



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 05:49 PM BST

PDB ID : 2QRB  
Title : Crystal structure of chloride saturated bovine lactoperoxidase at 2.5 Å resolution shows multiple halide binding sites  
Authors : Singh, A.K.; Singh, N.; Sharma, S.; Kaur, P.; Singh, T.P.  
Deposited on : 2007-07-28  
Resolution : 2.50 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

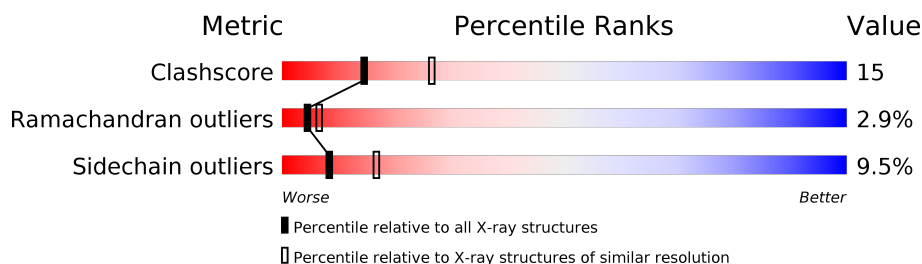
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	595	
2	B	3	
2	D	3	
3	C	2	
3	E	2	

## 2 Entry composition [i](#)

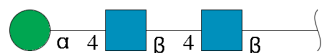
There are 8 unique types of molecules in this entry. The entry contains 5220 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 3 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
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

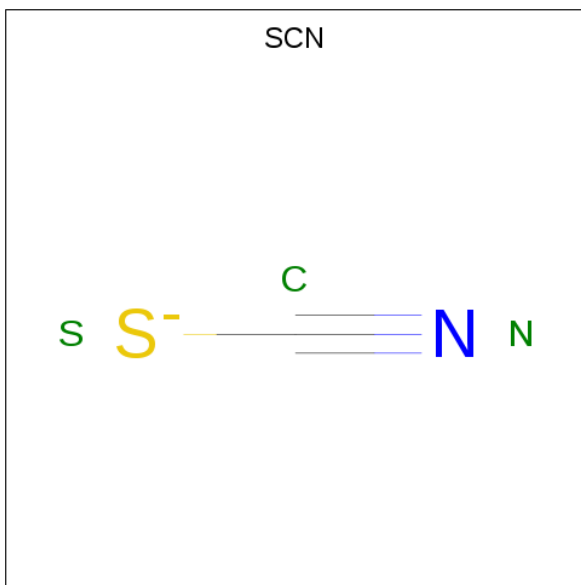
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	Cl	0	0
			11	11		

- Molecule 6 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



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

- Molecule 7 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
7	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is water.

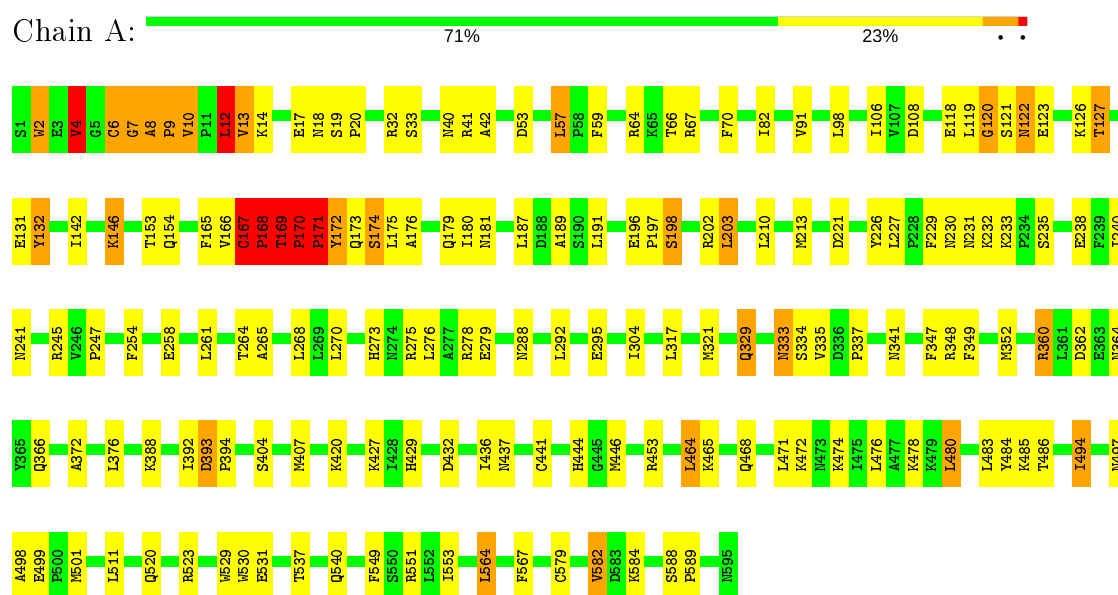
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	254	Total	O	0	0
			254	254		

### 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. 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. 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.

Note EDS was not executed.

