



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:45 AM UTC

PDB ID : 1LLP / pdb_00001llp
Title : LIGNIN PEROXIDASE (ISOZYME H2) PI 4.15
Authors : Choinowski, T.H.; Piontek, K.; Glumoff, T.
Deposited on : 1995-11-09
Resolution : 1.70 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

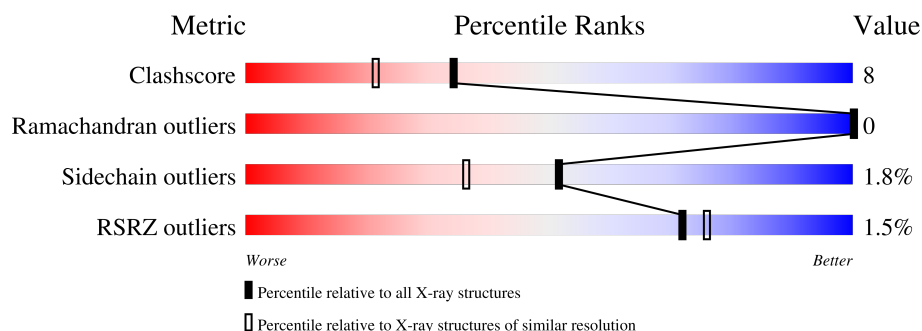
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	343	82% 15% .
2	B	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
4	A2G	A	380	-	-	X	-

2 Entry composition [i](#)

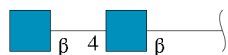
There are 8 unique types of molecules in this entry. The entry contains 3029 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LIGNIN PEROXIDASE.

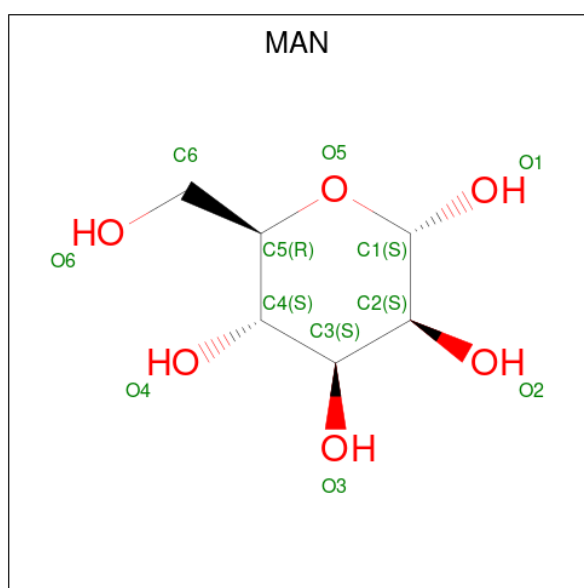
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	343	2560	1618	429	497	16	0	0	0

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



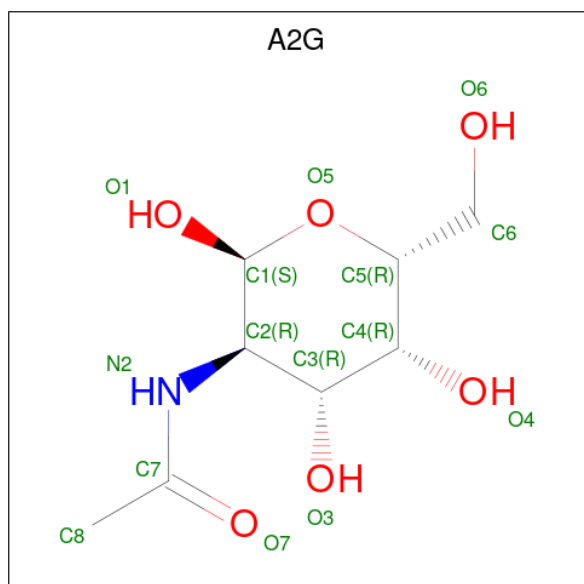
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

- Molecule 3 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is 2-acetamido-2-deoxy- α -D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$).

