



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:18 AM JST

PDB ID : 5B72 / pdb_00005b72
Title : Crystal structure of bovine lactoperoxidase with a broken covalent bond between Glu258 and heme moiety at 1.98 Å resolution.
Authors : Singh, P.K.; Sirohi, H.V.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2016-06-03
Resolution : 1.98 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	:	1.8.5 (274361), CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

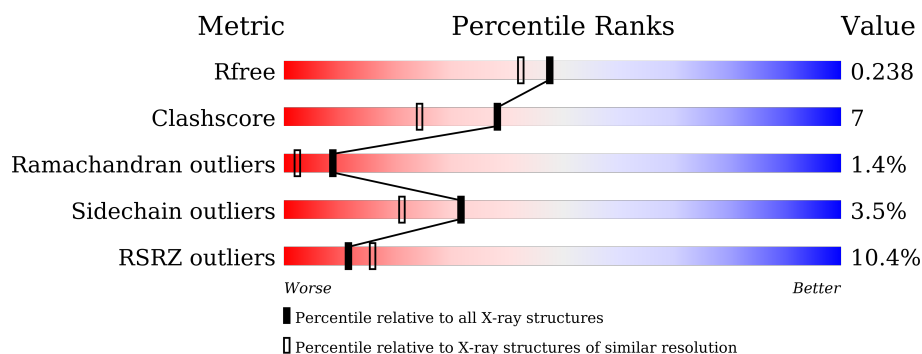
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

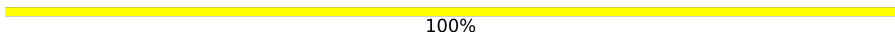
The reported resolution of this entry is 1.98 Å.

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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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

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

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 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5181 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	4767	3027	847	865	1	27	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

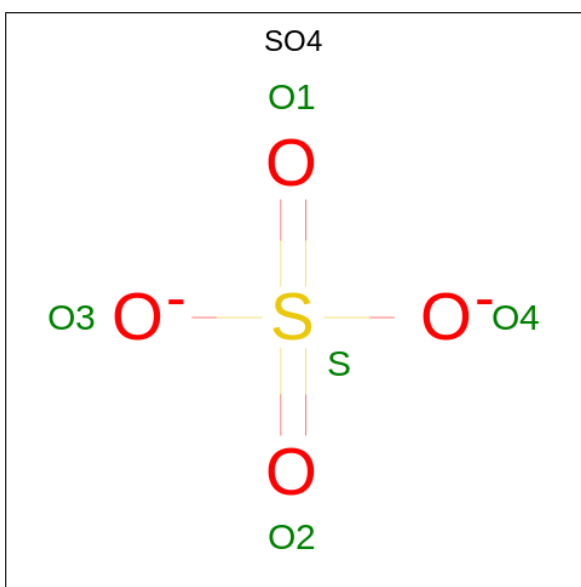
Chain	Residue	Modelled	Actual	Comment	Reference
A	220	SER	TRP	engineered mutation	UNP P80025
A	254	SER	PHE	engineered mutation	UNP P80025
A	410	LYS	ASP	engineered mutation	UNP P80025
A	547	MET	VAL	engineered mutation	UNP P80025

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



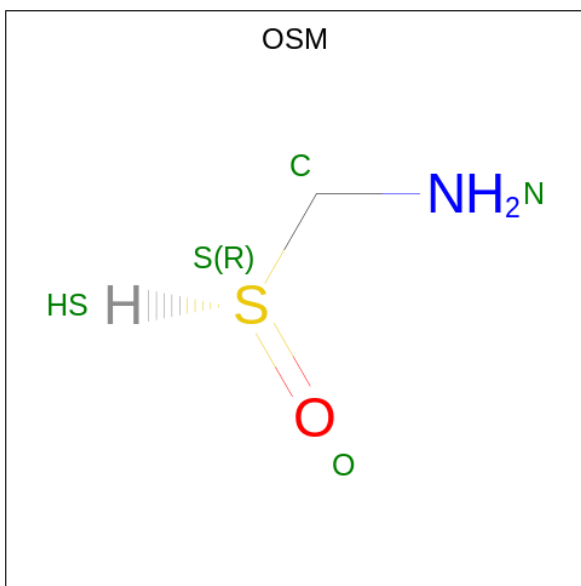
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1-(OXIDOSULFANYL)METHANAMINE (CCD ID: OSM) (formula: CH₅NOS).