- Molecule 1: Lactoperoxidase



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



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




- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

HA01  
HA02

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

HA01  
HA02

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.44 Å   80.56 Å   77.71 Å 90.00°   102.77°   90.00°	Depositor
Resolution (Å)	19.47 – 2.50	Depositor
% Data completeness (in resolution range)	90.7 (19.47-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.189 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5220	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SCN, NAG, SEP, CA, CL, HEM, MAN

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	0.44	4/4891 (0.1%)	0.79	9/6634 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	PRO	N-CA	5.90	1.57	1.47
1	A	171	PRO	N-CA	5.86	1.57	1.47
1	A	170	PRO	C-N	5.34	1.44	1.34
1	A	170	PRO	CA-C	5.18	1.63	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	CYS	N-CA-C	-8.96	86.82	111.00
1	A	167	CYS	N-CA-C	-7.63	90.40	111.00
1	A	168	PRO	CA-C-N	-6.77	102.30	117.20
1	A	232	LYS	N-CA-C	6.34	128.12	111.00
1	A	12	LEU	N-CA-C	5.65	126.25	111.00
1	A	171	PRO	N-CA-C	5.51	126.42	112.10
1	A	120	GLY	N-CA-C	5.45	126.72	113.10
1	A	233	LYS	N-CA-C	-5.28	96.75	111.00
1	A	170	PRO	N-CA-C	5.06	125.25	112.10

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	4688	143	0
2	B	39	0	34	2	0
2	D	39	0	34	1	0
3	C	28	0	25	2	0
3	E	28	0	25	0	0
4	A	1	0	0	0	0
5	A	11	0	0	2	0
6	A	3	0	0	0	0
7	A	43	0	30	11	0
8	A	254	0	0	18	0
All	All	5220	0	4836	151	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 15.