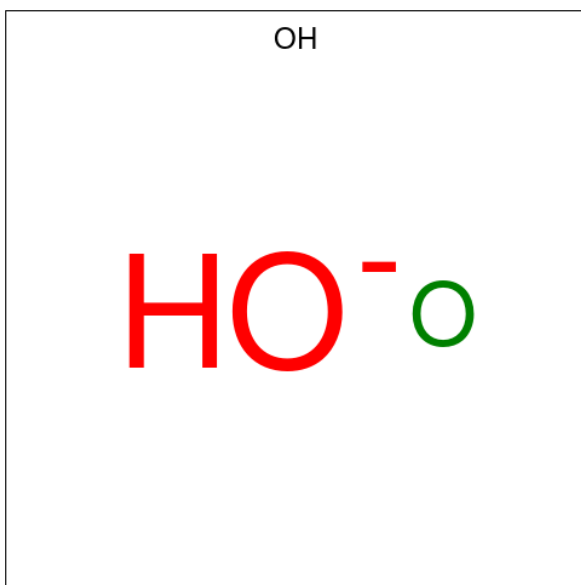


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

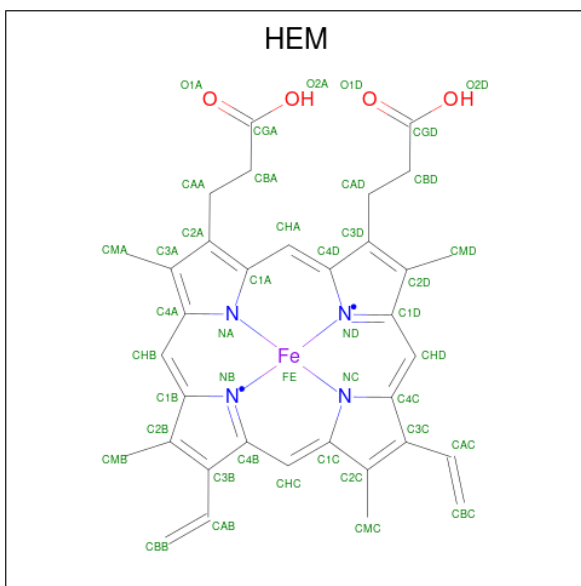
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		

- Molecule 6 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



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

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

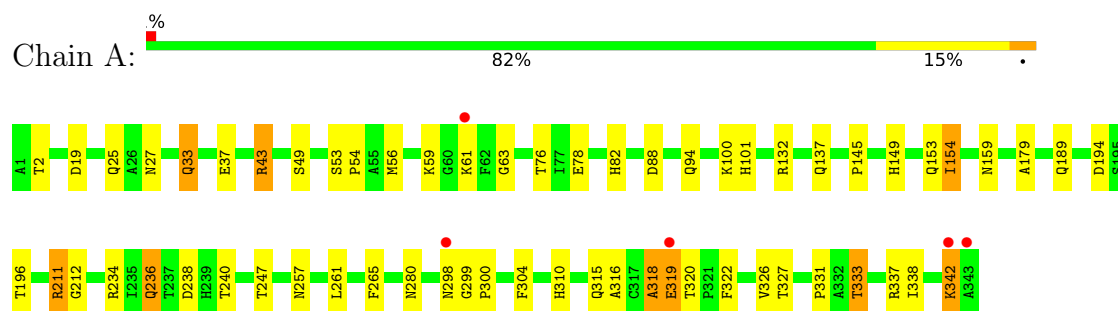


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	370	Total 370	O 370	0	0

3 Residue-property plots

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

• Molecule 1: LIGNIN PEROXIDASE



• 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.70Å 74.71Å 106.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.70 10.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.2 (10.00-1.70) 97.4 (10.00-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.70Å)	Xtriage
Refinement program	PROLSQ, X-PLOR 3.0	Depositor
R, R_{free}	0.162 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3029	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MAN, CA, HEM, OH, A2G

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	1.13	0/2630	1.99	67/3582 (1.9%)

