O	2.18	0.43
1:A:166:VAL:O	1:A:167:CYS:HB2	2.18	0.43
1:A:196:GLU:HA	1:A:197:PRO:HD3	1.90	0.43
1:A:9:PRO:CG	1:A:167:CYS:H	2.32	0.43
1:A:10:VAL:HG11	1:A:41:ARG:CZ	2.49	0.42
1:A:290:GLU:HA	1:A:290:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ASP:OD1	1:A:557:THR:HB	2.19	0.42
1:A:258:GLU:CD	9:A:623:3OP:H1	2.38	0.42
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.93	0.42
1:A:193:TYR:OH	1:A:297:ARG:HA	2.18	0.42
1:A:392:ILE:O	1:A:396:VAL:HG23	2.19	0.42
1:A:203:LEU:HD11	1:A:252:GLY:HA2	2.02	0.42
4:A:602:HEM:CMB	4:A:602:HEM:HBB2	2.49	0.42
1:A:9:PRO:HG2	1:A:167:CYS:H	1.84	0.42
1:A:184:THR:OG1	1:A:188:ASP:OD2	2.38	0.42
1:A:351:HIS:CE1	1:A:433:LEU:HD21	2.55	0.42
1:A:82:ILE:HD11	1:A:483:LEU:HD12	2.01	0.42
1:A:407:MET:HB3	1:A:501:MET:HE2	2.00	0.41
1:A:499:GLU:OE1	1:A:509:PRO:HD2	2.20	0.41
1:A:63:GLN:O	1:A:71:ARG:NH1	2.54	0.41
1:A:588:SER:N	1:A:589:PRO:CD	2.82	0.41
1:A:168:PRO:CG	1:A:172:TYR:HB2	2.49	0.41
1:A:188:ASP:O	1:A:189:ALA:HB3	2.20	0.41
1:A:77:GLU:HG3	6:A:610:IOD:I	2.91	0.41
1:A:339:ILE:CD1	1:A:522:ILE:HD11	2.51	0.41
1:A:120:GLY:HA3	1:A:126:LYS:CD	2.49	0.41
1:A:82:ILE:CD1	1:A:483:LEU:HD12	2.50	0.41
1:A:168:PRO:HG3	1:A:172:TYR:HD1	1.84	0.40
1:A:221:ASP:HB2	1:A:226:TYR:CE2	2.57	0.40
1:A:335:VAL:O	1:A:337:PRO:HD3	2.21	0.40
1:A:360:ARG:HB3	1:A:368:TRP:HB3	2.04	0.40
1:A:393:ASP:CB	1:A:394:PRO:HD3	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%)	562 (95%)	25 (4%)	5 (1%)	19 23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	167	CYS
1	A	11	PRO
1	A	169	THR
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%)	501 (97%)	16 (3%)	40 55

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	12	LEU
1	A	16	ASP
1	A	91	VAL
1	A	122	ASN
1	A	124	HIS
1	A	126	LYS
1	A	168	PRO
1	A	174	SER
1	A	218	GLU
1	A	347	PHE
1	A	360	ARG
1	A	486	THR
1	A	494	ILE
1	A	513	CYS
1	A	573	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	124	HIS
1	A	147	ASN
1	A	497	ASN
1	A	570	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	2.59	4 (50%)	8,12,14	3.25	7 (87%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O3P	-4.26	1.38	1.54
1	A	198	SEP	P-O1P	-4.23	1.36	1.50
1	A	198	SEP	P-O2P	-3.48	1.41	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	CA-N	-2.01	1.42	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	P-OG-CB	6.28	135.59	118.30
1	A	198	SEP	O2P-P-OG	3.33	115.59	106.73
1	A	198	SEP	O2P-P-O1P	2.90	122.04	110.68
1	A	198	SEP	OG-CB-CA	-2.82	105.40	108.14
1	A	198	SEP	O3P-P-OG	2.63	113.74	106.73
1	A	198	SEP	O3P-P-O2P	-2.27	98.97	107.64
1	A	198	SEP	OG-P-O1P	-2.03	100.78	106.47

There are no chirality outliers.