All (151) 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:169:THR:CG2	1:A:170:PRO:HD3	1.59	1.31
1:A:169:THR:HG22	1:A:170:PRO:CD	1.62	1.29
1:A:169:THR:CG2	1:A:170:PRO:CD	2.17	1.20
1:A:169:THR:HG22	1:A:170:PRO:HD2	1.14	1.10
1:A:169:THR:HG23	1:A:170:PRO:HD3	1.14	1.09
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.14	1.07
1:A:175:LEU:HD23	1:A:176:ALA:H	1.20	1.07
1:A:12:LEU:HD12	1:A:12:LEU:H	1.17	1.04
1:A:202:ARG:HH22	1:A:231:ASN:HB2	1.16	1.04
1:A:167:CYS:HB3	1:A:168:PRO:CD	1.88	1.02
1:A:10:VAL:HG23	1:A:10:VAL:O	1.65	0.96
1:A:108:ASP:OD2	7:A:619:HEM:HMD3	1.69	0.93
1:A:170:PRO:HB3	1:A:171:PRO:HD2	1.51	0.92
1:A:202:ARG:NH2	1:A:231:ASN:HB2	1.84	0.92
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.02	0.88
1:A:197:PRO:HD2	1:A:198:SEP:O3P	1.73	0.88
1:A:12:LEU:N	1:A:12:LEU:HD12	1.86	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:HD23	1:A:176:ALA:N	1.95	0.82
1:A:108:ASP:OD2	7:A:619:HEM:CMD	2.29	0.80
1:A:258:GLU:OE2	7:A:619:HEM:HMB3	1.83	0.78
1:A:2:TRP:HB3	1:A:4:VAL:HG22	1.67	0.76
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.68	0.76
1:A:82:ILE:HG21	1:A:494:ILE:HD11	1.68	0.75
1:A:231:ASN:HA	8:A:732:HOH:O	1.88	0.74
1:A:360:ARG:NH1	1:A:372:ALA:HA	2.05	0.72
1:A:8:ALA:HB3	1:A:9:PRO:CD	2.20	0.71
1:A:8:ALA:HB3	1:A:9:PRO:HD2	1.73	0.70
1:A:123:GLU:HB3	1:A:126:LYS:HG3	1.75	0.69
1:A:131:GLU:HB3	1:A:132:TYR:CD1	2.28	0.69
1:A:235:SER:HB3	1:A:238:GLU:HG2	1.75	0.68
1:A:427:LYS:HE2	8:A:808:HOH:O	1.93	0.68
1:A:231:ASN:HB3	8:A:799:HOH:O	1.93	0.68
1:A:329:GLN:HG3	8:A:748:HOH:O	1.94	0.67
1:A:427:LYS:HE3	8:A:783:HOH:O	1.92	0.67
1:A:348:ARG:HH11	1:A:437:ASN:ND2	1.92	0.67
1:A:131:GLU:HB3	1:A:132:TYR:HD1	1.59	0.67
7:A:619:HEM:HBB2	7:A:619:HEM:HMB1	1.76	0.67
1:A:169:THR:HG23	1:A:170:PRO:CD	2.00	0.66
1:A:432:ASP:O	1:A:436:ILE:HG12	1.95	0.66
1:A:362:ASP:HB2	8:A:823:HOH:O	1.95	0.65
1:A:170:PRO:CB	1:A:171:PRO:HD2	2.26	0.65
2:B:1:NAG:H61	2:B:2:NAG:C1	2.27	0.65
1:A:472:LYS:HE3	8:A:788:HOH:O	1.97	0.64
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.78	0.64
1:A:474:LYS:HD3	8:A:838:HOH:O	1.98	0.64
1:A:108:ASP:CG	7:A:619:HEM:HMD3	2.18	0.64
1:A:579:CYS:O	1:A:582:VAL:HG23	1.98	0.64
1:A:106:ILE:HD11	1:A:265:ALA:HB1	1.78	0.64
1:A:197:PRO:CD	1:A:198:SEP:O3P	2.45	0.63
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.80	0.63
1:A:167:CYS:CB	1:A:168:PRO:CD	2.63	0.62
1:A:258:GLU:OE2	7:A:619:HEM:CMB	2.48	0.61
1:A:127:THR:O	1:A:131:GLU:HB2	2.00	0.60
8:A:863:HOH:O	2:B:1:NAG:H83	2.01	0.60
1:A:333:ASN:HD22	1:A:333:ASN:C	2.03	0.60
1:A:349:PHE:HB2	1:A:497:ASN:HD21	1.67	0.59
1:A:567:PHE:HB2	5:A:617:CL:CL	2.40	0.59
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:C	1:A:10:VAL:H	2.07	0.58
1:A:537:THR:OG1	1:A:540:GLN:HG3	2.04	0.58
7:A:619:HEM:HMC1	7:A:619:HEM:HBC2	1.85	0.58
8:A:864:HOH:O	3:C:1:NAG:H3	2.03	0.58
1:A:333:ASN:HD22	1:A:334:SER:N	2.02	0.58
1:A:67:ARG:NH1	8:A:853:HOH:O	2.37	0.58
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.39	0.57
1:A:12:LEU:N	1:A:12:LEU:CD1	2.55	0.56
1:A:42:ALA:HB2	1:A:166:VAL:HG11	1.87	0.56
1:A:121:SER:O	1:A:122:ASN:HB3	2.06	0.56
1:A:82:ILE:HD13	1:A:480:LEU:CD1	2.36	0.56
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.18	0.56
1:A:170:PRO:HB3	1:A:171:PRO:CD	2.32	0.55
1:A:166:VAL:O	1:A:167:CYS:HB2	2.06	0.55
1:A:258:GLU:HG3	5:A:608:CL:CL	2.43	0.55
1:A:169:THR:CG2	1:A:170:PRO:HD2	2.00	0.54
1:A:123:GLU:HB3	1:A:126:LYS:HE2	1.90	0.54
1:A:166:VAL:O	1:A:167:CYS:CB	2.56	0.54
1:A:360:ARG:HH12	1:A:372:ALA:HA	1.71	0.54
1:A:122:ASN:H	1:A:126:LYS:HZ3	1.56	0.53
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.44	0.53
1:A:8:ALA:CB	1:A:9:PRO:CD	2.85	0.53
1:A:82:ILE:HD13	1:A:480:LEU:HD13	1.91	0.52
1:A:240:ILE:O	1:A:240:ILE:HD12	2.10	0.52
1:A:53:ASP:OD2	1:A:57:LEU:HD22	2.09	0.52
1:A:264:THR:HG23	1:A:392:ILE:HB	1.91	0.52
1:A:12:LEU:O	1:A:13:VAL:HG13	2.10	0.51
1:A:335:VAL:O	1:A:337:PRO:HD3	2.10	0.51
1:A:341:ASN:HB3	1:A:446:MET:HE1	1.92	0.51
1:A:529:TRP:CD1	1:A:531:GLU:HB2	2.45	0.51
1:A:170:PRO:CB	1:A:171:PRO:CD	2.89	0.51
1:A:59:PHE:CE2	1:A:67:ARG:HG3	2.46	0.50
1:A:407:MET:HB3	1:A:501:MET:HE3	1.92	0.49
8:A:864:HOH:O	3:C:1:NAG:H5	2.11	0.49
1:A:146:LYS:HE3	8:A:738:HOH:O	2.13	0.49
1:A:165:PHE:N	1:A:165:PHE:CD2	2.80	0.49
1:A:82:ILE:HD12	1:A:483:LEU:HD12	1.94	0.49
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.48	0.48
1:A:407:MET:HB3	1:A:501:MET:CE	2.43	0.48
1:A:321:MET:HB3	8:A:790:HOH:O	2.13	0.48
1:A:175:LEU:CD2	1:A:176:ALA:N	2.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ASN:HB3	1:A:446:MET:CE	2.43	0.47
2:D:2:NAG:H4	2:D:3:MAN:H2	1.61	0.47
1:A:8:ALA:O	1:A:10:VAL:N	2.46	0.47
1:A:121:SER:HA	1:A:126:LYS:NZ	2.29	0.47
1:A:9:PRO:O	1:A:40:ASN:HB3	2.15	0.46
1:A:230:ASN:OD1	1:A:231:ASN:N	2.49	0.46
1:A:82:ILE:CG2	1:A:494:ILE:HD11	2.42	0.46
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.51	0.46
1:A:123:GLU:CB	1:A:126:LYS:HE2	2.46	0.46
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.98	0.46
1:A:549:PHE:O	1:A:553:ILE:HG12	2.15	0.46
1:A:210:LEU:HB3	8:A:663:HOH:O	2.16	0.45
1:A:229:PHE:CG	1:A:247:PRO:HG2	2.51	0.45
1:A:108:ASP:OD2	7:A:619:HEM:HMD2	2.16	0.45
1:A:333:ASN:ND2	1:A:333:ASN:C	2.70	0.45
1:A:254:PHE:HB3	8:A:810:HOH:O	2.16	0.45
1:A:258:GLU:CD	7:A:619:HEM:HMB3	2.37	0.45
1:A:106:ILE:HD11	1:A:265:ALA:CB	2.47	0.45
1:A:588:SER:N	1:A:589:PRO:CD	2.80	0.45
1:A:121:SER:HA	1:A:126:LYS:HZ3	1.82	0.45
1:A:179:GLN:HG2	1:A:444:HIS:CE1	2.52	0.45
1:A:132:TYR:CD1	1:A:132:TYR:N	2.86	0.44
1:A:142:ILE:CD1	1:A:436:ILE:HD13	2.47	0.44
1:A:7:GLY:HA2	1:A:10:VAL:HG11	2.00	0.44
1:A:453:ARG:NH1	1:A:499:GLU:OE2	2.50	0.43
1:A:196:GLU:HB3	1:A:198:SEP:O2P	2.17	0.43
1:A:478:LYS:HB2	1:A:478:LYS:HE3	1.67	0.43
1:A:108:ASP:OD1	7:A:619:HEM:HMD3	2.18	0.43
1:A:180:ILE:HG22	1:A:181:ASN:N	2.33	0.43
1:A:10:VAL:CG2	1:A:10:VAL:O	2.38	0.43
1:A:221:ASP:HB2	1:A:226:TYR:CE2	2.54	0.43
1:A:295:GLU:HG3	8:A:760:HOH:O	2.18	0.43
1:A:196:GLU:HA	1:A:197:PRO:HD3	1.89	0.42
1:A:19:SER:HA	1:A:20:PRO:HD3	1.86	0.42
1:A:203:LEU:HB3	1:A:213:MET:CE	2.49	0.42
1:A:10:VAL:HB	1:A:41:ARG:CZ	2.49	0.42
7:A:619:HEM:HBB2	7:A:619:HEM:CMB	2.46	0.42
1:A:564:LEU:HA	1:A:564:LEU:HD12	1.87	0.42
1:A:420:LYS:HA	1:A:429:HIS:O	2.19	0.42
1:A:362:ASP:OD1	1:A:366:GLN:HB2	2.20	0.42
1:A:288:ASN:O	1:A:292:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:O	1:A:122:ASN:CG	2.57	0.41
1:A:66:THR:HB	1:A:70:PHE:O	2.20	0.41
1:A:14:LYS:HB2	8:A:845:HOH:O	2.19	0.41
1:A:173:GLN:HG3	1:A:174:SER:H	1.86	0.41
1:A:464:LEU:O	1:A:468:GLN:HG3	2.21	0.41
1:A:588:SER:OG	1:A:589:PRO:HD3	2.21	0.41
1:A:476:LEU:HD21	1:A:498:ALA:HB1	2.03	0.41
1:A:484:TYR:O	1:A:485:LYS:HB2	2.20	0.41
1:A:275:ARG:O	1:A:279:GLU:HB2	2.21	0.40
1:A:32:ARG:HH11	1:A:32:ARG:HB3	1.85	0.40
1:A:106:ILE:HG23	1:A:191:LEU:HD11	2.03	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%)	542 (92%)	33 (6%)	17 (3%)	<b>4</b> <b>6</b>