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	29.46	165.65	124.40
1	A	33	GLN	OE1-CD-NE2	15.56	138.16	122.60
1	A	280	ASN	CA-CB-CG	-10.35	102.25	112.60
1	A	337	ARG	CD-NE-CZ	9.91	138.28	124.40
1	A	49	SER	N-CA-C	9.08	121.26	111.36
1	A	137	GLN	O-C-N	7.97	127.47	121.65
1	A	53	SER	O-C-N	7.59	125.82	121.27
1	A	82	HIS	CA-CB-CG	-7.35	106.45	113.80
1	A	247	THR	N-CA-CB	-7.19	100.95	110.88
1	A	298	ASN	CA-CB-CG	-7.19	105.41	112.60
1	A	63	GLY	CA-C-O	-7.05	112.63	119.04
1	A	299	GLY	N-CA-C	-6.87	103.76	112.00
1	A	327	THR	CA-C-O	-6.64	113.19	120.43
1	A	94	GLN	N-CA-C	6.53	119.72	111.69
1	A	153	GLN	OE1-CD-NE2	6.50	129.10	122.60
1	A	179	ALA	N-CA-CB	-6.48	101.52	111.56
1	A	315	GLN	OE1-CD-NE2	6.44	129.04	122.60
1	A	322	PHE	O-C-N	6.31	126.91	121.30
1	A	319	GLU	N-CA-C	6.30	120.97	113.28
1	A	27	ASN	N-CA-C	6.30	121.13	113.38
1	A	189	GLN	CB-CG-CD	-6.25	101.98	112.60
1	A	342	LYS	O-C-N	6.20	130.55	122.68
1	A	236	GLN	N-CA-C	6.08	117.91	111.28
1	A	194	ASP	CA-CB-CG	6.01	118.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	PRO	O-C-N	5.96	130.43	123.21
1	A	101	HIS	CA-CB-CG	-5.96	107.84	113.80
1	A	54	PRO	O-C-N	-5.95	115.39	122.24
1	A	159	ASN	CB-CG-ND2	5.92	125.28	116.40
1	A	234	ARG	CD-NE-CZ	-5.88	116.17	124.40
1	A	78	GLU	N-CA-C	5.82	117.62	111.28
1	A	265	PHE	CA-CB-CG	-5.79	108.01	113.80
1	A	304	PHE	N-CA-C	-5.74	102.55	109.72
1	A	333	THR	CA-CB-CG2	5.74	120.26	110.50
1	A	137	GLN	CB-CA-C	-5.71	101.12	109.97
1	A	153	GLN	CB-CA-C	-5.68	101.36	110.79
1	A	153	GLN	CG-CD-NE2	-5.65	107.92	116.40
1	A	196	THR	O-C-N	5.65	126.42	121.17
1	A	19	ASP	CA-CB-CG	-5.62	106.97	112.60
1	A	316	ALA	CA-C-O	-5.59	112.07	119.06
1	A	33	GLN	O-C-N	5.59	129.20	122.94
1	A	238	ASP	O-C-N	5.55	128.47	122.15
1	A	54	PRO	CA-C-N	5.53	127.63	120.44
1	A	54	PRO	C-N-CA	5.53	127.63	120.44
1	A	322	PHE	CA-CB-CG	-5.50	108.30	113.80
1	A	76	THR	CA-CB-OG1	-5.47	101.39	109.60
1	A	212	GLY	CA-C-O	-5.47	115.86	120.89
1	A	189	GLN	CG-CD-NE2	5.43	124.54	116.40
1	A	43	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	A	2	THR	N-CA-CB	5.36	119.00	110.65
1	A	153	GLN	O-C-N	5.34	127.78	122.12
1	A	159	ASN	CA-CB-CG	5.34	117.94	112.60
1	A	132	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	A	33	GLN	CA-CB-CG	-5.30	103.50	114.10
1	A	236	GLN	CB-CG-CD	-5.27	103.64	112.60
1	A	310	HIS	CE1-NE2-CD2	5.27	114.27	109.00
1	A	37	GLU	CA-C-O	-5.26	114.97	120.55
1	A	318	ALA	CA-C-O	-5.26	114.85	120.42
1	A	88	ASP	CB-CG-OD1	5.24	130.45	118.40
1	A	100	LYS	N-CA-C	5.19	116.94	111.28
1	A	257	ASN	O-C-N	5.16	130.70	122.81
1	A	78	GLU	O-C-N	5.14	127.56	122.12
1	A	88	ASP	OD1-CG-OD2	-5.10	110.67	122.90
1	A	27	ASN	CA-CB-CG	-5.09	107.51	112.60
1	A	261	LEU	CA-C-N	5.07	127.04	120.56
1	A	261	LEU	C-N-CA	5.07	127.04	120.56
1	A	132	ARG	NE-CZ-NH2	-5.05	114.65	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	ILE	CB-CA-C	-5.04	106.29	111.08

