



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:53 PM UTC

PDB ID : 7DLQ / pdb_00007dlq
Title : CRYSTAL STRUCTURE OF THE COMPLEX OF LACTOPEROXIDASE
WITH HYDROGEN PEROXIDE AT 1.77Å RESOLUTION
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Deposited on : 2020-11-29
Resolution : 1.77 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

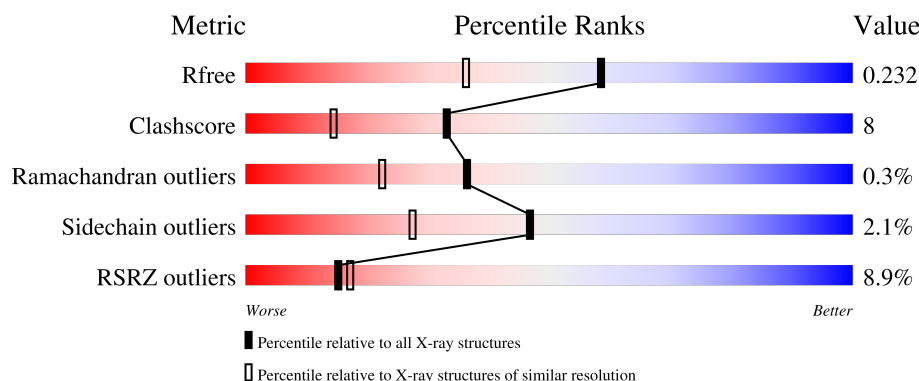
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	9% 82% 16%
2	B	2	100%
2	C	2	50% 50%

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
10	OSM	A	617	-	-	X	-
10	OSM	A	619	-	-	X	-
11	PEO	A	627	-	-	X	-

2 Entry composition [i](#)

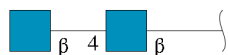
There are 12 unique types of molecules in this entry. The entry contains 5585 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

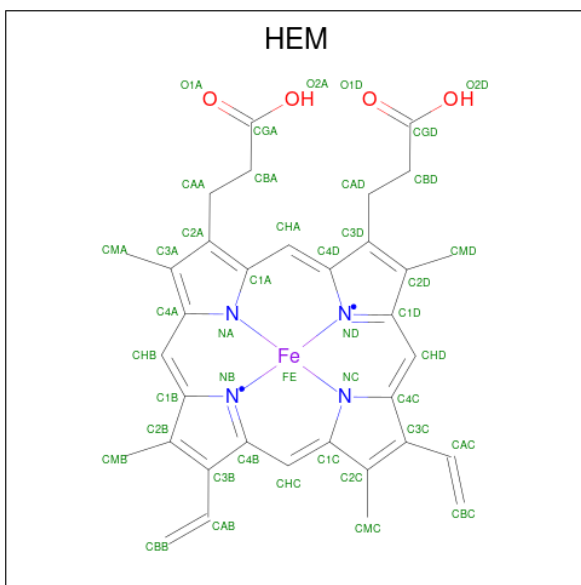
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4770	3037	847	860	26			

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



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).

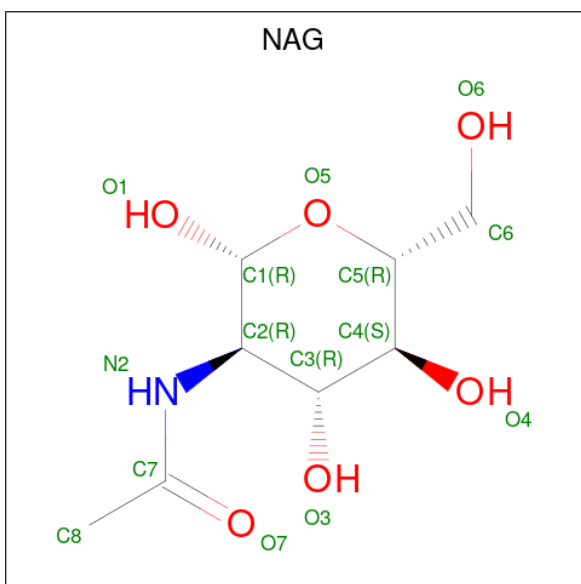


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).

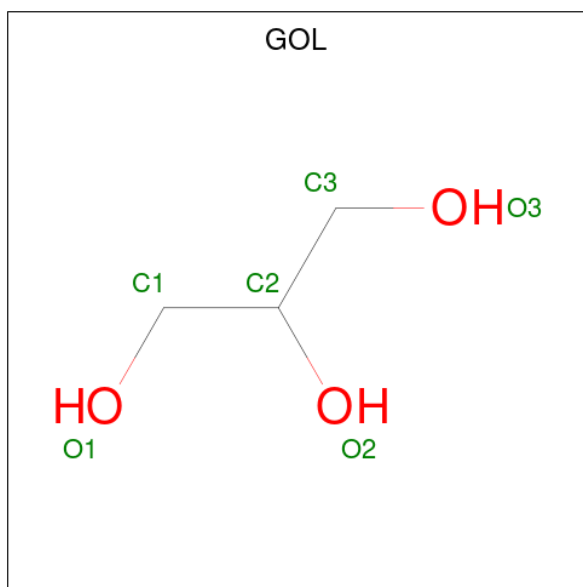


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	I	0	0
			19	19		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