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	168	PRO
1	A	174	SER
1	A	241	ASN
1	A	169	THR
1	A	170	PRO
1	A	172	TYR
1	A	64	ARG
1	A	8	ALA
1	A	122	ASN

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Mol	Chain	Res	Type
1	A	171	PRO
1	A	9	PRO
1	A	17	GLU
1	A	120	GLY
1	A	7	GLY
1	A	4	VAL
1	A	10	VAL

### 5.3.2 Protein sidechains ⓘ

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%)	468 (90%)	49 (10%)	8 17

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	4	VAL
1	A	6	CYS
1	A	12	LEU
1	A	13	VAL
1	A	18	ASN
1	A	33	SER
1	A	57	LEU
1	A	91	VAL
1	A	98	LEU
1	A	118	GLU
1	A	119	LEU
1	A	127	THR
1	A	132	TYR
1	A	146	LYS
1	A	153	THR
1	A	154	GLN
1	A	167	CYS
1	A	169	THR

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Mol	Chain	Res	Type
1	A	172	TYR
1	A	187	LEU
1	A	203	LEU
1	A	245	ARG
1	A	261	LEU
1	A	268	LEU
1	A	276	LEU
1	A	278	ARG
1	A	317	LEU
1	A	329	GLN
1	A	333	ASN
1	A	347	PHE
1	A	352	MET
1	A	360	ARG
1	A	364	ASN
1	A	376	LEU
1	A	388	LYS
1	A	393	ASP
1	A	404	SER
1	A	441	CYS
1	A	464	LEU
1	A	465	LYS
1	A	471	LEU
1	A	480	LEU
1	A	486	THR
1	A	494	ILE
1	A	511	LEU
1	A	520	GLN
1	A	564	LEU
1	A	582	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	333	ASN
1	A	423	GLN
1	A	437	ASN
1	A	468	GLN
1	A	497	ASN
1	A	520	GLN



### 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	1.40	1 (12%)	8,12,14	3.16	5 (62%)

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	O-C	2.15	1.28	1.19

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-P-O1P	6.70	125.27	106.47
1	A	198	SEP	P-OG-CB	3.60	128.21	118.30
1	A	198	SEP	O3P-P-O2P	2.84	118.51	107.64
1	A	198	SEP	O3P-P-OG	-2.70	99.54	106.73
1	A	198	SEP	O2P-P-O1P	-2.03	102.74	110.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

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	CB-OG-P-O1P
1	A	198	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	3	0

## 5.5 Carbohydrates [i](#)

10 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	0.74	0	17,19,21	1.52	4 (23%)
2	NAG	B	2	2	14,14,15	0.65	0	17,19,21	0.79	1 (5%)
2	MAN	B	3	2	11,11,12	0.66	0	15,15,17	0.42	0
3	NAG	C	1	1,3	14,14,15	0.62	0	17,19,21	0.73	0
3	NAG	C	2	3	14,14,15	0.88	1 (7%)	17,19,21	1.51	2 (11%)
2	NAG	D	1	1,2	14,14,15	0.68	0	17,19,21	0.76	0
2	NAG	D	2	2	14,14,15	0.83	0	17,19,21	1.13	3 (17%)
2	MAN	D	3	2	11,11,12	0.89	1 (9%)	15,15,17	1.43	2 (13%)
3	NAG	E	1	1,3	14,14,15	0.61	0	17,19,21	1.35	2 (11%)
3	NAG	E	2	3	14,14,15	0.70	0	17,19,21	1.44	2 (11%)