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	2560	0	2420	39	0
2	B	28	0	25	0	0
3	A	11	0	10	0	0
4	A	14	0	11	18	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
7	A	43	0	30	0	0
8	A	370	0	0	1	0
All	All	3029	0	2496	39	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 (39) 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:319:GLU:OE2	4:A:380:A2G:C8	1.65	1.40
1:A:319:GLU:CD	4:A:380:A2G:C8	2.17	1.17
1:A:319:GLU:CG	4:A:380:A2G:H8B	1.85	1.06
1:A:319:GLU:CD	4:A:380:A2G:H8A	1.86	0.95
1:A:319:GLU:CG	4:A:380:A2G:C8	2.47	0.91
1:A:319:GLU:OE2	4:A:380:A2G:H8B	1.73	0.88
1:A:319:GLU:HG2	4:A:380:A2G:H8B	1.55	0.85
1:A:59:LYS:HB2	1:A:61:LYS:HE2	1.59	0.85
1:A:56:MET:HG3	1:A:61:LYS:NZ	1.91	0.84
1:A:319:GLU:HB2	4:A:380:A2G:C8	2.13	0.78
1:A:319:GLU:HB2	4:A:380:A2G:H8A	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLU:CD	4:A:380:A2G:H8B	2.01	0.71
1:A:319:GLU:CB	4:A:380:A2G:C8	2.69	0.70
1:A:25:GLN:HE21	1:A:25:GLN:HA	1.61	0.65
1:A:56:MET:HG3	1:A:61:LYS:HZ1	1.62	0.64
1:A:318:ALA:HB3	1:A:319:GLU:OE1	1.98	0.62
1:A:319:GLU:HB2	4:A:380:A2G:N2	2.17	0.60
1:A:149:HIS:HB2	1:A:154:ILE:HD11	1.83	0.59
1:A:59:LYS:HD2	1:A:61:LYS:NZ	2.18	0.58
1:A:43:ARG:HG3	8:A:398:HOH:O	2.03	0.58
1:A:319:GLU:CB	4:A:380:A2G:H8B	2.34	0.57
1:A:56:MET:HG3	1:A:61:LYS:CE	2.34	0.56
1:A:319:GLU:CB	4:A:380:A2G:H8A	2.33	0.54
1:A:300:PRO:HG3	1:A:326:VAL:CG2	2.39	0.53
1:A:59:LYS:CB	1:A:61:LYS:HE2	2.36	0.53
1:A:236:GLN:O	1:A:240:THR:HG23	2.09	0.52
1:A:319:GLU:CG	4:A:380:A2G:H8A	2.32	0.50
1:A:25:GLN:HA	1:A:25:GLN:NE2	2.27	0.49
1:A:319:GLU:HB2	4:A:380:A2G:HN2	1.79	0.47
1:A:145:PRO:HB3	1:A:154:ILE:HD12	1.97	0.47
1:A:300:PRO:HG3	1:A:326:VAL:HG21	1.97	0.46
1:A:149:HIS:CB	1:A:154:ILE:HD11	2.46	0.45
1:A:56:MET:HE3	1:A:56:MET:HB2	1.84	0.43
1:A:56:MET:HG3	1:A:61:LYS:HE3	1.99	0.42
1:A:319:GLU:CB	4:A:380:A2G:HN2	2.33	0.42
1:A:59:LYS:HD2	1:A:61:LYS:HZ3	1.85	0.41
1:A:59:LYS:HD2	1:A:61:LYS:CE	2.51	0.41
1:A:320:THR:HG21	4:A:380:A2G:C5	2.50	0.41
1:A:56:MET:HG3	1:A:61:LYS:HZ2	1.82	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	341/343 (99%)	335 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	274/274 (100%)	269 (98%)	5 (2%)	51	36

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	154	ILE
1	A	211	ARG
1	A	333	THR
1	A	342	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	27	ASN
1	A	119	ASN
1	A	182	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

2 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	2,1	14,14,15	1.34	2 (14%)	17,19,21	2.96	9 (52%)
2	NAG	B	2	2	14,14,15	3.04	9 (64%)	17,19,21	2.80	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	5.50	1.52	1.43
2	B	2	NAG	O5-C5	5.30	1.53	1.43
2	B	2	NAG	C1-C2	4.39	1.58	1.52
2	B	2	NAG	C2-N2	4.21	1.53	1.46
2	B	1	NAG	C2-N2	3.26	1.51	1.46
2	B	2	NAG	O4-C4	2.73	1.49	1.43
2	B	1	NAG	O7-C7	-2.61	1.17	1.23
2	B	2	NAG	C4-C5	2.57	1.58	1.53
2	B	2	NAG	O7-C7	-2.47	1.17	1.23
2	B	2	NAG	C3-C2	2.19	1.57	1.52
2	B	2	NAG	C4-C3	2.06	1.57	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C2-N2-C7	-7.24	113.20	122.90
2	B	2	NAG	C2-N2-C7	6.65	131.81	122.90
2	B	2	NAG	C1-O5-C5	-6.12	103.98	112.19
2	B	1	NAG	C1-O5-C5	-4.65	105.96	112.19
2	B	1	NAG	C8-C7-N2	-4.20	109.15	116.12
2	B	2	NAG	C1-C2-N2	-3.45	104.99	110.43
2	B	1	NAG	C3-C4-C5	3.28	116.18	110.23
2	B	2	NAG	O3-C3-C2	-3.21	102.73	109.40
2	B	1	NAG	O5-C1-C2	-3.13	106.45	111.29
2	B	1	NAG	O7-C7-C8	2.92	127.25	122.05
2	B	1	NAG	O5-C5-C4	-2.90	103.78	110.83
2	B	2	NAG	C8-C7-N2	-2.47	112.02	116.12
2	B	2	NAG	O3-C3-C4	2.40	116.04	110.38
2	B	1	NAG	C6-C5-C4	-2.34	107.27	113.02
2	B	1	NAG	C4-C3-C2	-2.32	107.62	111.02

There are no chirality outliers.