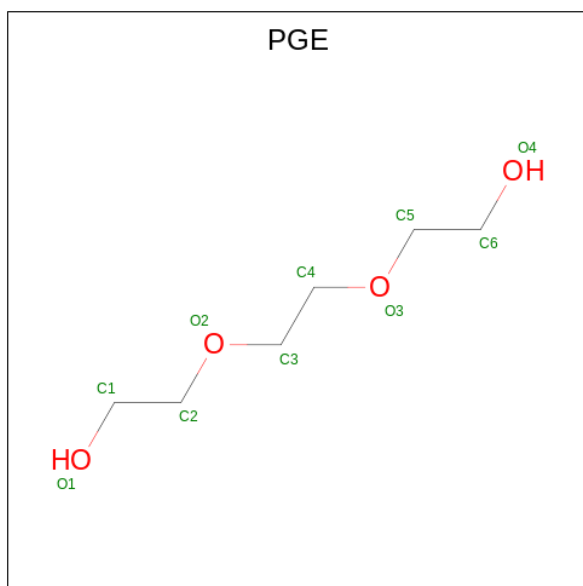


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0
			4	1	1	1	1	0

- Molecule 5 is IODIDE ION (CCD ID: IOD) (formula: I).

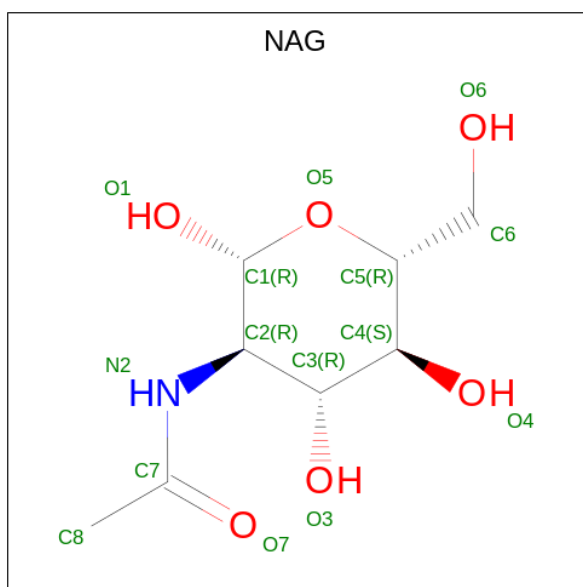
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	9	Total I 9 9	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 6 4	0	0
6	A	1	Total C O 10 6 4	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