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	-	1/6/23/26	0/1/1/1
2	MAN	B	3	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	MAN	D	3	2	-	1/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	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)
3	C	2	NAG	C1-C2	2.41	1.55	1.52
2	D	3	MAN	C2-C3	2.11	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C1-O5-C5	4.62	118.45	112.19
3	E	2	NAG	C4-C3-C2	4.57	117.72	111.02
2	D	3	MAN	C1-C2-C3	4.45	115.13	109.67
3	E	1	NAG	C4-C3-C2	4.26	117.26	111.02
2	B	1	NAG	C1-O5-C5	3.54	116.99	112.19
3	C	2	NAG	O5-C1-C2	3.03	116.07	111.29
2	B	1	NAG	C2-N2-C7	-2.89	118.78	122.90
2	D	2	NAG	C2-N2-C7	-2.66	119.12	122.90
2	D	3	MAN	C2-C3-C4	2.48	115.19	110.89
2	B	2	NAG	C2-N2-C7	-2.48	119.38	122.90
2	D	2	NAG	C1-O5-C5	2.41	115.45	112.19
3	E	1	NAG	C3-C4-C5	2.25	114.26	110.24
2	D	2	NAG	C4-C3-C2	-2.25	107.72	111.02
2	B	1	NAG	C4-C3-C2	-2.10	107.94	111.02
3	E	2	NAG	C3-C4-C5	2.09	113.97	110.24
2	B	1	NAG	O5-C5-C6	-2.01	104.05	107.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

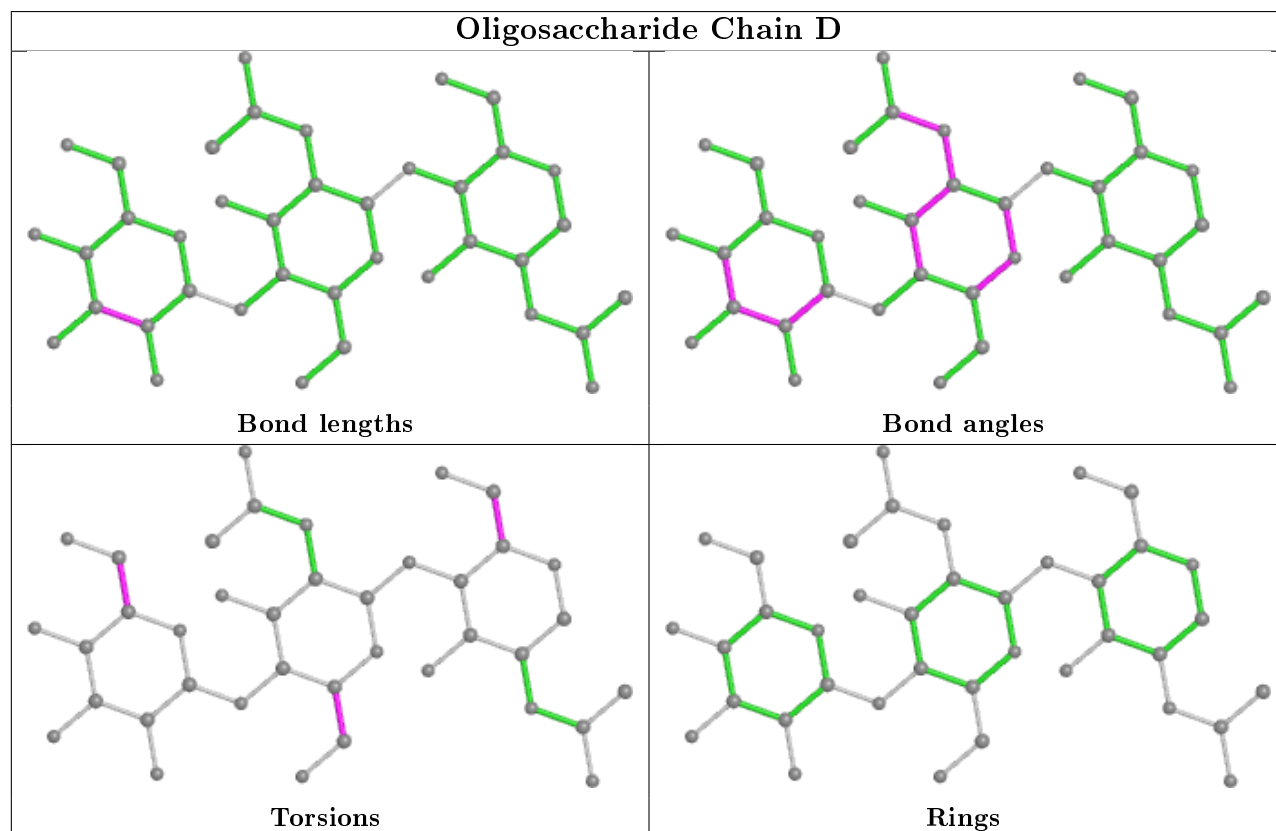
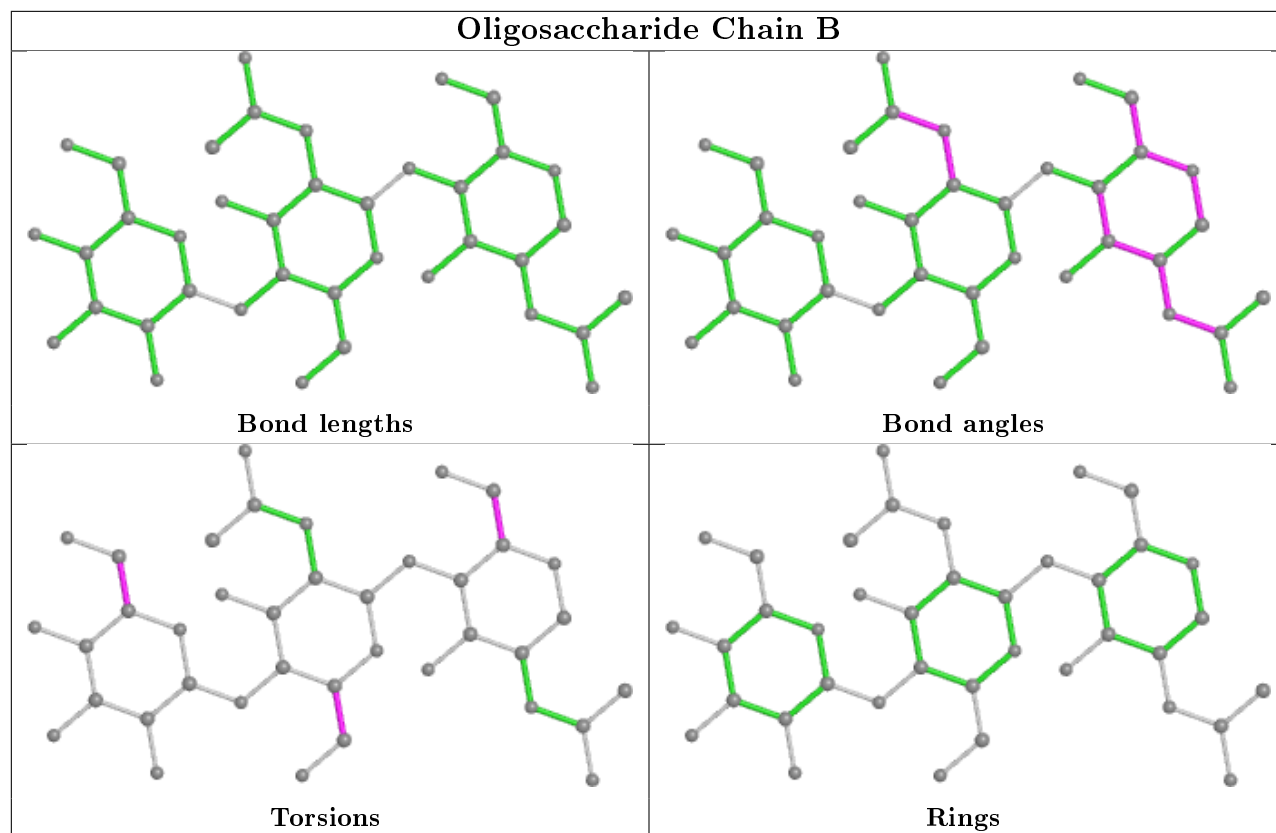
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	B	3	MAN	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	3	MAN	O5-C5-C6-O6
2	D	3	MAN	C4-C5-C6-O6