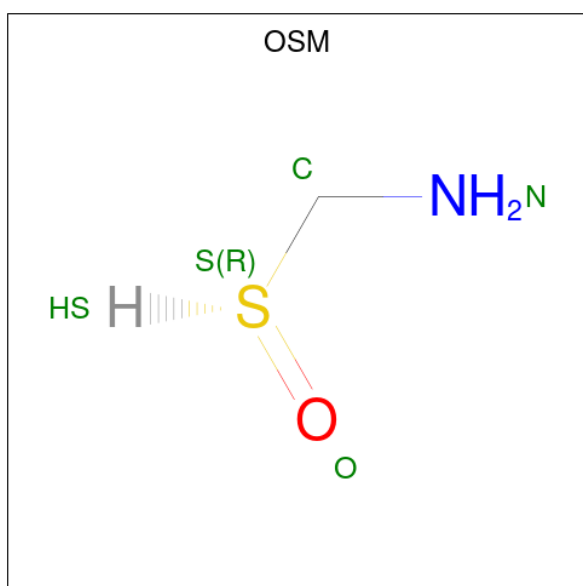


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

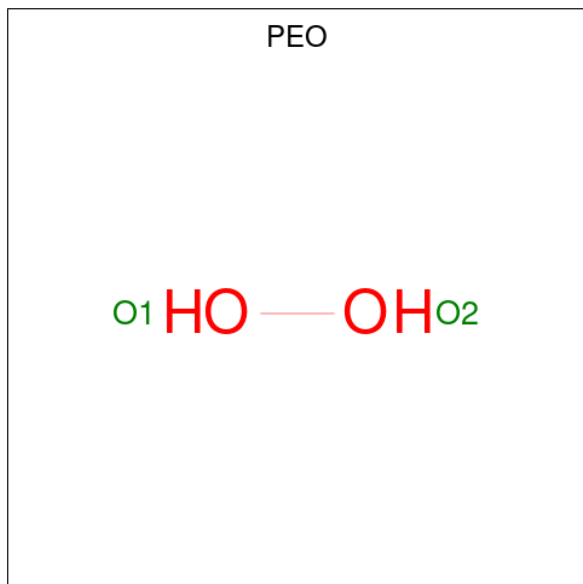
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Zn	0	0
			1	1		

- Molecule 10 is 1-(OXIDOSULFANYL)METHANAMINE (CCD ID: OSM) (formula: CH₅NOS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C N O S 4 1 1 1 1	0	0
10	A	1	Total C N O S 4 1 1 1 1	0	0
10	A	1	Total C N O S 4 1 1 1 1	0	0

- Molecule 11 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H₂O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total O 2 2	0	0

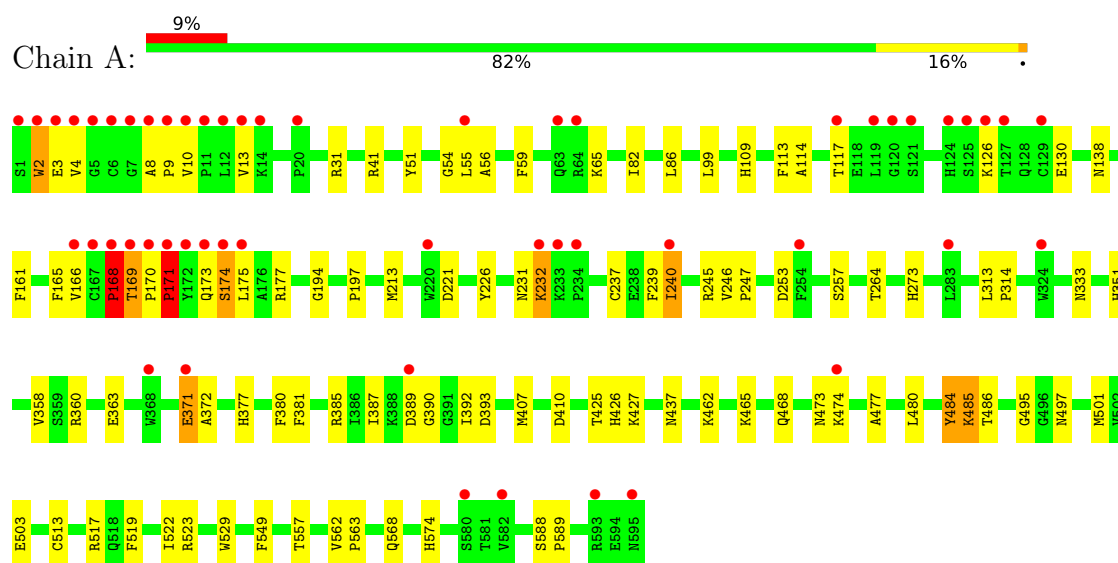
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	657	Total O 657 657	0	0

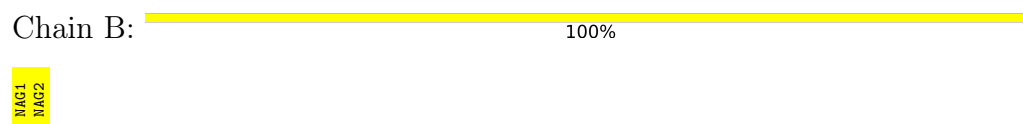
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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	54.23Å 79.84Å 77.55Å 90.00° 102.67° 90.00°	Depositor
Resolution (Å)	34.57 – 1.77 34.57 – 1.77	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.57-1.77) 98.2 (34.57-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.187 , 0.226 0.194 , 0.232	Depositor DCC
R_{free} test set	3107 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5585	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: NAG, EDO, OSM, HEM, GOL, IOD, CA, PEO, ZN

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	1.12	11/4898 (0.2%)	1.44	30/6645 (0.5%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	ALA	CA-CB	-12.30	1.35	1.53
1	A	114	ALA	CA-C	9.32	1.62	1.52
1	A	562	VAL	C-N	-8.79	1.22	1.33
1	A	486	THR	CA-C	-8.31	1.43	1.52
1	A	113	PHE	CA-CB	8.28	1.67	1.53
1	A	114	ALA	N-CA	6.23	1.53	1.46
1	A	495	GLY	C-O	5.28	1.30	1.23
1	A	563	PRO	C-N	-5.25	1.25	1.33
1	A	358	VAL	C-O	5.14	1.29	1.24
1	A	477	ALA	C-O	5.10	1.30	1.24
1	A	473	ASN	C-O	5.07	1.29	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	ILE	CB-CA-C	13.76	129.58	111.97
1	A	562	VAL	O-C-N	-13.25	112.45	121.72
1	A	562	VAL	CA-C-N	12.83	136.67	120.51
1	A	562	VAL	C-N-CA	12.83	136.67	120.51
1	A	372	ALA	N-CA-C	-12.40	97.61	113.12
1	A	168	PRO	CB-CA-C	11.72	130.89	111.56
1	A	426	HIS	CB-CA-C	10.51	127.63	109.24
1	A	485	LYS	CB-CA-C	-9.58	100.35	109.83
1	A	168	PRO	CA-N-CD	-9.23	99.07	112.00
1	A	240	ILE	N-CA-C	-9.07	101.71	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	PRO	N-CA-C	8.25	120.77	110.70
1	A	484	TYR	CB-CA-C	7.76	124.77	110.56
1	A	390	GLY	N-CA-C	7.59	126.23	115.30
1	A	114	ALA	N-CA-C	-7.51	91.38	108.27
1	A	174	SER	CB-CA-C	7.41	121.37	110.26
1	A	114	ALA	CB-CA-C	6.33	120.97	110.97
1	A	171	PRO	N-CA-CB	-5.96	97.00	103.25
1	A	166	VAL	CA-C-O	-5.57	115.95	122.13
1	A	194	GLY	CA-C-O	-5.57	117.78	122.29
1	A	56	ALA	N-CA-CB	-5.55	102.23	111.06
1	A	484	TYR	N-CA-C	-5.42	104.24	112.04
1	A	253	ASP	CA-C-N	5.38	128.24	120.38
1	A	253	ASP	C-N-CA	5.38	128.24	120.38
1	A	177	ARG	CB-CG-CD	-5.38	98.93	111.30
1	A	161	PHE	CA-CB-CG	-5.30	108.50	113.80
1	A	231	ASN	CB-CA-C	5.29	120.28	112.03
1	A	59	PHE	CB-CA-C	5.23	117.68	109.84
1	A	138	ASN	N-CA-C	5.18	119.22	113.01
1	A	13	VAL	CB-CA-C	5.09	116.75	111.09
1	A	371	GLU	N-CA-C	-5.09	96.49	107.49