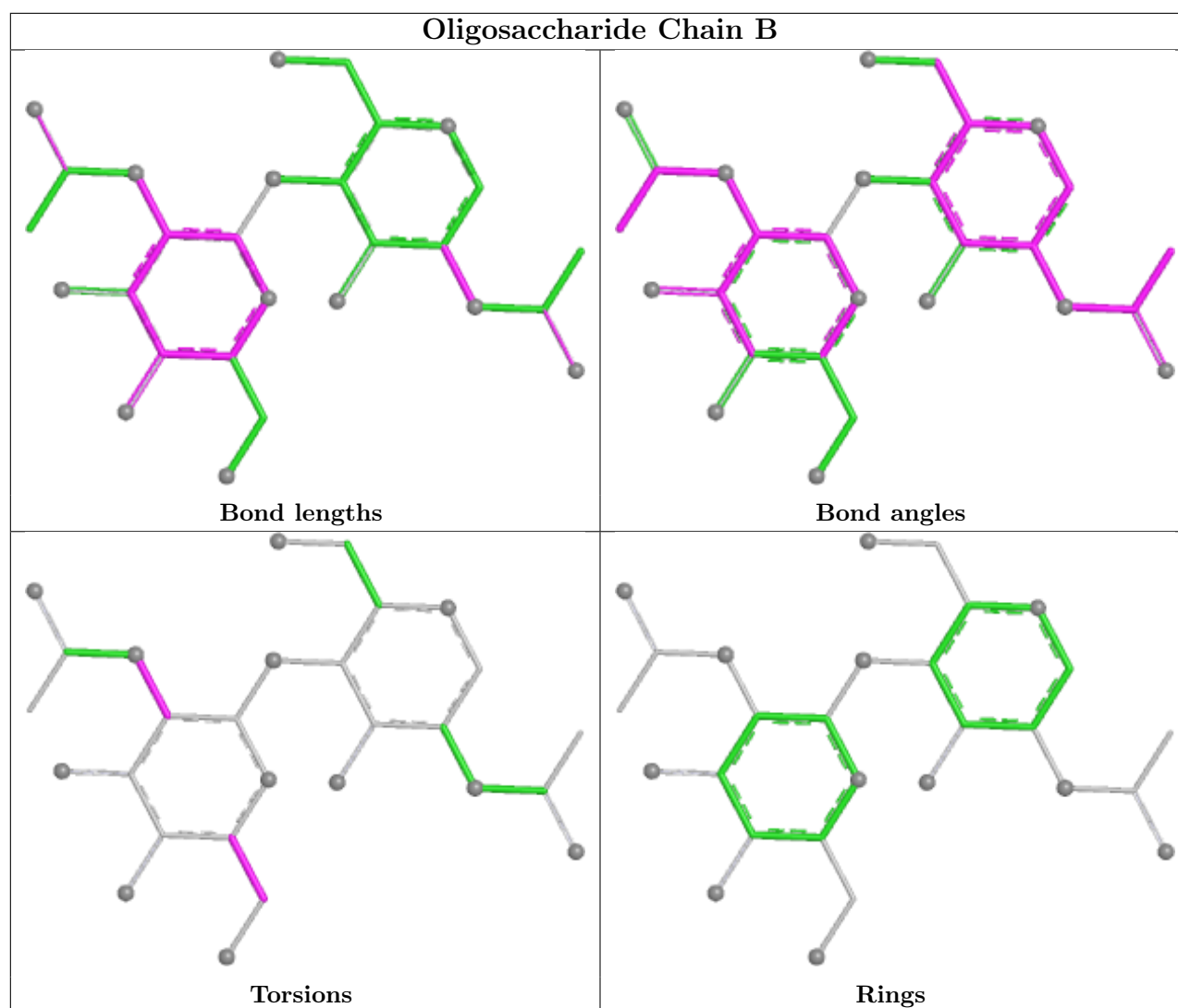
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7
2	B	2	NAG	C1-C2-N2-C7