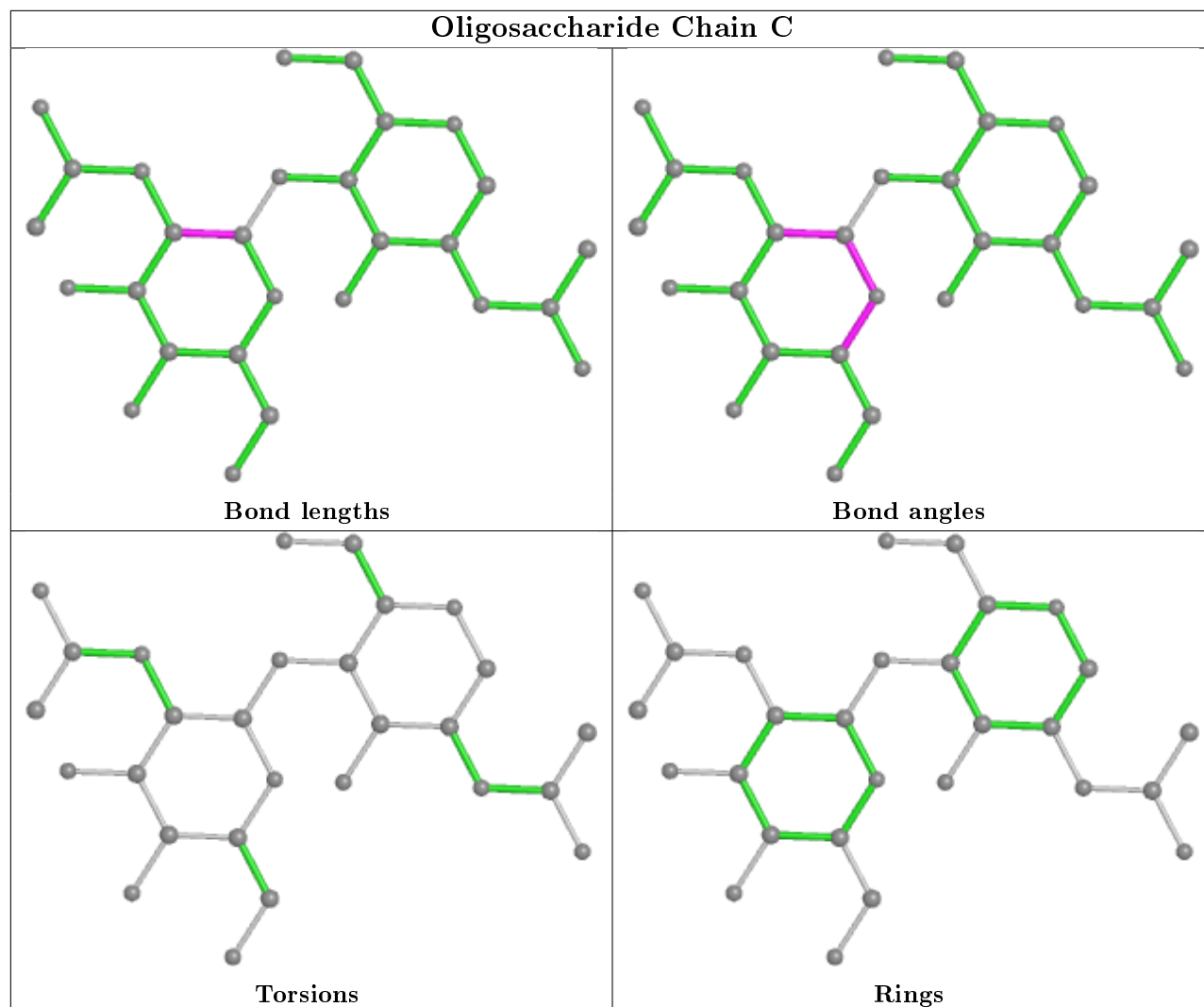
There are no ring outliers.