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	4770	0	4689	70	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
3	A	43	0	30	1	0
4	A	1	0	0	0	0
5	A	14	0	13	0	0
6	A	19	0	0	6	0
7	A	6	0	8	2	0
8	A	4	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	1	0	0	0	0
10	A	12	0	13	5	0
11	A	2	0	0	2	0
12	A	657	0	0	20	0
All	All	5585	0	4807	76	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 8.

All (76) 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:165:PHE:CZ	1:A:169:THR:O	1.90	1.25
1:A:3:GLU:HG2	1:A:174:SER:OG	1.41	1.19
1:A:333:ASN:HD22	10:A:619:OSM:HS	1.05	0.96
1:A:109:HIS:NE2	11:A:627:PEO:O1	2.04	0.90
1:A:165:PHE:HZ	1:A:169:THR:O	1.56	0.89
1:A:173:GLN:OE1	12:A:702:HOH:O	1.92	0.86
6:A:622:IOD:I	12:A:1339:HOH:O	2.63	0.85
6:A:623:IOD:I	12:A:1198:HOH:O	2.65	0.84
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.27	0.79
1:A:169:THR:HG21	12:A:1029:HOH:O	1.84	0.77
1:A:410:ASP:OD1	12:A:703:HOH:O	2.02	0.77
1:A:117:THR:HG22	1:A:169:THR:CG2	2.18	0.73
1:A:126:LYS:O	12:A:704:HOH:O	2.06	0.72
1:A:65:LYS:NZ	12:A:708:HOH:O	2.25	0.70
1:A:3:GLU:CG	1:A:174:SER:OG	2.33	0.68
1:A:117:THR:HG22	1:A:169:THR:HG22	1.74	0.67
1:A:3:GLU:HG2	1:A:174:SER:HG	1.58	0.64
1:A:3:GLU:HG2	1:A:174:SER:CB	2.28	0.63
1:A:407:MET:HE3	1:A:497:ASN:O	1.98	0.63
10:A:617:OSM:H2	12:A:860:HOH:O	1.97	0.62
6:A:620:IOD:I	11:A:627:PEO:O1	2.88	0.62
1:A:10:VAL:O	1:A:10:VAL:HG12	2.02	0.59
1:A:86:LEU:O	12:A:705:HOH:O	2.17	0.59
1:A:245:ARG:NH2	12:A:715:HOH:O	2.35	0.59
1:A:51:TYR:CD2	1:A:55:LEU:O	2.56	0.59
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.39	0.57
1:A:41:ARG:NH1	12:A:716:HOH:O	2.36	0.57
1:A:117:THR:HG22	1:A:169:THR:HG21	1.86	0.57
1:A:385:ARG:O	1:A:389:ASP:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ASN:ND2	10:A:619:OSM:S	2.76	0.57
1:A:2:TRP:O	1:A:2:TRP:HE3	1.89	0.55
1:A:8:ALA:HB3	1:A:9:PRO:HD3	1.89	0.55
1:A:165:PHE:CE1	1:A:169:THR:O	2.56	0.55
1:A:197:PRO:HD2	6:A:625:IOD:I	2.78	0.54
1:A:232:LYS:NZ	10:A:617:OSM:HS	2.06	0.53
1:A:393:ASP:OD1	1:A:557:THR:HB	2.09	0.53
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.44	0.52
1:A:3:GLU:CG	1:A:174:SER:CB	2.87	0.52
1:A:462:LYS:HD2	12:A:768:HOH:O	2.09	0.52
1:A:99:LEU:HD21	1:A:549:PHE:CD1	2.46	0.51
1:A:237:CYS:HA	1:A:381:PHE:O	2.11	0.51
1:A:363:GLU:H	8:A:615:EDO:H21	1.76	0.51
1:A:8:ALA:N	1:A:9:PRO:CD	2.75	0.49
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.47	0.49
1:A:568:GLN:HG3	12:A:1064:HOH:O	2.12	0.49
1:A:574:HIS:O	12:A:706:HOH:O	2.20	0.48
1:A:54:GLY:HA2	12:A:1092:HOH:O	2.14	0.47
3:A:601:HEM:HMC2	3:A:601:HEM:HBC2	1.96	0.47
1:A:360:ARG:NH2	1:A:371:GLU:O	2.41	0.46
1:A:257:SER:O	1:A:381:PHE:HA	2.16	0.46
1:A:484:TYR:O	1:A:485:LYS:CB	2.63	0.46
1:A:239:PHE:HZ	1:A:427:LYS:HB3	1.82	0.45
1:A:377:HIS:CD2	7:A:614:GOL:H2	2.52	0.45
1:A:377:HIS:HD2	7:A:614:GOL:H2	1.82	0.44
1:A:517:ARG:NE	12:A:737:HOH:O	2.45	0.43
1:A:31:ARG:HD2	6:A:613:IOD:I	2.88	0.43
1:A:239:PHE:CZ	1:A:427:LYS:HB3	2.53	0.43
1:A:246:VAL:HG11	1:A:387:ILE:HG13	1.99	0.43
1:A:313:LEU:N	1:A:314:PRO:CD	2.82	0.42
1:A:130:GLU:HB2	12:A:704:HOH:O	2.19	0.42
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.55	0.42
1:A:246:VAL:HA	1:A:247:PRO:HD3	1.93	0.42
1:A:407:MET:HB3	1:A:501:MET:CE	2.50	0.42
1:A:484:TYR:O	1:A:485:LYS:HB2	2.19	0.42
1:A:169:THR:CG2	12:A:1029:HOH:O	2.58	0.42
1:A:232:LYS:HZ1	10:A:617:OSM:HS	1.67	0.42
1:A:2:TRP:O	1:A:2:TRP:CE3	2.70	0.42
1:A:588:SER:OG	1:A:589:PRO:HD3	2.21	0.41
1:A:82:ILE:HD13	1:A:480:LEU:HD23	2.03	0.41
1:A:519:PHE:O	1:A:522:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:GLN:HG2	1:A:474:LYS:HA	2.03	0.41
1:A:484:TYR:O	1:A:485:LYS:HG2	2.21	0.41
1:A:264:THR:HG23	1:A:392:ILE:HB	2.03	0.41
1:A:465:LYS:NZ	12:A:736:HOH:O	2.45	0.41
1:A:588:SER:N	1:A:589:PRO:CD	2.84	0.41
6:A:612:IOD:I	12:A:1235:HOH:O	2.93	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	593/595 (100%)	578 (98%)	13 (2%)	2 (0%)	36 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	PRO
1	A	171	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	518/518 (100%)	507 (98%)	11 (2%)	47 27