All (4) 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-O3P
1	A	198	SEP	CB-OG-P-O1P
1	A	198	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

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	0.58	0	17,19,21	1.26	2 (11%)
2	NAG	B	2	2	14,14,15	0.79	1 (7%)	17,19,21	1.65	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	1,2	14,14,15	0.76	0	17,19,21	1.52	3 (17%)
2	NAG	C	2	2	14,14,15	0.65	0	17,19,21	2.91	7 (41%)

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	-	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	-	1/6/23/26	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	O5-C1	-2.11	1.40	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	7.58	122.46	112.19
2	C	2	NAG	C4-C3-C2	-5.59	102.82	111.02
2	C	2	NAG	C1-C2-N2	4.00	117.31	110.49
2	B	2	NAG	C1-C2-N2	-3.65	104.25	110.49
2	C	2	NAG	O5-C5-C6	3.58	112.81	107.20
2	B	2	NAG	C4-C3-C2	3.58	116.26	111.02
2	B	2	NAG	C1-O5-C5	-3.13	107.95	112.19
2	C	2	NAG	O3-C3-C2	2.88	115.42	109.47
2	C	1	NAG	C1-O5-C5	-2.79	108.42	112.19
2	C	1	NAG	O5-C1-C2	-2.71	107.02	111.29
2	C	2	NAG	O5-C1-C2	-2.48	107.37	111.29
2	C	1	NAG	C3-C4-C5	-2.21	106.29	110.24
2	B	1	NAG	C1-C2-N2	2.18	114.21	110.49
2	C	2	NAG	O5-C5-C4	2.06	115.85	110.83
2	B	1	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

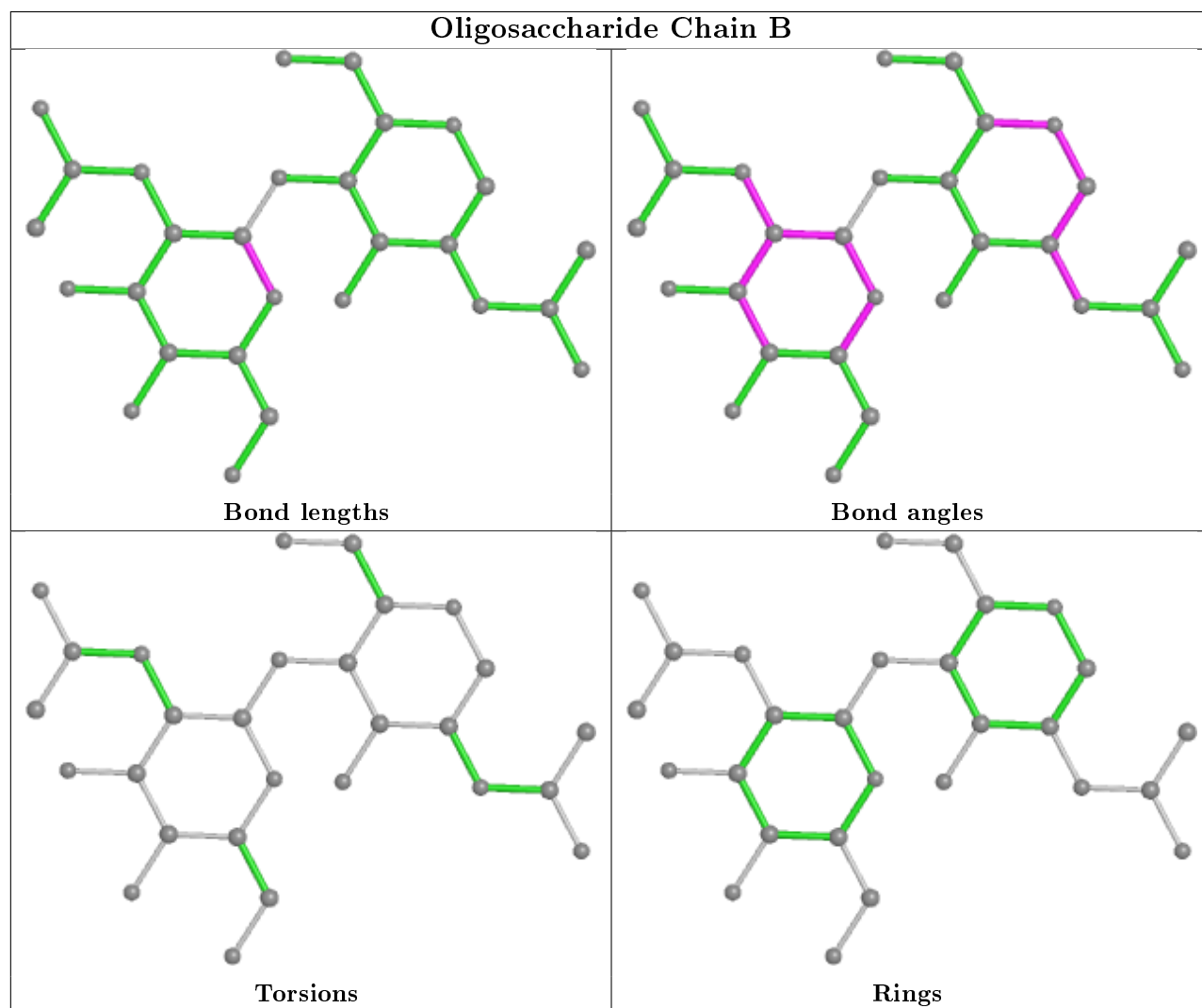
All (1) torsion outliers are listed below:

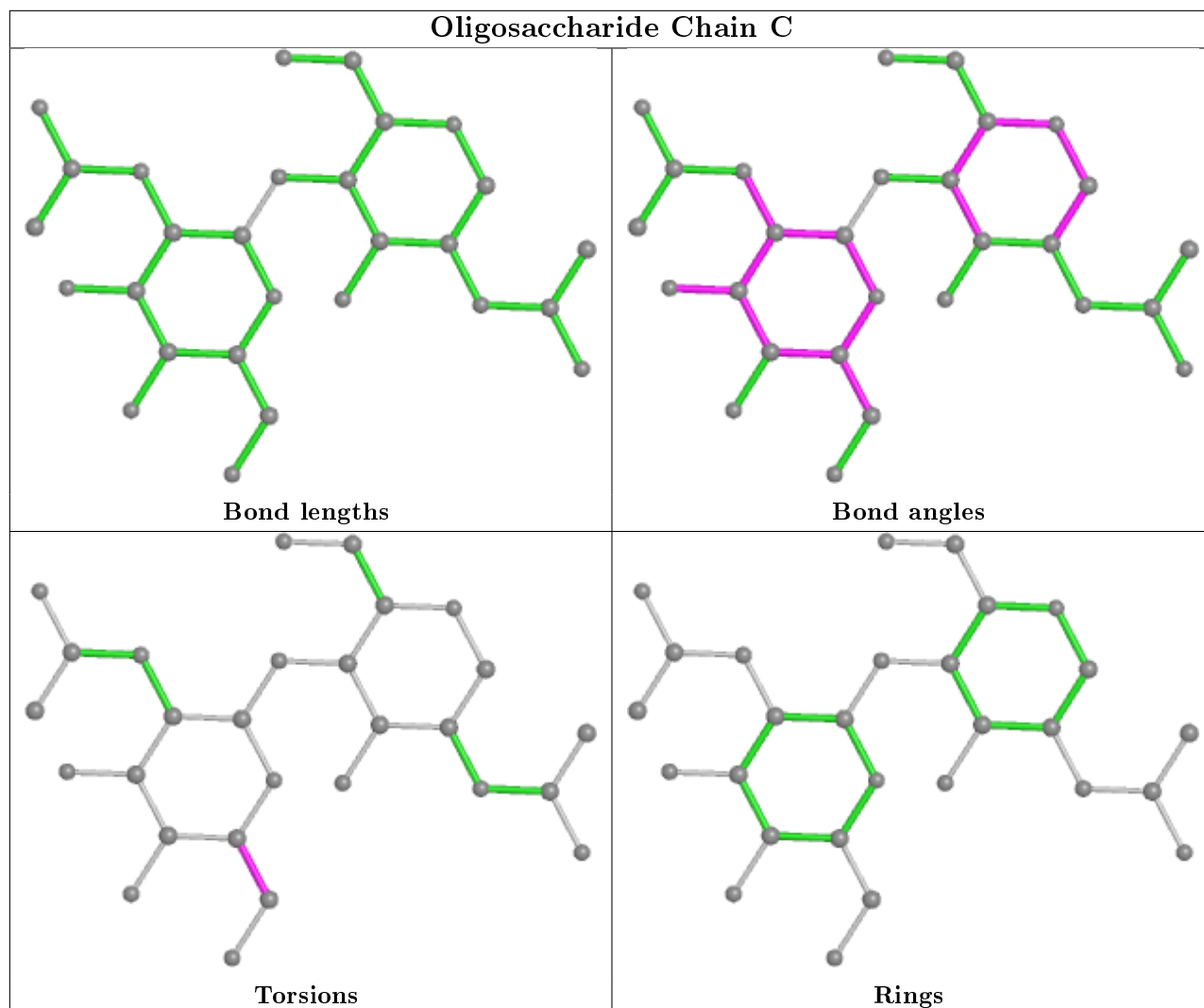
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6