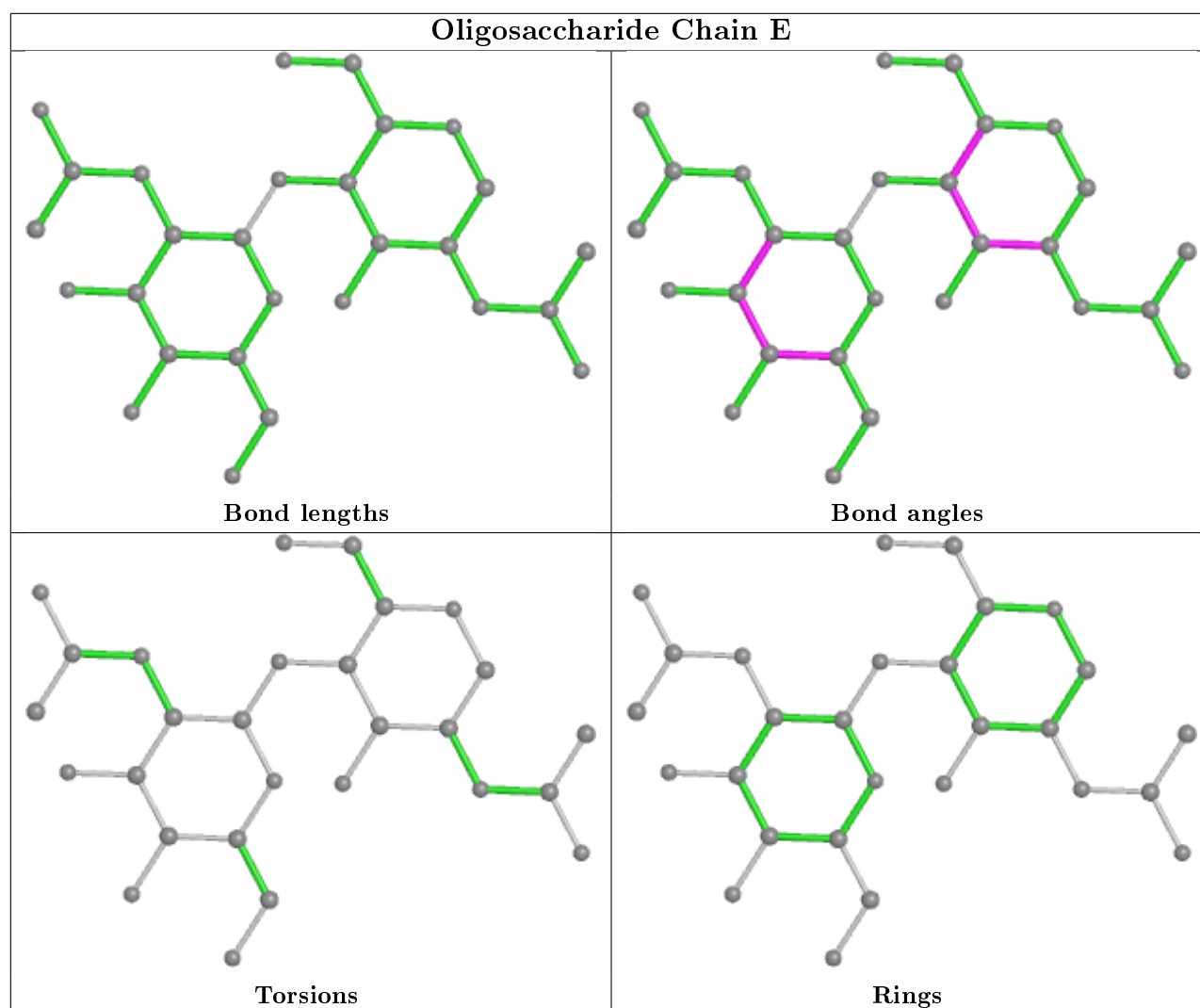
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0
2	D	2	NAG	1	0
2	D	3	MAN	1	0
3	C	1	NAG	2	0
2	B	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 [i](#)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	SCN	A	618	-	1,2,2	1.16	0	0,1,1	0.00	-
7	HEM	A	619	1,8	27,50,50	2.52	10 (37%)	17,82,82	1.78	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
7	HEM	A	619	1,8	-	0/6/54/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	619	HEM	C3D-C2D	5.50	1.54	1.37
7	A	619	HEM	C3C-CAC	4.96	1.58	1.47
7	A	619	HEM	C3B-CAB	4.78	1.57	1.47
7	A	619	HEM	CAD-C3D	4.00	1.59	1.52
7	A	619	HEM	C1D-ND	3.95	1.44	1.36
7	A	619	HEM	C4D-C3D	3.43	1.50	1.42
7	A	619	HEM	CMC-C2C	3.38	1.59	1.51
7	A	619	HEM	C1B-C2B	3.08	1.49	1.42
7	A	619	HEM	C1A-CHA	-2.46	1.34	1.41
7	A	619	HEM	CAA-C2A	2.22	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	619	HEM	CAD-CBD-CGD	3.71	118.89	112.67
7	A	619	HEM	CBD-CAD-C3D	-3.50	106.04	112.48
7	A	619	HEM	CAA-CBA-CGA	2.57	116.99	112.67
7	A	619	HEM	CMC-C2C-C3C	2.56	129.48	124.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