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	4	VAL
1	A	168	PRO
1	A	169	THR
1	A	171	PRO
1	A	175	LEU
1	A	232	LYS
1	A	240	ILE
1	A	425	THR
1	A	503	GLU
1	A	513	CYS

Sometimes 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	173	GLN
1	A	329	GLN
1	A	364	ASN
1	A	556	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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	0.95	0	17,19,21	1.56	4 (23%)
2	NAG	B	2	2	14,14,15	0.58	0	17,19,21	1.18	2 (11%)
2	NAG	C	1	1,2	14,14,15	0.93	0	17,19,21	1.06	0
2	NAG	C	2	2	14,14,15	0.52	0	17,19,21	2.66	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	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	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	6.93	121.47	112.19
2	C	2	NAG	C4-C3-C2	-5.52	102.93	111.02
2	C	2	NAG	O5-C1-C2	-3.72	105.53	111.29
2	B	2	NAG	C1-O5-C5	2.99	116.20	112.19
2	B	1	NAG	O4-C4-C5	2.94	116.57	109.32
2	B	1	NAG	O5-C5-C6	-2.75	102.31	107.66
2	C	2	NAG	C2-N2-C7	-2.71	119.27	122.90
2	B	1	NAG	C1-O5-C5	-2.64	108.65	112.19
2	C	2	NAG	O3-C3-C2	2.56	114.72	109.40
2	C	2	NAG	C1-C2-N2	2.39	114.20	110.43
2	B	1	NAG	C6-C5-C4	2.14	118.28	113.02
2	B	2	NAG	C4-C3-C2	2.14	114.15	111.02

There are no chirality outliers.

All (6) 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
2	C	2	NAG	C4-C5-C6-O6

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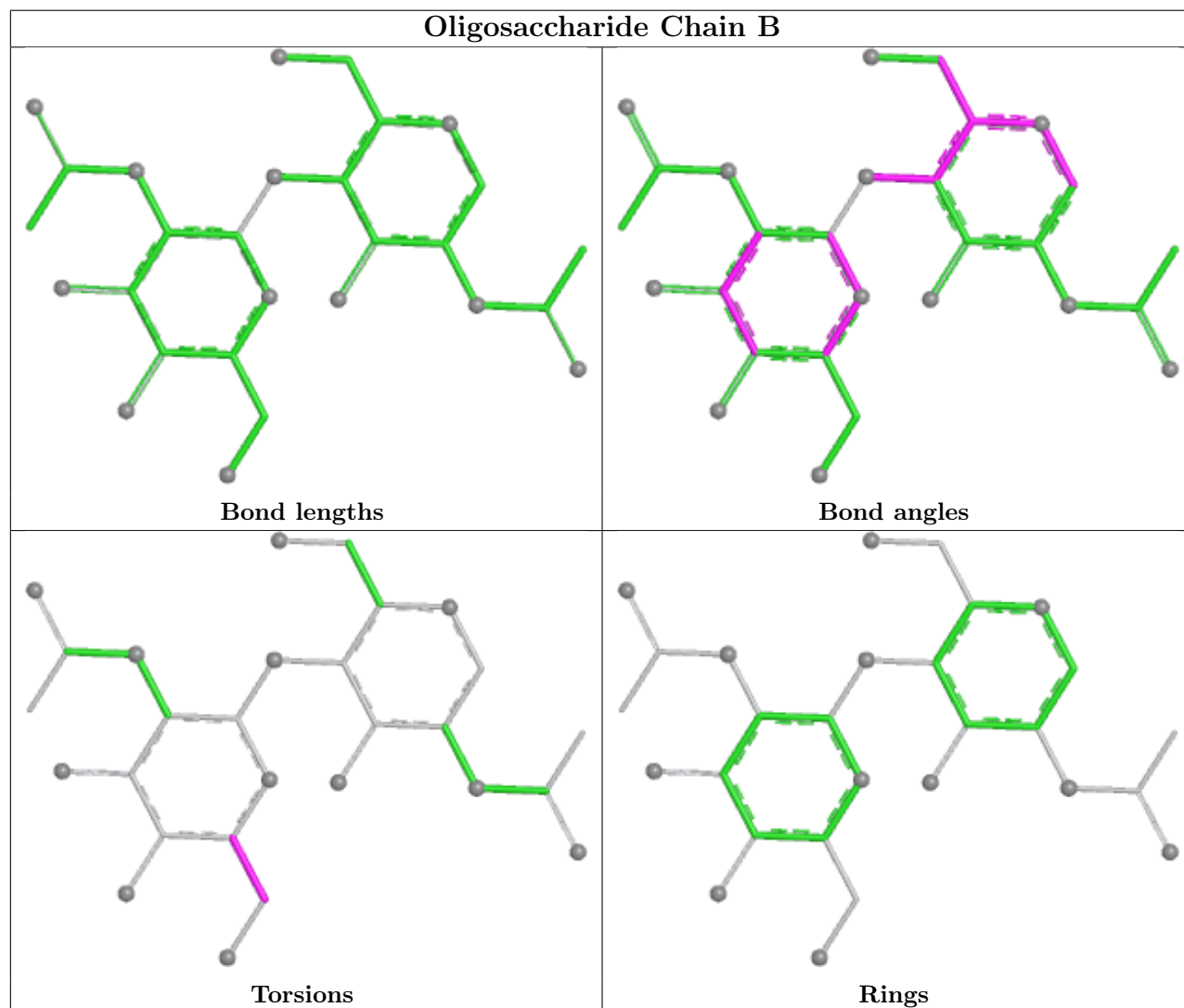
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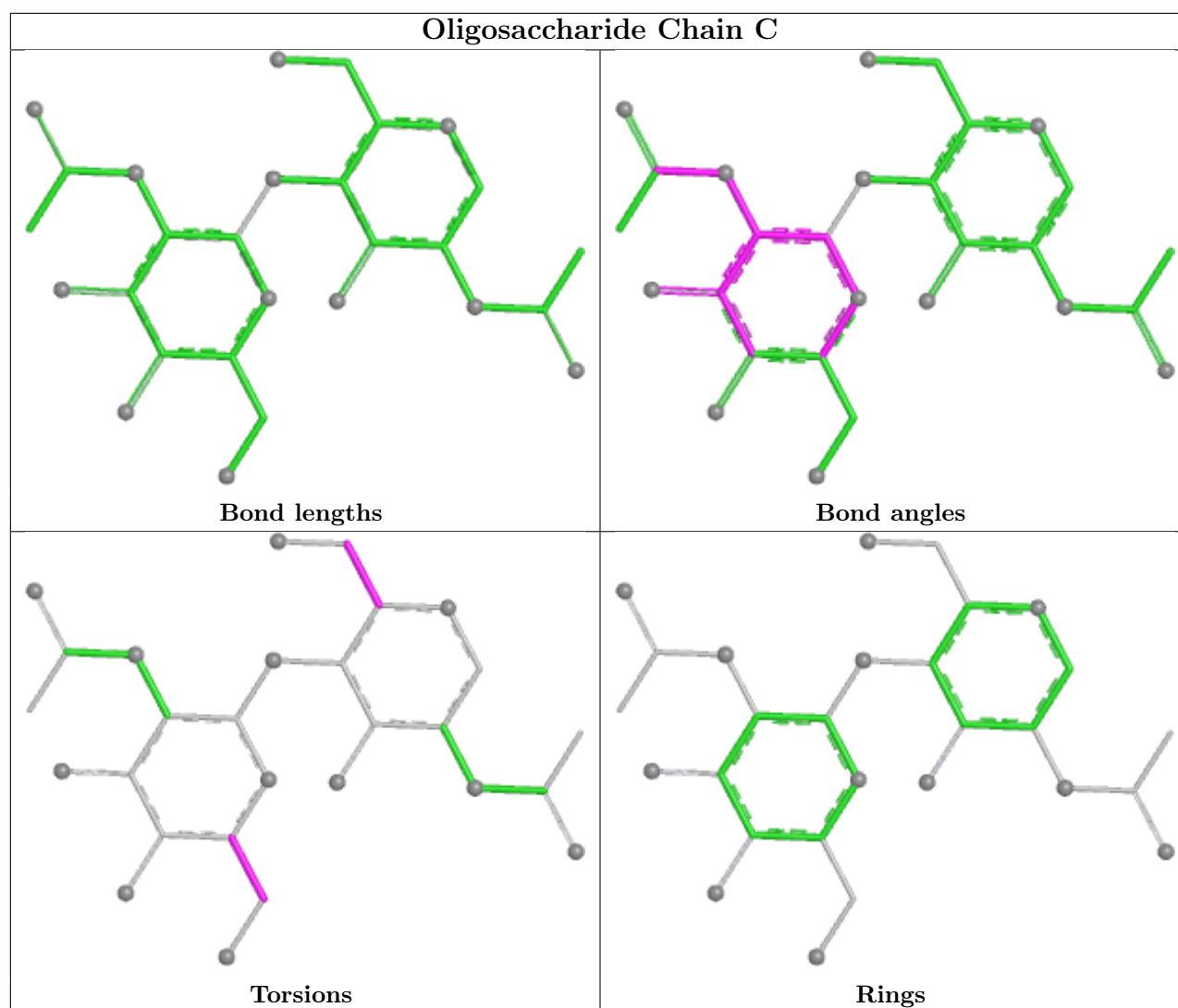
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