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 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 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	$\# Z > 2$
7	PEG	A	620	-	6,6,6	1.88	2 (33%)	5,5,5	0.98	0
5	NAG	A	603	1	14,14,15	0.67	0	17,19,21	1.30	2 (11%)
9	3OP	A	623	-	14,14,14	2.41	5 (35%)	17,17,17	1.14	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	A	621	-	3,3,3	0.83	0	2,2,2	0.75	0
5	NAG	A	608	1	14,14,15	0.52	0	17,19,21	1.39	2 (11%)
4	HEM	A	602	1,10	27,50,50	2.67	11 (40%)	17,82,82	3.06	11 (64%)
8	EDO	A	622	-	3,3,3	0.77	0	2,2,2	0.78	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
7	PEG	A	620	-	-	3/4/4/4	-
5	NAG	A	603	1	-	1/6/23/26	0/1/1/1
9	3OP	A	623	-	-	2/4/4/4	0/2/2/2
8	EDO	A	621	-	-	0/1/1/1	-
5	NAG	A	608	1	-	0/6/23/26	0/1/1/1
4	HEM	A	602	1,10	-	0/6/54/54	-
8	EDO	A	622	-	-	1/1/1/1	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	HEM	CMA-C3A	-8.01	1.35	1.51
9	A	623	3OP	C1-C3	-5.40	1.30	1.38
4	A	602	HEM	C4A-CHB	4.75	1.54	1.41
4	A	602	HEM	CMC-C2C	4.68	1.62	1.51
9	A	623	3OP	C2-C4	-4.19	1.32	1.38
4	A	602	HEM	C3C-C2C	-3.87	1.35	1.40
7	A	620	PEG	O1-C1	-3.51	1.24	1.42
4	A	602	HEM	CMB-C2B	3.31	1.59	1.51
9	A	623	3OP	C7-C5	-3.13	1.32	1.38
4	A	602	HEM	C3D-C2D	3.08	1.46	1.37
4	A	602	HEM	C3C-CAC	3.05	1.54	1.47
9	A	623	3OP	O13-C4	-2.88	1.33	1.39
7	A	620	PEG	C2-C1	-2.67	1.35	1.49
4	A	602	HEM	C1A-CHA	-2.37	1.34	1.41
4	A	602	HEM	CAA-C2A	2.21	1.55	1.52
4	A	602	HEM	C1D-CHD	2.08	1.46	1.41
4	A	602	HEM	C1D-ND	2.06	1.40	1.36
9	A	623	3OP	C5-C3	-2.06	1.34	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	HEM	CBD-CAD-C3D	-6.43	100.64	112.48
4	A	602	HEM	C4A-C3A-C2A	6.32	111.39	107.00
4	A	602	HEM	C3C-C4C-NC	-3.48	104.37	110.94
4	A	602	HEM	CMC-C2C-C3C	3.29	130.83	124.68
4	A	602	HEM	C4C-C3C-C2C	3.22	109.14	106.90
4	A	602	HEM	CMD-C2D-C1D	2.97	133.04	128.46
5	A	608	NAG	O5-C5-C6	2.89	111.74	107.20
5	A	608	NAG	C3-C4-C5	-2.76	105.32	110.24
5	A	603	NAG	O4-C4-C5	2.73	116.09	109.30
4	A	602	HEM	CMA-C3A-C4A	-2.63	124.42	128.46
4	A	602	HEM	CAA-CBA-CGA	2.58	117.00	112.67
4	A	602	HEM	CMB-C2B-C3B	2.52	129.39	124.68
4	A	602	HEM	CMD-C2D-C3D	-2.48	120.26	124.94
9	A	623	3OP	C7-C5-C3	2.35	122.73	118.96
5	A	603	NAG	C1-O5-C5	2.34	115.36	112.19
4	A	602	HEM	CAD-CBD-CGD	-2.20	108.97	112.67
9	A	623	3OP	C9-N11-C1	2.06	120.42	116.85

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	620	PEG	O2-C3-C4-O4
8	A	622	EDO	O1-C1-C2-O2
7	A	620	PEG	O1-C1-C2-O2
5	A	603	NAG	C4-C5-C6-O6
9	A	623	3OP	C2-C4-O13-C3
7	A	620	PEG	C4-C3-O2-C2
9	A	623	3OP	C1-C3-O13-C4