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 6 ligands modelled in this entry, 2 are monoatomic and 1 is modelled with single atom - leaving 3 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	HEM	A	350	1,8	50,50,50	1.57	9 (18%)	67,82,82	1.23	6 (8%)
3	MAN	A	370	1	11,11,12	1.17	1 (9%)	15,15,17	2.09	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	A2G	A	380	1	14,14,15	0.84	0	17,19,21	2.60	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
7	HEM	A	350	1,8	-	1/14/54/54	-
3	MAN	A	370	1	-	0/2/19/22	0/1/1/1
4	A2G	A	380	1	-	4/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	350	HEM	FE-NA	4.19	2.09	1.95
7	A	350	HEM	FE-NC	4.16	2.08	1.95
7	A	350	HEM	CAB-C3B	3.55	1.56	1.47
7	A	350	HEM	FE-NB	3.16	2.04	1.94
7	A	350	HEM	FE-ND	2.48	2.02	1.94
3	A	370	MAN	C1-C2	2.46	1.58	1.52
7	A	350	HEM	CAC-C3C	2.42	1.53	1.47
7	A	350	HEM	CMC-C2C	2.35	1.55	1.50
7	A	350	HEM	CBD-CGD	2.32	1.55	1.50
7	A	350	HEM	CMA-C3A	2.12	1.55	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	380	A2G	O5-C1-C2	-8.35	98.38	111.29
3	A	370	MAN	C1-O5-C5	4.07	117.65	112.19
4	A	380	A2G	C1-O5-C5	3.91	117.43	112.19
3	A	370	MAN	O6-C6-C5	-3.07	100.88	111.33
3	A	370	MAN	O4-C4-C3	3.03	117.52	110.38
7	A	350	HEM	CBB-CAB-C3B	-2.88	113.14	127.53
3	A	370	MAN	C1-C2-C3	2.81	113.73	109.64
4	A	380	A2G	O7-C7-N2	2.59	126.56	121.98
7	A	350	HEM	O1D-CGD-CBD	-2.57	114.94	123.09
7	A	350	HEM	C2A-C1A-NA	-2.57	107.30	110.15
7	A	350	HEM	CBC-CAC-C3C	-2.52	114.94	127.53
7	A	350	HEM	CHD-C4C-C3C	2.44	129.33	125.21
7	A	350	HEM	O2D-CGD-O1D	2.35	129.37	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	380	A2G	C3-C4-C5	2.23	114.27	110.23
3	A	370	MAN	C2-C3-C4	2.17	114.68	110.86
3	A	370	MAN	O5-C5-C4	2.11	115.96	110.83
4	A	380	A2G	C2-N2-C7	-2.08	120.11	122.90
4	A	380	A2G	C1-C2-N2	2.05	113.66	110.43
4	A	380	A2G	O7-C7-C8	-2.02	118.45	122.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

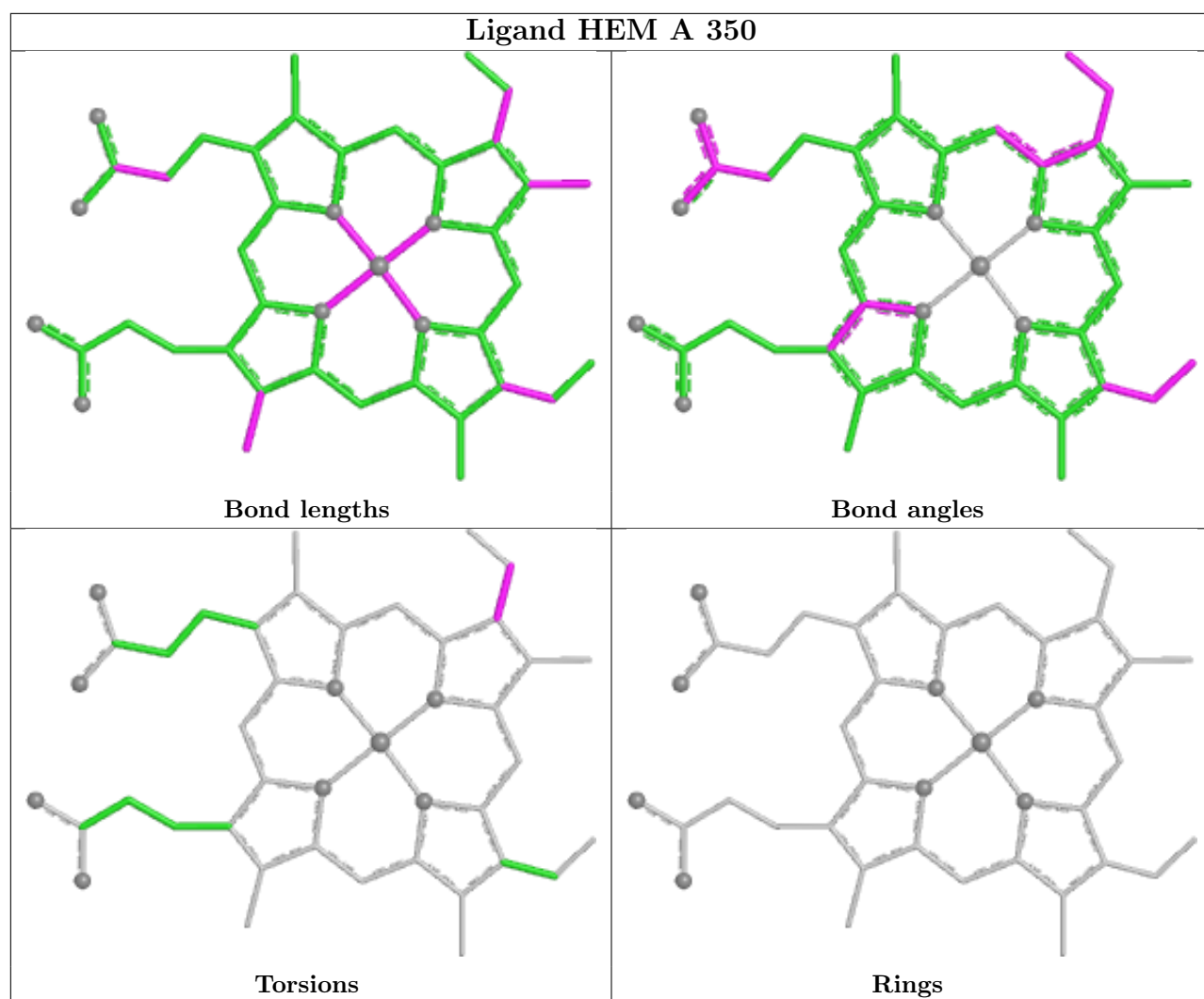
Mol	Chain	Res	Type	Atoms
4	A	380	A2G	O5-C5-C6-O6
4	A	380	A2G	C4-C5-C6-O6
4	A	380	A2G	C8-C7-N2-C2
4	A	380	A2G	O7-C7-N2-C2
7	A	350	HEM	C4C-C3C-CAC-CBC