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 29 ligands modelled in this entry, 21 are monoatomic - leaving 8 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	$\# Z > 2$
3	HEM	A	601	1,11	50,50,50	1.83	12 (24%)	67,82,82	1.55	12 (17%)
10	OSM	A	617	-	1,3,3	0.22	0	0,2,2	-	-
5	NAG	A	603	1	14,14,15	0.71	0	17,19,21	1.71	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	A	614	-	5,5,5	0.16	0	5,5,5	0.59	0
8	EDO	A	615	-	3,3,3	1.90	2 (66%)	2,2,2	0.97	0
10	OSM	A	618	-	1,3,3	0.27	0	0,2,2	-	-
11	PEO	A	627	3	1,1,1	0.50	0	-	-	-
10	OSM	A	619	-	1,3,3	0.16	0	0,2,2	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	601	1,11	-	4/14/54/54	-
10	OSM	A	617	-	-	0/0/1/1	-
5	NAG	A	603	1	-	0/6/23/26	0/1/1/1
7	GOL	A	614	-	-	2/4/4/4	-
8	EDO	A	615	-	-	0/1/1/1	-
10	OSM	A	618	-	-	0/0/1/1	-
10	OSM	A	619	-	-	0/0/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	HEM	C1B-NB	-4.86	1.31	1.40
3	A	601	HEM	FE-NC	4.70	2.10	1.95
3	A	601	HEM	FE-NB	4.65	2.09	1.94
3	A	601	HEM	C4D-ND	-3.29	1.34	1.40
3	A	601	HEM	C4C-NC	-2.63	1.34	1.39
3	A	601	HEM	C1C-C2C	-2.60	1.40	1.45
3	A	601	HEM	FE-NA	2.58	2.03	1.95
3	A	601	HEM	CBD-CGD	2.58	1.56	1.50
8	A	615	EDO	O2-C2	-2.42	1.29	1.42
3	A	601	HEM	CBD-CAD	2.41	1.60	1.51
3	A	601	HEM	C4A-NA	-2.23	1.35	1.39
3	A	601	HEM	C4D-C3D	2.22	1.48	1.45
3	A	601	HEM	C1A-NA	-2.17	1.35	1.39
8	A	615	EDO	O1-C1	-2.04	1.31	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	HEM	C1B-NB-C4B	5.03	111.16	105.21
5	A	603	NAG	O5-C1-C2	-4.12	104.91	111.29
3	A	601	HEM	CHC-C4B-NB	3.75	128.46	124.42
3	A	601	HEM	C2D-C1D-ND	3.23	113.64	109.90
3	A	601	HEM	CHD-C1D-C2D	-3.21	119.96	125.03
5	A	603	NAG	C4-C3-C2	-2.98	106.65	111.02
3	A	601	HEM	CMB-C2B-C1B	-2.69	120.83	125.03
3	A	601	HEM	C3B-C4B-NB	-2.61	107.59	109.47
3	A	601	HEM	CBD-CAD-C3D	-2.53	105.54	112.53
3	A	601	HEM	C1D-C2D-C3D	-2.39	104.47	106.98
3	A	601	HEM	CAD-C3D-C4D	2.32	128.74	124.70
3	A	601	HEM	C3D-C4D-ND	2.21	112.60	110.17
3	A	601	HEM	O2A-CGA-CBA	2.21	120.98	114.00
3	A	601	HEM	CHB-C1B-NB	2.18	127.06	124.37
5	A	603	NAG	O5-C5-C6	2.10	111.75	107.66
5	A	603	NAG	O4-C4-C5	2.01	114.28	109.32