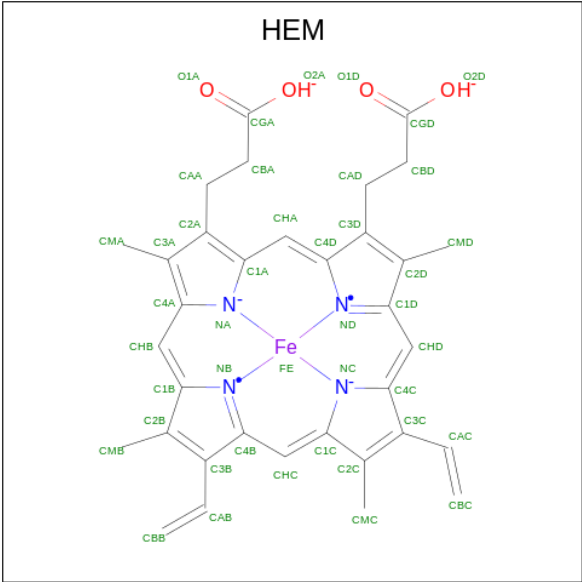


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

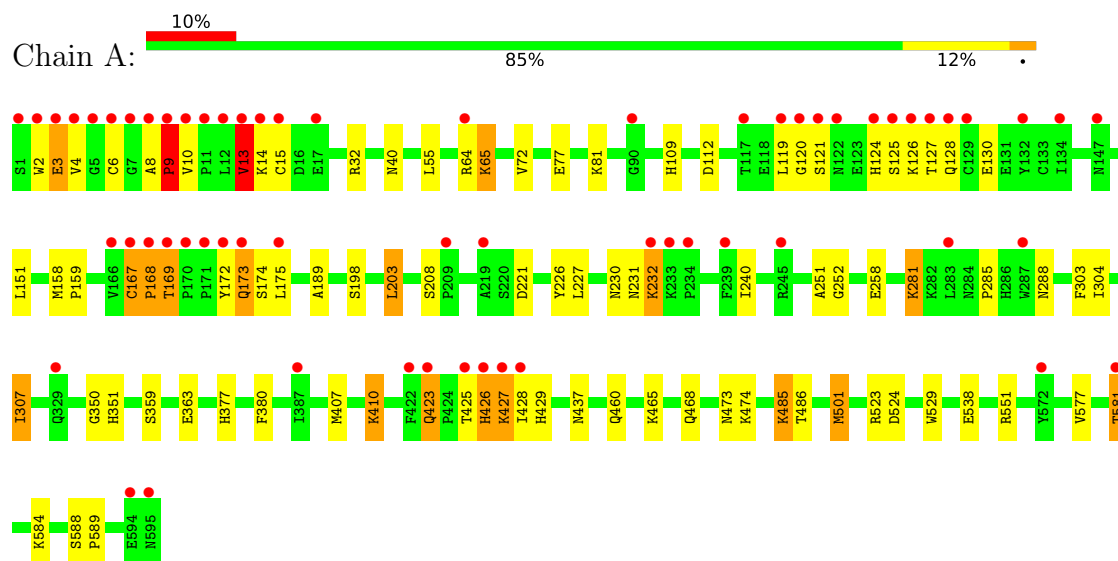
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	262	Total	O	0	0
			262	262		

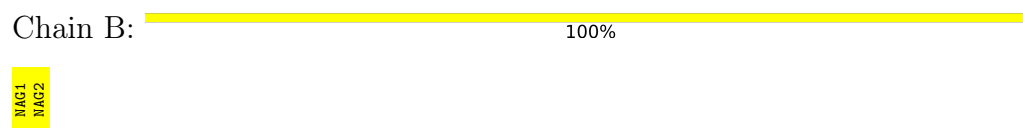
3 Residue-property plots [i](#)

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.85Å 80.19Å 75.09Å 90.00° 105.41° 90.00°	Depositor
Resolution (Å)	72.39 – 1.98 72.39 – 1.98	Depositor EDS
% Data completeness (in resolution range)	95.8 (72.39-1.98) 96.0 (72.39-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.188 , 0.235 0.195 , 0.238	Depositor DCC
R_{free} test set	1676 reflections (3.90%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 58.9	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	0.95	EDS
Total number of atoms	5181	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, HEM, IOD, SEP, OSM, NAG, PGE, SO4

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	1.11	3/4886 (0.1%)	1.17	19/6623 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	485	LYS	C-O	-7.37	1.14	1.24
1	A	426	HIS	N-CA	6.28	1.53	1.46
1	A	501	MET	C-O	-5.37	1.17	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	LYS	N-CA-C	-9.46	93.84	108.42
1	A	258[A]	GLU	CA-CB-CG	8.56	131.22	114.10
1	A	258[B]	GLU	CA-CB-CG	8.56	131.22	114.10
1	A	428	ILE	N-CA-C	8.46	120.53	108.17
1	A	426	HIS	N-CA-C	7.59	122.62	112.30
1	A	112	ASP	N-CA-C	6.30	118.99	109.23
1	A	13	VAL	N-CA-C	6.03	121.88	109.34
1	A	64	ARG	N-CA-C	6.00	119.70	112.38
1	A	72	VAL	N-CA-CB	5.83	116.47	110.23
1	A	474	LYS	N-CA-C	5.57	117.03	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	524	ASP	N-CA-C	5.55	118.26	111.82
1	A	72	VAL	N-CA-C	-5.53	103.87	108.63
1	A	9	PRO	CA-N-CD	-5.53	104.26	112.00
1	A	167	CYS	N-CA-C	-5.39	97.89	109.81
1	A	468	GLN	CB-CA-C	-5.31	101.98	110.79
1	A	208	SER	N-CA-C	5.25	116.69	110.07
1	A	363	GLU	N-CA-C	5.21	118.73	112.38
1	A	158	MET	CA-C-N	-5.15	114.48	119.78
1	A	158	MET	C-N-CA	-5.15	114.48	119.78

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	CYS	Peptide
1	A	167	CYS	Peptide

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	4767	0	4689	62	0
2	B	28	0	25	0	0
3	A	5	0	0	0	0
4	A	4	0	5	0	0
5	A	9	0	0	2	0
6	A	20	0	28	1	0
7	A	42	0	39	0	0
8	A	1	0	0	0	0
9	A	43	0	30	5	0
10	A	262	0	0	10	1
All	All	5181	0	4816	67	1

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 7.