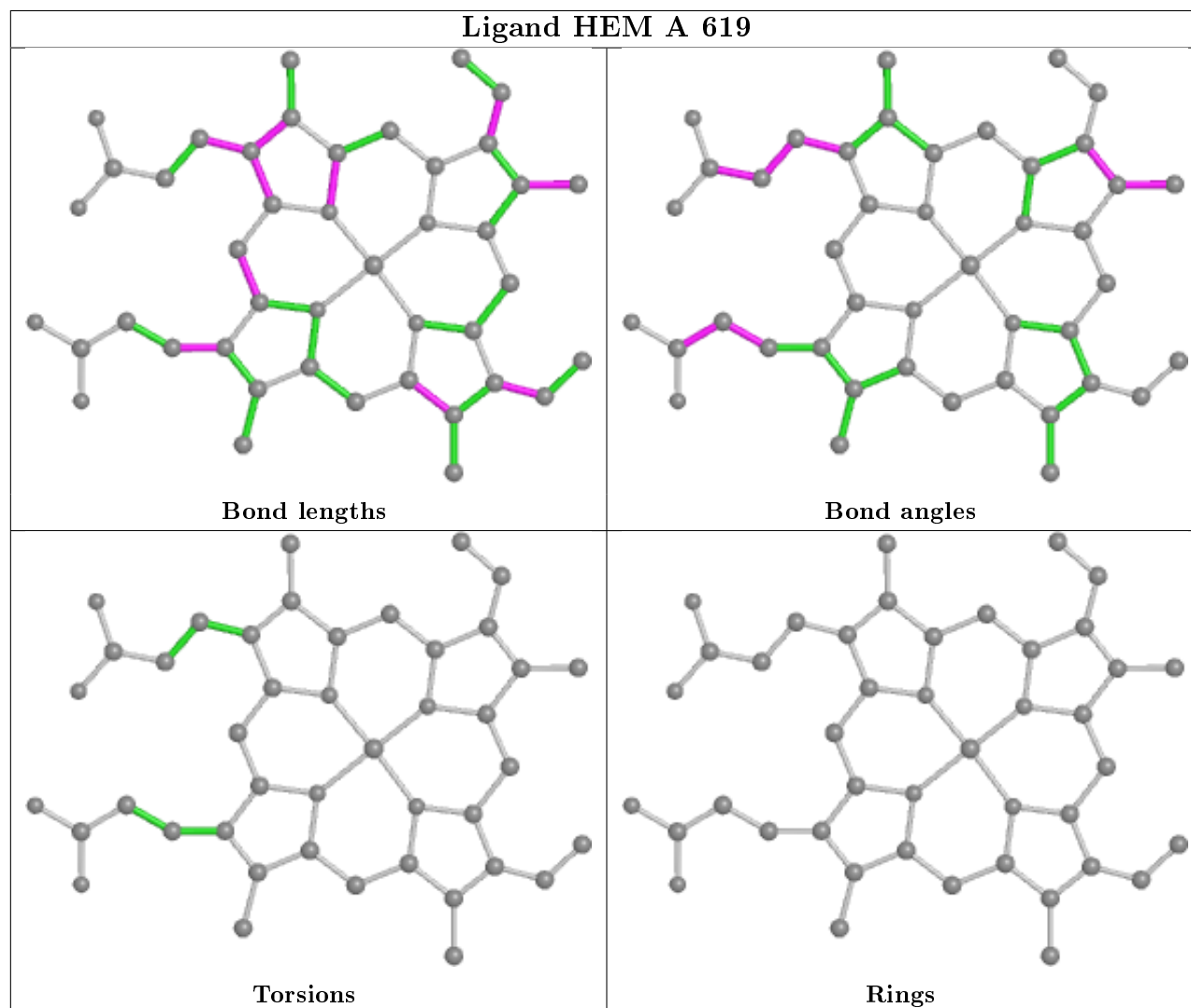
1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	619	HEM	11	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.