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	614	GOL	O1-C1-C2-C3
7	A	614	GOL	O1-C1-C2-O2
3	A	601	HEM	CAD-CBD-CGD-O2D
3	A	601	HEM	CAA-CBA-CGA-O1A
3	A	601	HEM	CAA-CBA-CGA-O2A
3	A	601	HEM	CAD-CBD-CGD-O1D

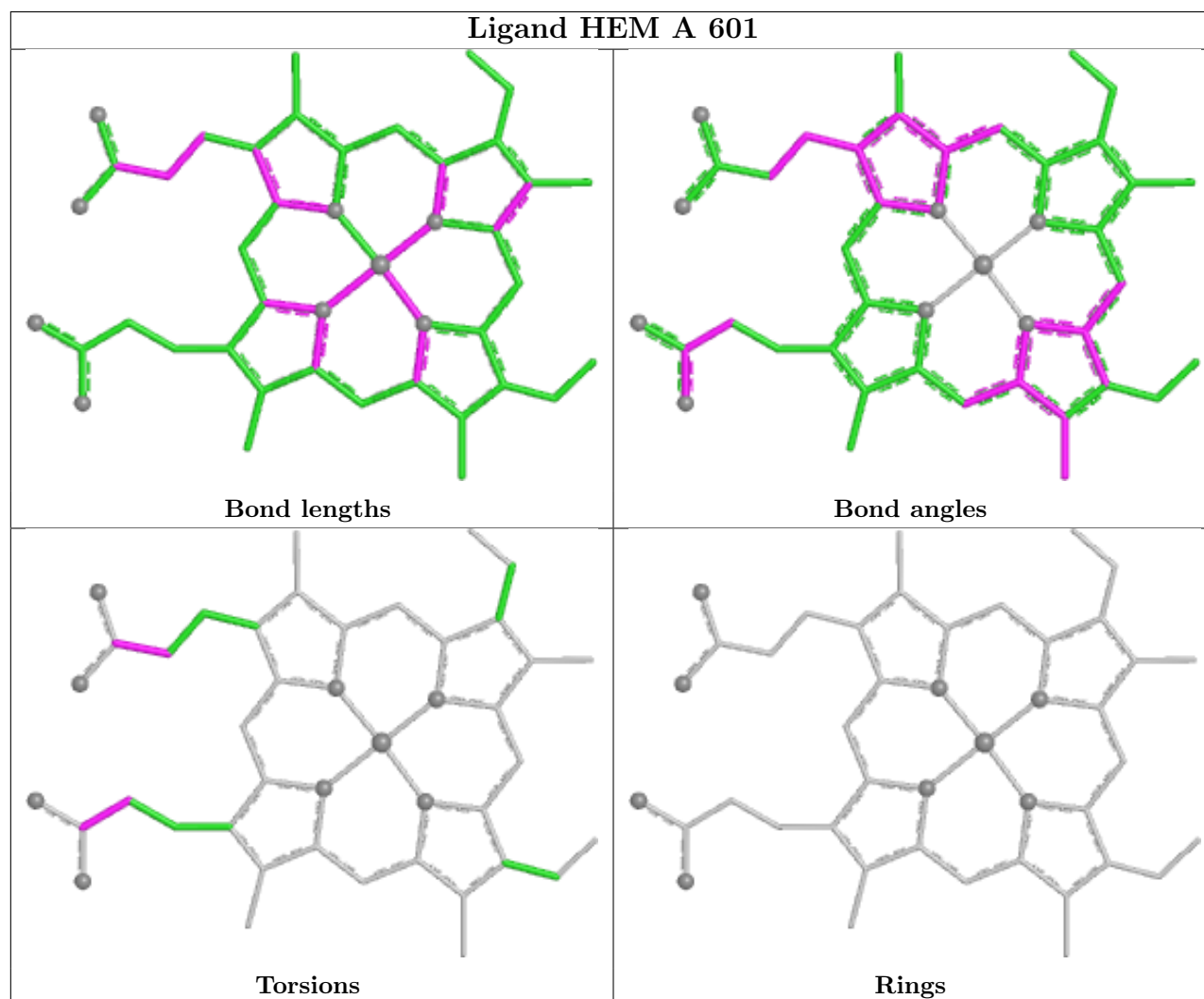
There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	HEM	1	0
10	A	617	OSM	3	0
7	A	614	GOL	2	0
8	A	615	EDO	1	0
11	A	627	PEO	2	0
10	A	619	OSM	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	595/595 (100%)	0.57	53 (8%)	15 17	14, 26, 94, 171	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	SER	8.5
1	A	10	VAL	8.0
1	A	168	PRO	6.8
1	A	173	GLN	6.6
1	A	175	LEU	6.4
1	A	119	LEU	6.3
1	A	169	THR	6.2
1	A	4	VAL	6.2
1	A	172	TYR	6.1
1	A	8	ALA	5.8
1	A	171	PRO	5.6
1	A	5	GLY	5.4
1	A	2	TRP	5.1
1	A	12	LEU	5.0
1	A	9	PRO	4.8
1	A	240	ILE	4.5
1	A	170	PRO	4.5
1	A	1	SER	4.3
1	A	125	SER	4.3
1	A	13	VAL	4.2
1	A	283	LEU	4.0
1	A	167	CYS	4.0
1	A	7	GLY	4.0
1	A	6	CYS	3.9
1	A	11	PRO	3.5
1	A	124	HIS	3.5
1	A	121	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	120	GLY	3.2
1	A	166	VAL	3.2
1	A	254	PHE	3.1
1	A	127	THR	3.1
1	A	3	GLU	3.1
1	A	389	ASP	3.0
1	A	593	ARG	2.9
1	A	117	THR	2.7
1	A	64	ARG	2.5
1	A	55	LEU	2.5
1	A	63	GLN	2.5
1	A	368	TRP	2.5
1	A	220	TRP	2.4
1	A	232	LYS	2.4
1	A	20	PRO	2.4
1	A	595	ASN	2.4
1	A	126	LYS	2.4
1	A	129	CYS	2.3
1	A	14	LYS	2.2
1	A	233	LYS	2.2
1	A	234	PRO	2.2
1	A	324	TRP	2.1
1	A	474	LYS	2.1
1	A	371	GLU	2.0
1	A	580	SER	2.0
1	A	582	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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.