There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	380	A2G	18	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	343/343 (100%)	-0.58	5 (1%) 72 76	6, 12, 27, 44	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	ASN	5.2
1	A	343	ALA	4.7
1	A	342	LYS	3.7
1	A	61	LYS	3.3
1	A	319	GLU	2.3

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

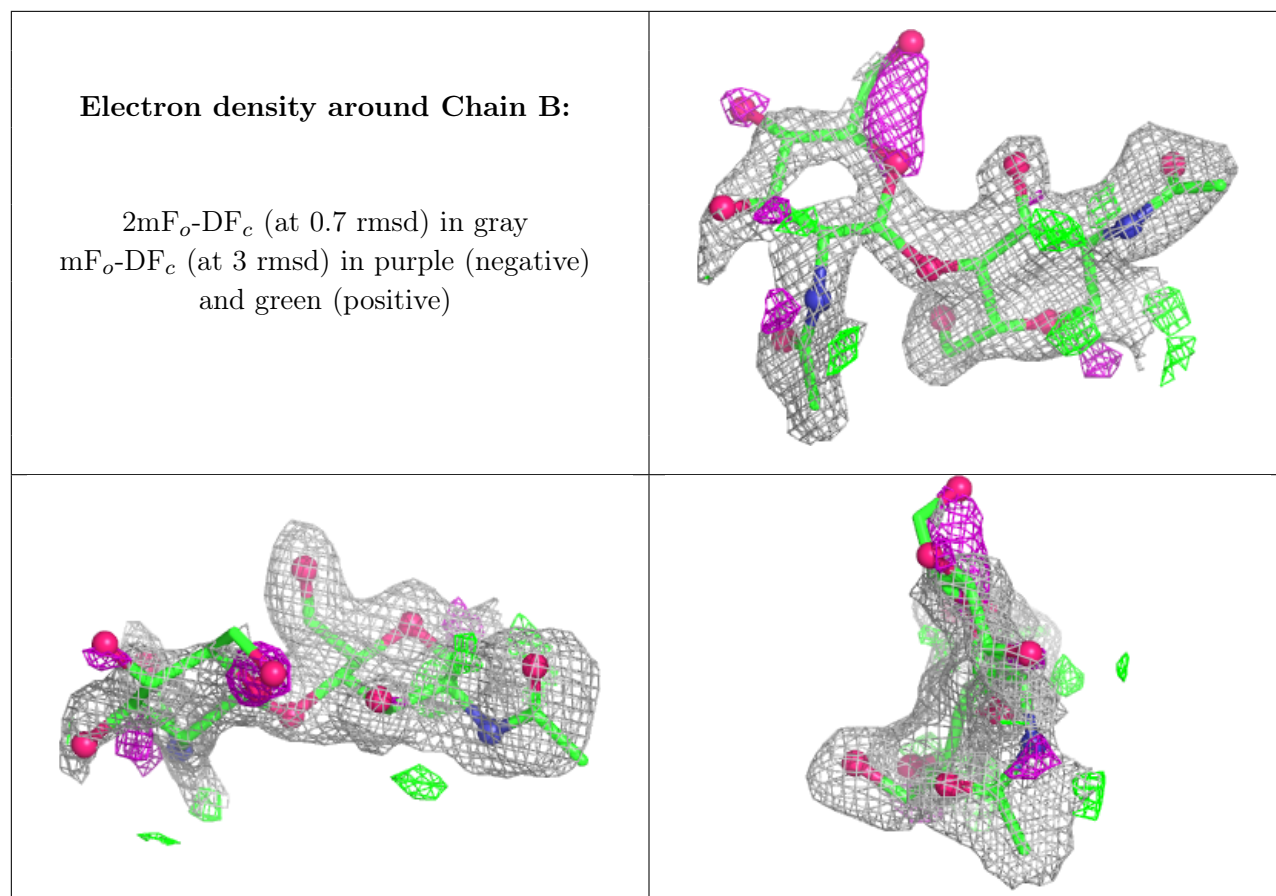
There are no non-standard protein/DNA/RNA residues in this entry.