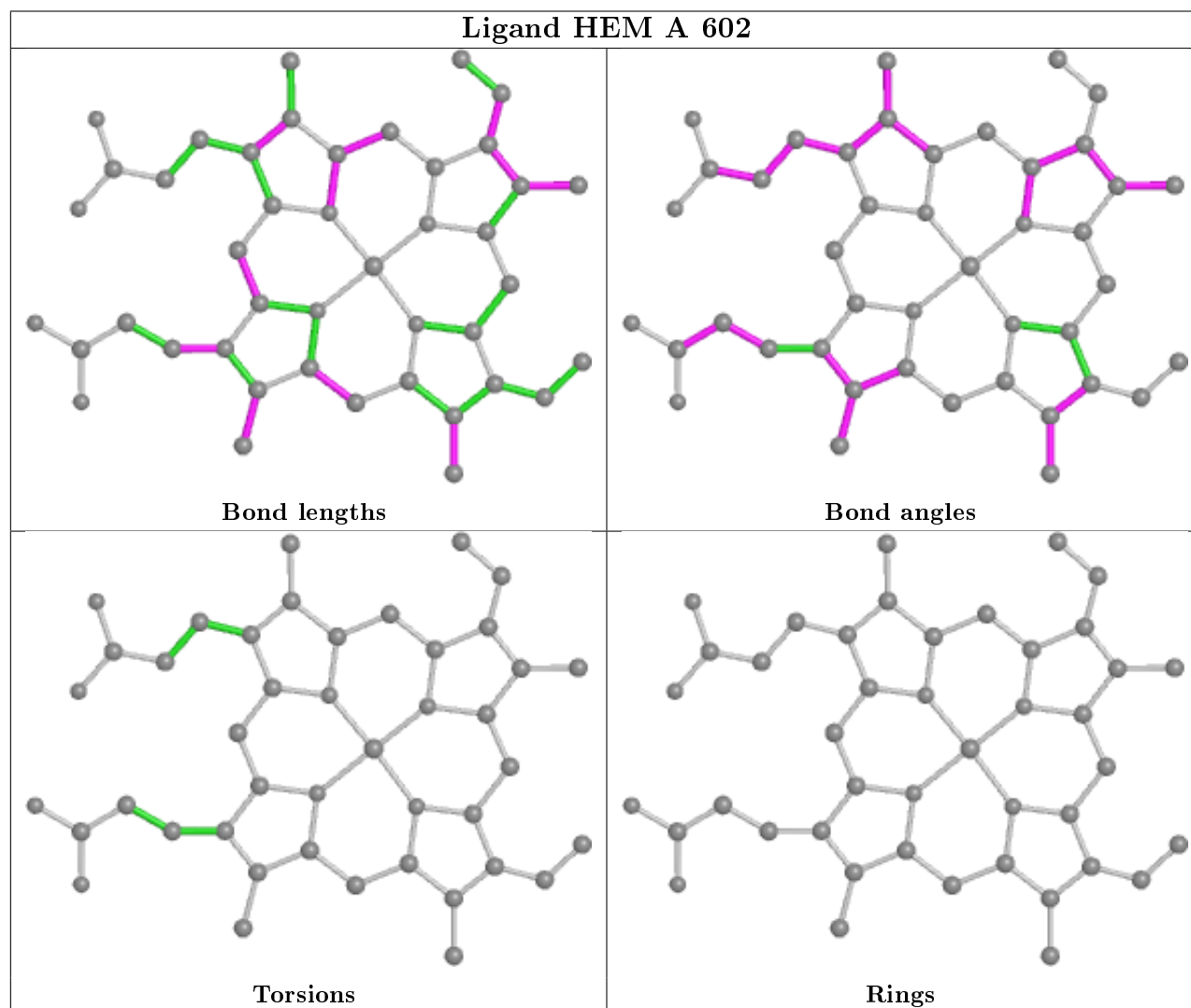
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	623	3OP	4	0
4	A	602	HEM	7	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%)	0.60	67 (11%) 5 7	29, 49, 98, 100	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	15.8
1	A	173	GLN	15.5
1	A	172	TYR	15.2
1	A	8	ALA	13.0
1	A	7	GLY	12.9
1	A	12	LEU	8.4
1	A	13	VAL	8.4
1	A	174	SER	8.2
1	A	9	PRO	8.2
1	A	1	SER	8.1
1	A	121	SER	7.5
1	A	170	PRO	6.4
1	A	122	ASN	6.4
1	A	595	ASN	6.4
1	A	120	GLY	6.3
1	A	6	CYS	6.2
1	A	10	VAL	6.1
1	A	169	THR	5.1
1	A	107	VAL	4.7
1	A	593	ARG	4.7
1	A	4	VAL	4.6
1	A	5	GLY	4.4
1	A	11	PRO	4.3
1	A	106	ILE	4.3
1	A	17	GLU	4.1
1	A	171	PRO	4.1
1	A	124	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	132	TYR	3.7
1	A	3	GLU	3.6
1	A	119	LEU	3.4
1	A	223	GLY	3.4
1	A	125	SER	3.4
1	A	123	GLU	3.2
1	A	183	VAL	3.2
1	A	279	GLU	3.2
1	A	14	LYS	3.2
1	A	191	LEU	3.2
1	A	118	GLU	3.1
1	A	111	LEU	3.0
1	A	354	VAL	3.0
1	A	134	ILE	2.9
1	A	594	GLU	2.9
1	A	269	LEU	2.8
1	A	105	GLN	2.8
1	A	18	ASN	2.8
1	A	261	LEU	2.7
1	A	192	VAL	2.6
1	A	128	GLN	2.5
1	A	376	LEU	2.5
1	A	108	ASP	2.4
1	A	102	GLN	2.4
1	A	137	ASP	2.4
1	A	530	TRP	2.4
1	A	592	SER	2.3
1	A	104	GLY	2.3
1	A	259	GLN	2.2
1	A	109	HIS	2.2
1	A	286	HIS	2.2
1	A	300	LEU	2.2
1	A	101	MET	2.2
1	A	190	SER	2.2
1	A	131	GLU	2.1
1	A	344	THR	2.1
1	A	348	ARG	2.1
1	A	167	CYS	2.1
1	A	246	VAL	2.1
1	A	579	CYS	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	0.97	0.11	25,46,51,54	0