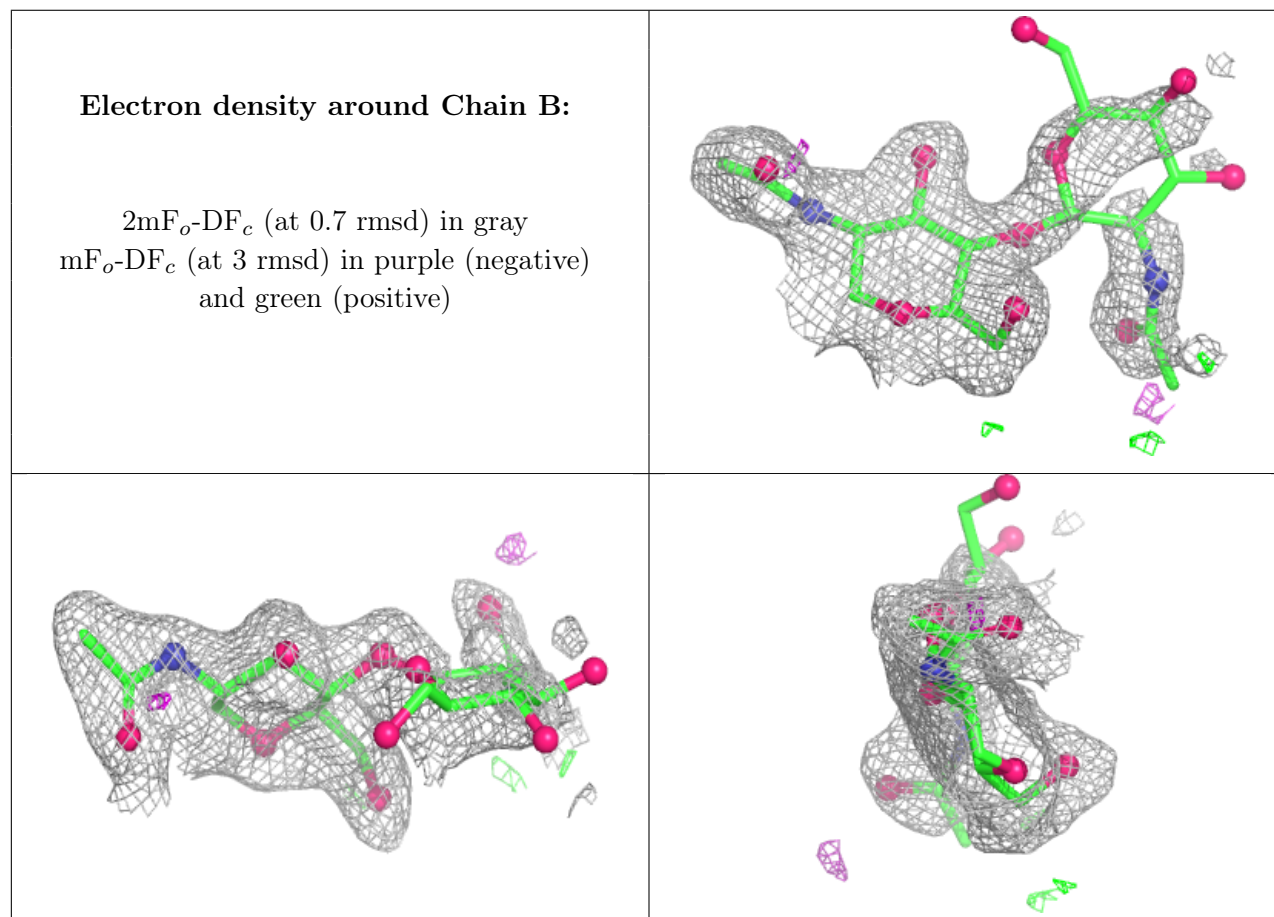
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.54	0.15	60,73,80,81	0
2	NAG	B	2	14/15	0.56	0.17	64,82,87,90	0

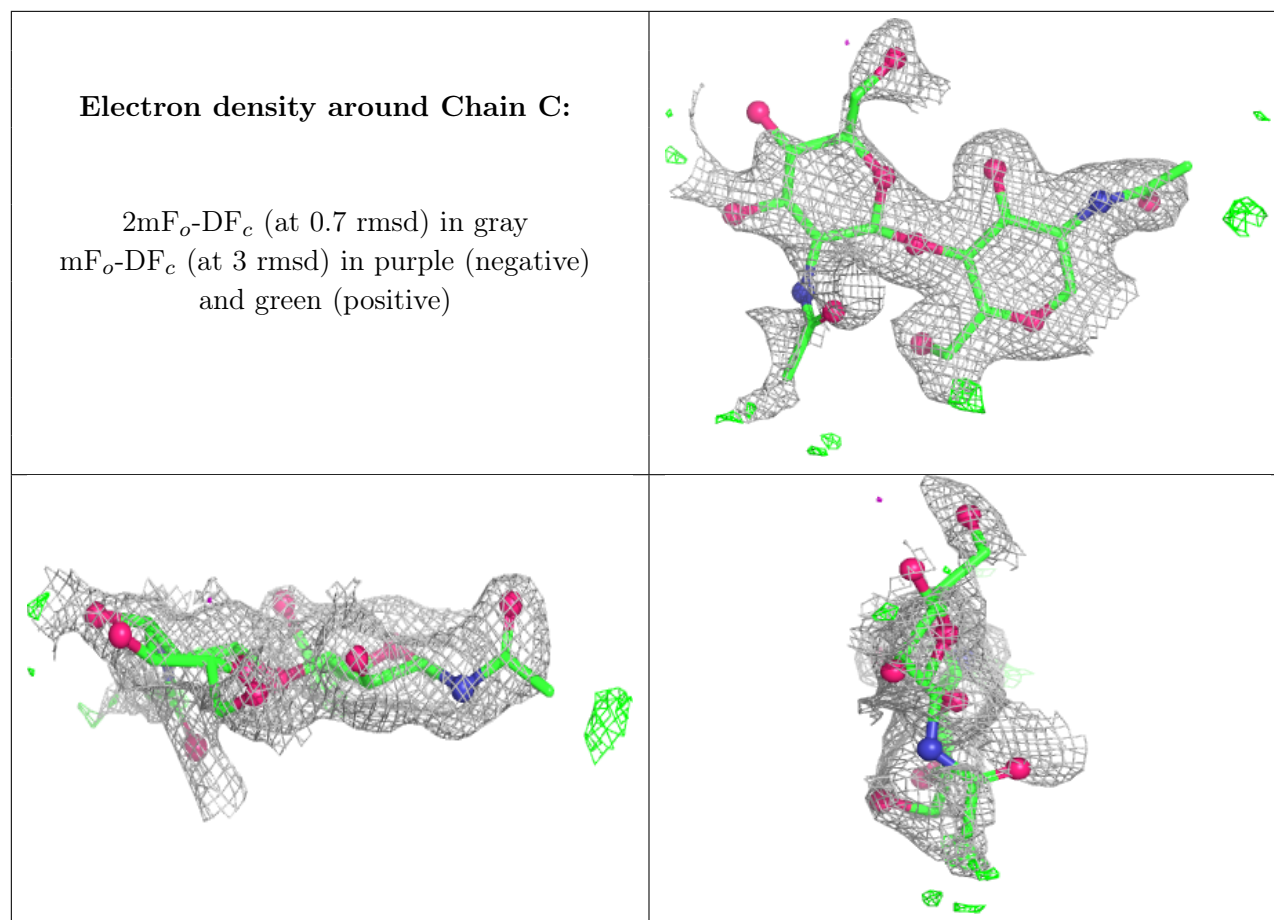
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	1	14/15	0.86	0.10	29,35,44,46	0
2	NAG	C	1	14/15	0.92	0.09	24,33,41,45	0