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	B	2	14/15	0.56	0.14	44,47,48,49	0
2	NAG	B	1	14/15	0.80	0.11	31,36,38,42	0

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

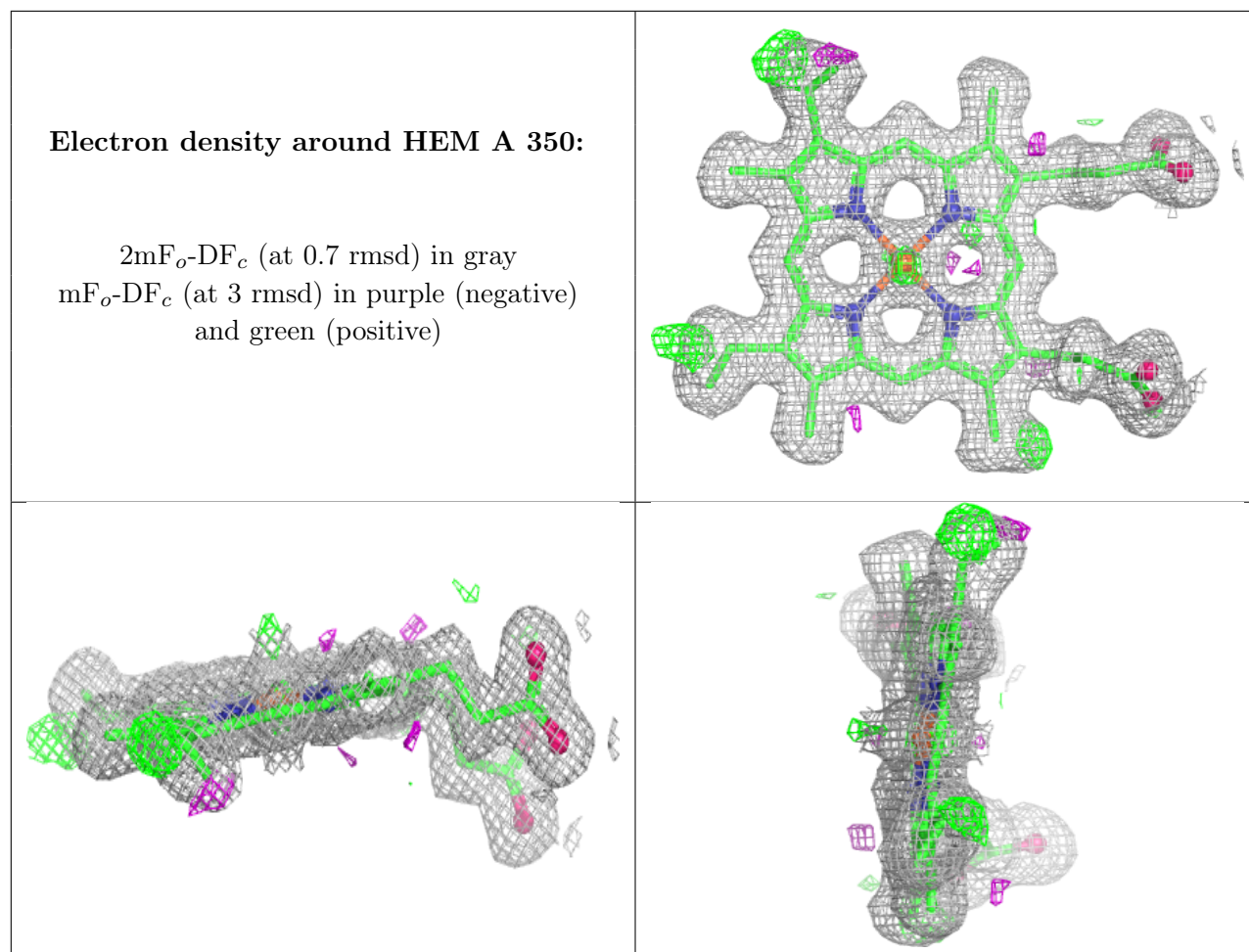


6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
4	A2G	A	380	14/15	0.63	0.15	42,45,46,47	0
3	MAN	A	370	11/12	0.92	0.07	21,22,23,26	0
6	OH	A	381	1/1	0.99	0.03	9,9,9,9	0
7	HEM	A	350	43/43	0.99	0.03	5,6,9,9	0
5	CA	A	351	1/1	1.00	0.02	7,7,7,7	0
5	CA	A	352	1/1	1.00	0.01	7,7,7,7	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.