6.3 Carbohydrates [i](#)

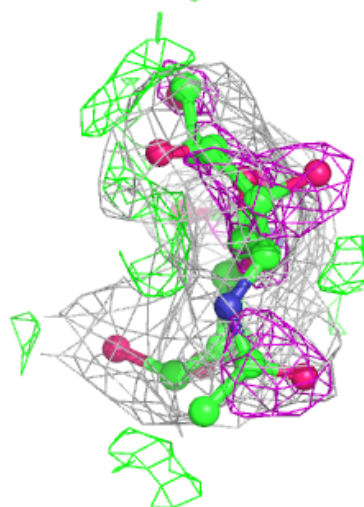
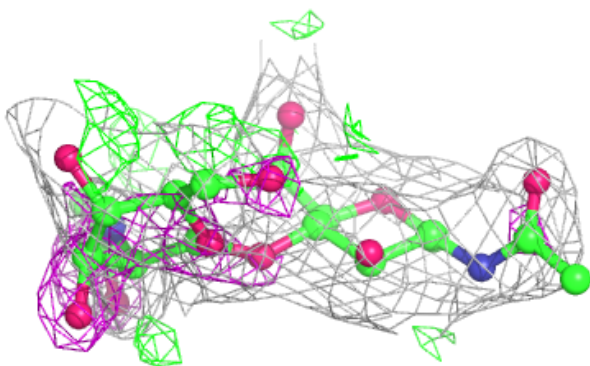
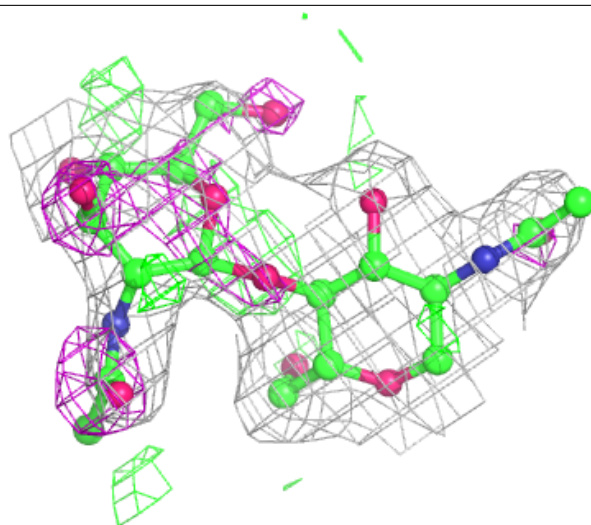
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