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
10	OSM	A	619	4/4	0.74	0.26	33,36,37,38	4
5	NAG	A	603	14/15	0.85	0.10	39,45,52,54	0
7	GOL	A	614	6/6	0.87	0.15	32,38,48,48	0
10	OSM	A	618	4/4	0.92	0.15	30,36,37,38	0
6	IOD	A	610	1/1	0.92	0.10	55,55,55,55	1
6	IOD	A	629	1/1	0.95	0.18	74,74,74,74	1
10	OSM	A	617	4/4	0.95	0.11	34,35,37,45	0
11	PEO	A	627	2/2	0.95	0.07	19,19,19,23	0
6	IOD	A	613	1/1	0.96	0.08	33,33,33,33	1
6	IOD	A	626	1/1	0.96	0.06	34,34,34,34	0
6	IOD	A	606	1/1	0.96	0.05	41,41,41,41	1
6	IOD	A	611	1/1	0.96	0.07	38,38,38,38	1

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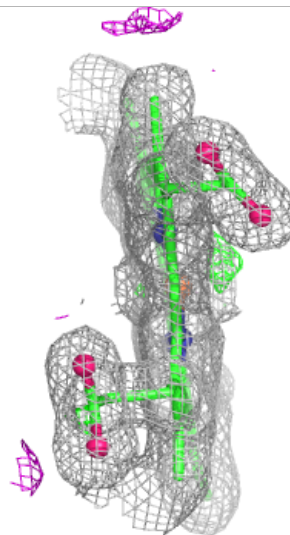
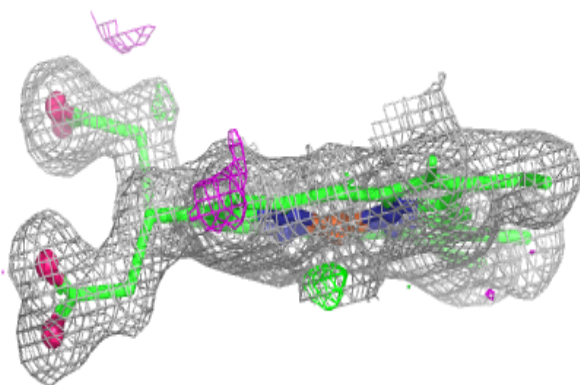
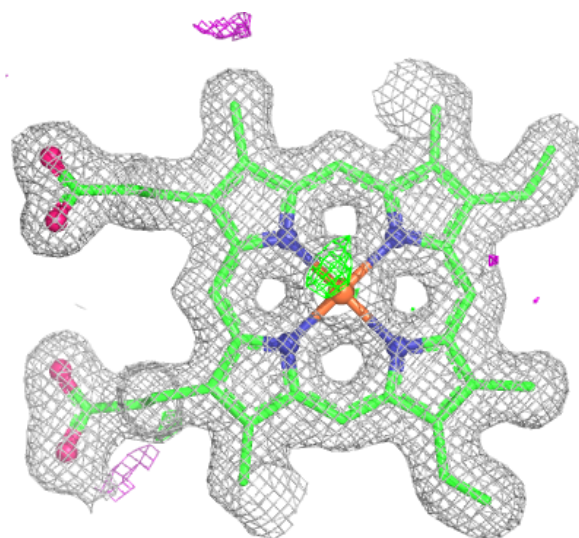
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	IOD	A	609	1/1	0.97	0.05	32,32,32,32	1
6	IOD	A	622	1/1	0.97	0.06	38,38,38,38	1
6	IOD	A	625	1/1	0.97	0.05	35,35,35,35	1
8	EDO	A	615	4/4	0.97	0.06	18,19,19,21	0
3	HEM	A	601	43/43	0.98	0.06	14,15,19,19	0
6	IOD	A	623	1/1	0.98	0.05	43,43,43,43	1
9	ZN	A	616	1/1	0.98	0.05	32,32,32,32	0
6	IOD	A	607	1/1	0.98	0.04	36,36,36,36	1
6	IOD	A	612	1/1	0.98	0.04	37,37,37,37	1
6	IOD	A	628	1/1	0.98	0.08	43,43,43,43	0
6	IOD	A	605	1/1	0.98	0.03	29,29,29,29	1
6	IOD	A	624	1/1	0.99	0.03	34,34,34,34	1
6	IOD	A	621	1/1	0.99	0.05	39,39,39,39	1
6	IOD	A	608	1/1	0.99	0.03	26,26,26,26	0
6	IOD	A	620	1/1	0.99	0.02	24,24,24,24	1
6	IOD	A	604	1/1	1.00	0.01	17,17,17,17	1
4	CA	A	602	1/1	1.00	0.02	16,16,16,16	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.

Electron density around HEM A 601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.