All (67) 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:159:PRO:HG3	1:A:426:HIS:CE1	2.07	0.89
1:A:126:LYS:O	1:A:130:GLU:OE1	2.00	0.80
1:A:159:PRO:HG3	1:A:426:HIS:HE1	1.47	0.77
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.66	0.76
1:A:172:TYR:HB2	1:A:173:GLN:HB3	1.69	0.75
1:A:303:PHE:CZ	1:A:307:ILE:HD13	2.27	0.70
1:A:127:THR:HA	1:A:130:GLU:CD	2.16	0.70
1:A:230:ASN:O	10:A:902:HOH:O	2.10	0.69
1:A:159:PRO:CG	1:A:426:HIS:HE1	2.06	0.69
9:A:820:HEM:HMB1	9:A:820:HEM:HBB2	1.74	0.69
1:A:303:PHE:CE1	1:A:307:ILE:CD1	2.76	0.68
1:A:159:PRO:CG	1:A:426:HIS:CE1	2.76	0.68
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.41	0.66
9:A:820:HEM:HMC1	9:A:820:HEM:HBC2	1.79	0.65
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.80	0.62
1:A:303:PHE:CE1	1:A:307:ILE:HD11	2.34	0.62
1:A:303:PHE:CZ	1:A:307:ILE:CD1	2.84	0.61
1:A:3:GLU:HB2	1:A:175:LEU:HD21	1.81	0.61
1:A:127:THR:HA	1:A:130:GLU:OE2	2.00	0.60
1:A:8:ALA:N	1:A:9:PRO:HD2	2.17	0.60
1:A:65:LYS:NZ	10:A:906:HOH:O	2.35	0.60
1:A:231:ASN:O	1:A:232:LYS:HG3	2.04	0.58
1:A:281:LYS:HE2	1:A:285:PRO:O	2.08	0.53
1:A:460:GLN:H	6:A:807:PGE:H12	1.75	0.52
1:A:423:GLN:NE2	10:A:912:HOH:O	2.42	0.52
1:A:426:HIS:O	1:A:427:LYS:HB2	2.10	0.52
1:A:130:GLU:OE1	1:A:130:GLU:N	2.24	0.52
9:A:820:HEM:HBB2	9:A:820:HEM:CMB	2.39	0.51
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.46	0.51
5:A:804:IOD:I	5:A:805:IOD:I	3.70	0.50
1:A:3:GLU:CB	1:A:175:LEU:HD21	2.40	0.50
1:A:125:SER:HA	1:A:128:GLN:HB3	1.95	0.49
1:A:407:MET:HB3	1:A:501:MET:HE3	1.94	0.49
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.48	0.49
1:A:127:THR:O	1:A:130:GLU:HG2	2.13	0.49
1:A:124:HIS:O	1:A:127:THR:N	2.47	0.48
1:A:426:HIS:CD2	1:A:426:HIS:N	2.82	0.48
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.96	0.47
1:A:120:GLY:CA	1:A:126:LYS:HB2	2.45	0.47
1:A:423:GLN:O	10:A:903:HOH:O	2.20	0.47
1:A:231:ASN:O	1:A:232:LYS:CG	2.62	0.47
1:A:350:GLY:HA3	9:A:820:HEM:CBC	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:CD	1:A:175:LEU:HD11	2.40	0.47
1:A:577:VAL:HG21	1:A:581:THR:CG2	2.44	0.47
1:A:14:LYS:HA	1:A:14:LYS:HE2	1.96	0.47
1:A:359:SER:OG	5:A:818:IOD:I	2.98	0.47
1:A:288:ASN:ND2	10:A:916:HOH:O	2.48	0.46
1:A:407:MET:HB3	1:A:501:MET:CE	2.46	0.46
1:A:410:LYS:HE2	1:A:473:ASN:HD21	1.80	0.46
1:A:10:VAL:HG11	1:A:40:ASN:HB2	1.98	0.45
1:A:203:LEU:HD21	1:A:252:GLY:HA2	1.99	0.45
1:A:9:PRO:HG3	1:A:168:PRO:CG	2.46	0.45
1:A:9:PRO:HG3	1:A:168:PRO:HG3	1.98	0.44
1:A:130:GLU:HB3	1:A:159:PRO:HG3	2.00	0.44
1:A:168:PRO:O	1:A:169:THR:CB	2.66	0.43
1:A:232:LYS:O	10:A:902:HOH:O	2.21	0.43
1:A:429:HIS:O	10:A:904:HOH:O	2.21	0.43
9:A:820:HEM:HBC2	9:A:820:HEM:CMC	2.47	0.43
1:A:77:GLU:OE2	1:A:81:LYS:NZ	2.42	0.43
1:A:120:GLY:HA2	1:A:126:LYS:HB2	2.01	0.43
1:A:240:ILE:HD12	10:A:1070:HOH:O	2.20	0.42
1:A:109:HIS:CD2	10:A:922:HOH:O	2.72	0.42
1:A:465:LYS:NZ	10:A:907:HOH:O	2.35	0.42
1:A:2:TRP:C	1:A:4:VAL:N	2.78	0.42
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.56	0.41
1:A:227:LEU:CD2	1:A:251:ALA:HB2	2.51	0.40
1:A:172:TYR:CD2	1:A:173:GLN:HG3	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:964:HOH:O	10:A:1094:HOH:O[2_445]	1.91	0.29