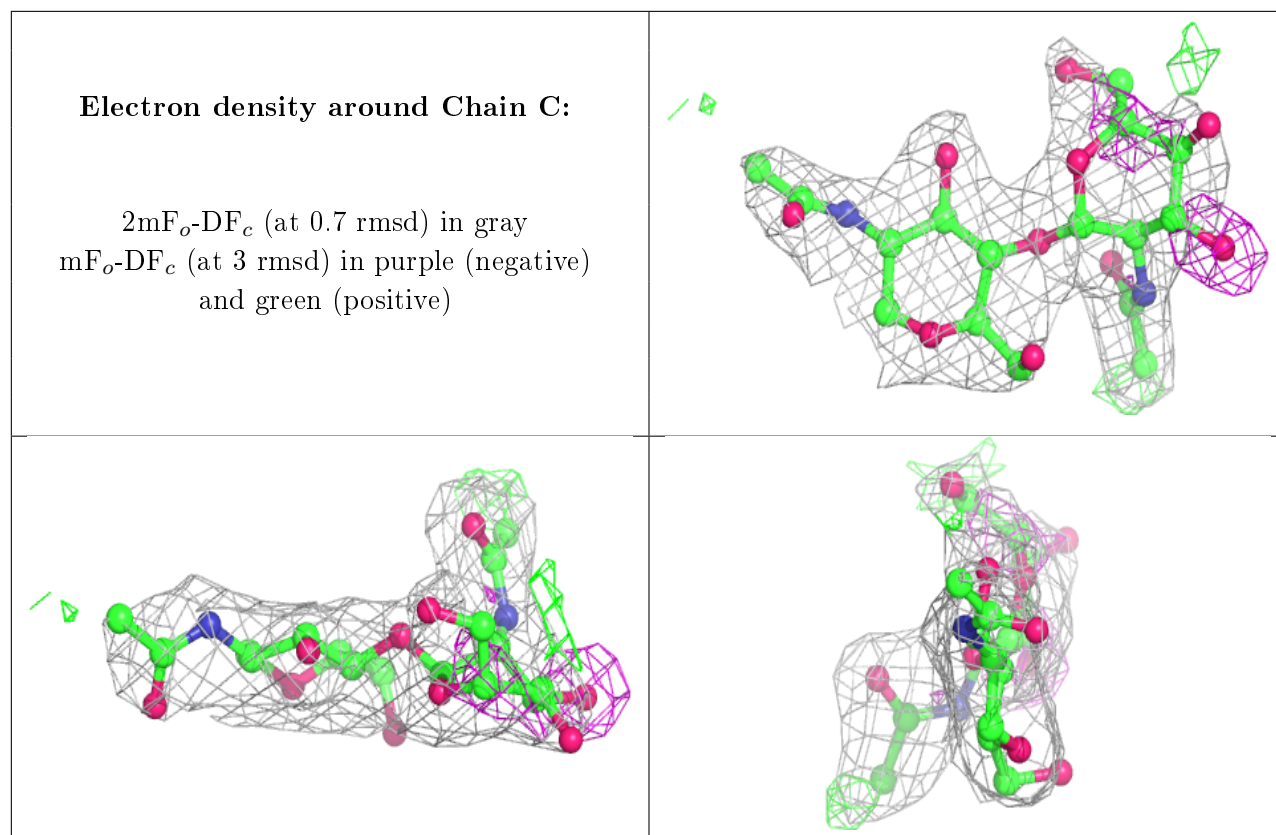
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	2	14/15	0.67	0.42	42,49,57,57	0
2	NAG	C	2	14/15	0.71	0.32	50,54,58,68	0
2	NAG	B	1	14/15	0.84	0.19	40,48,52,55	0
2	NAG	C	1	14/15	0.93	0.15	49,56,68,70	0

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.

Electron density around Chain B:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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.

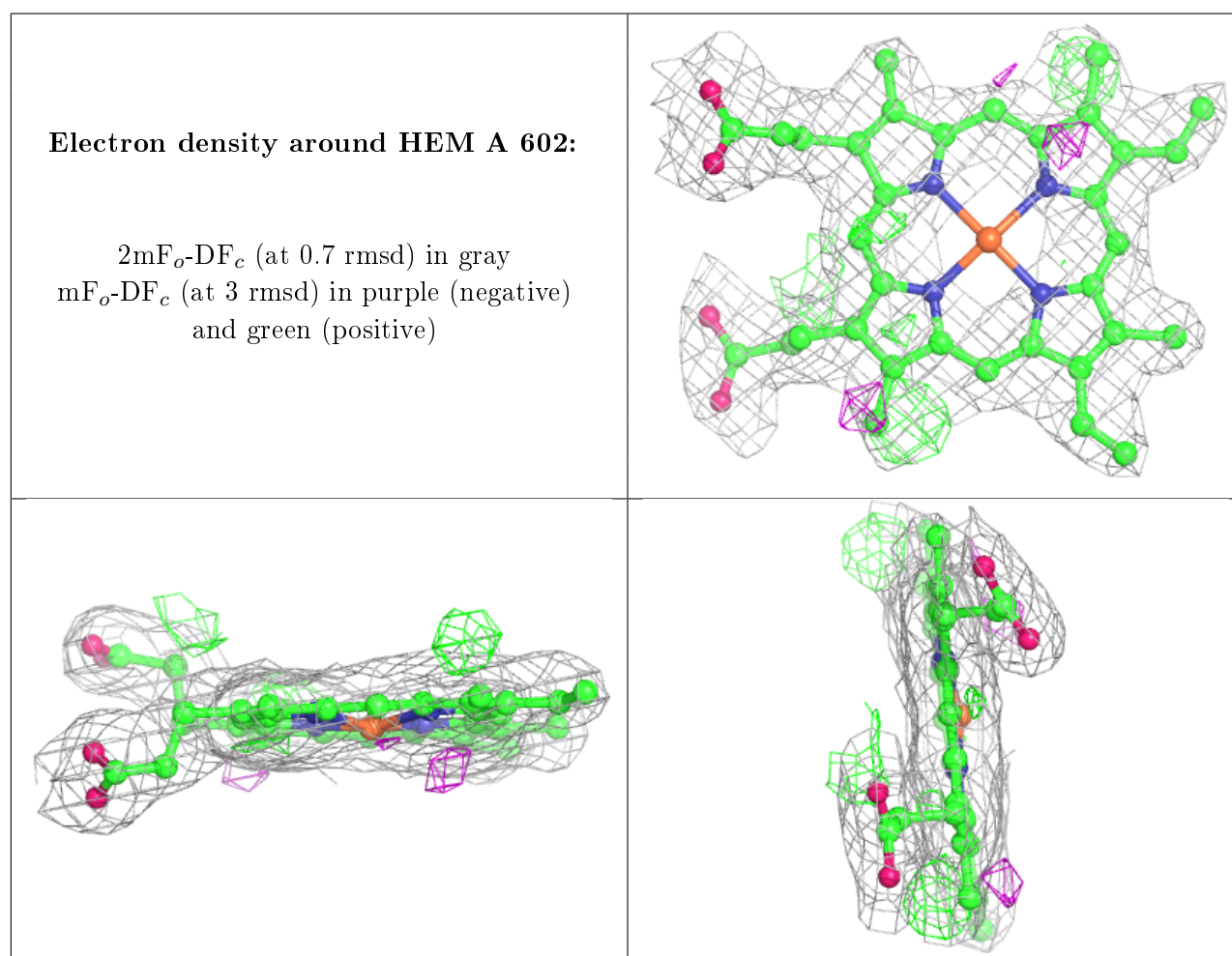
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	603	14/15	0.70	0.46	46,54,59,66	0
7	PEG	A	620	7/7	0.80	0.22	36,44,48,49	0
9	3OP	A	623	13/13	0.83	0.32	44,61,69,69	0
5	NAG	A	608	14/15	0.86	0.23	50,52,58,59	0
8	EDO	A	622	4/4	0.90	0.17	55,55,57,57	0
8	EDO	A	621	4/4	0.90	0.12	46,48,51,53	0
6	IOD	A	614	1/1	0.95	0.07	67,67,67,67	1
4	HEM	A	602	43/43	0.96	0.30	27,33,40,41	0
6	IOD	A	612	1/1	0.97	0.13	66,66,66,66	0
6	IOD	A	615	1/1	0.97	0.37	60,60,60,60	1
6	IOD	A	613	1/1	0.98	0.10	63,63,63,63	0
6	IOD	A	619	1/1	0.98	0.27	61,61,61,61	0
6	IOD	A	609	1/1	0.98	0.06	63,63,63,63	0
6	IOD	A	611	1/1	0.99	0.04	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	A	601	1/1	0.99	0.20	39,39,39,39	0
6	IOD	A	610	1/1	0.99	0.04	62,62,62,62	0
6	IOD	A	616	1/1	1.00	0.05	44,44,44,44	0
6	IOD	A	618	1/1	1.00	0.02	65,65,65,65	0
6	IOD	A	617	1/1	1.00	0.06	56,56,56,56	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 ⓘ

There are no such residues in this entry.