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%)	565 (95%)	20 (3%)	8 (1%)	9 3

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	13	VAL
1	A	169	THR
1	A	427	LYS
1	A	425	THR
1	A	174	SER
1	A	168	PRO
1	A	485	LYS

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	518/517 (100%)	500 (96%)	18 (4%)	32 21

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	6	CYS
1	A	13	VAL
1	A	32	ARG
1	A	55	LEU
1	A	65	LYS
1	A	119	LEU
1	A	121	SER
1	A	151	LEU
1	A	173	GLN
1	A	203	LEU

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Mol	Chain	Res	Type
1	A	281	LYS
1	A	307	ILE
1	A	410	LYS
1	A	423	GLN
1	A	486	THR
1	A	538	GLU
1	A	581	THR

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

Mol	Chain	Res	Type
1	A	68	ASN
1	A	173	GLN
1	A	341	ASN
1	A	426	HIS
1	A	520	GLN
1	A	556	ASN
1	A	571	ASN

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	2.39	4 (50%)	8,12,14	8.18	6 (75%)

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	-	5/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-OG	3.81	1.72	1.60
1	A	198	SEP	OG-CB	3.49	1.58	1.44
1	A	198	SEP	CB-CA	3.28	1.61	1.52
1	A	198	SEP	P-O3P	-2.03	1.47	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-CB-CA	18.64	126.29	108.14
1	A	198	SEP	P-OG-CB	12.42	152.50	118.30
1	A	198	SEP	O3P-P-O1P	-3.28	97.83	110.68
1	A	198	SEP	O3P-P-OG	2.84	114.29	106.73
1	A	198	SEP	O3P-P-O2P	2.53	117.30	107.64
1	A	198	SEP	O2P-P-O1P	2.32	119.75	110.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	N-CA-CB-OG
1	A	198	SEP	CA-CB-OG-P
1	A	198	SEP	CB-OG-P-O1P
1	A	198	SEP	CB-OG-P-O2P
1	A	198	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

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	1,2	14,14,15	0.69	0	17,19,21	1.28	3 (17%)
2	NAG	B	2	2	14,14,15	0.66	0	17,19,21	2.16	4 (23%)

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

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	7.05	121.74	112.19
2	B	2	NAG	C4-C3-C2	-3.16	106.39	111.02
2	B	2	NAG	C1-C2-N2	2.76	115.21	110.49
2	B	1	NAG	O4-C4-C5	2.76	116.15	109.30
2	B	1	NAG	C1-C2-N2	2.30	114.41	110.49
2	B	1	NAG	O4-C4-C3	-2.27	105.10	110.35
2	B	2	NAG	O5-C5-C6	2.10	110.49	107.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

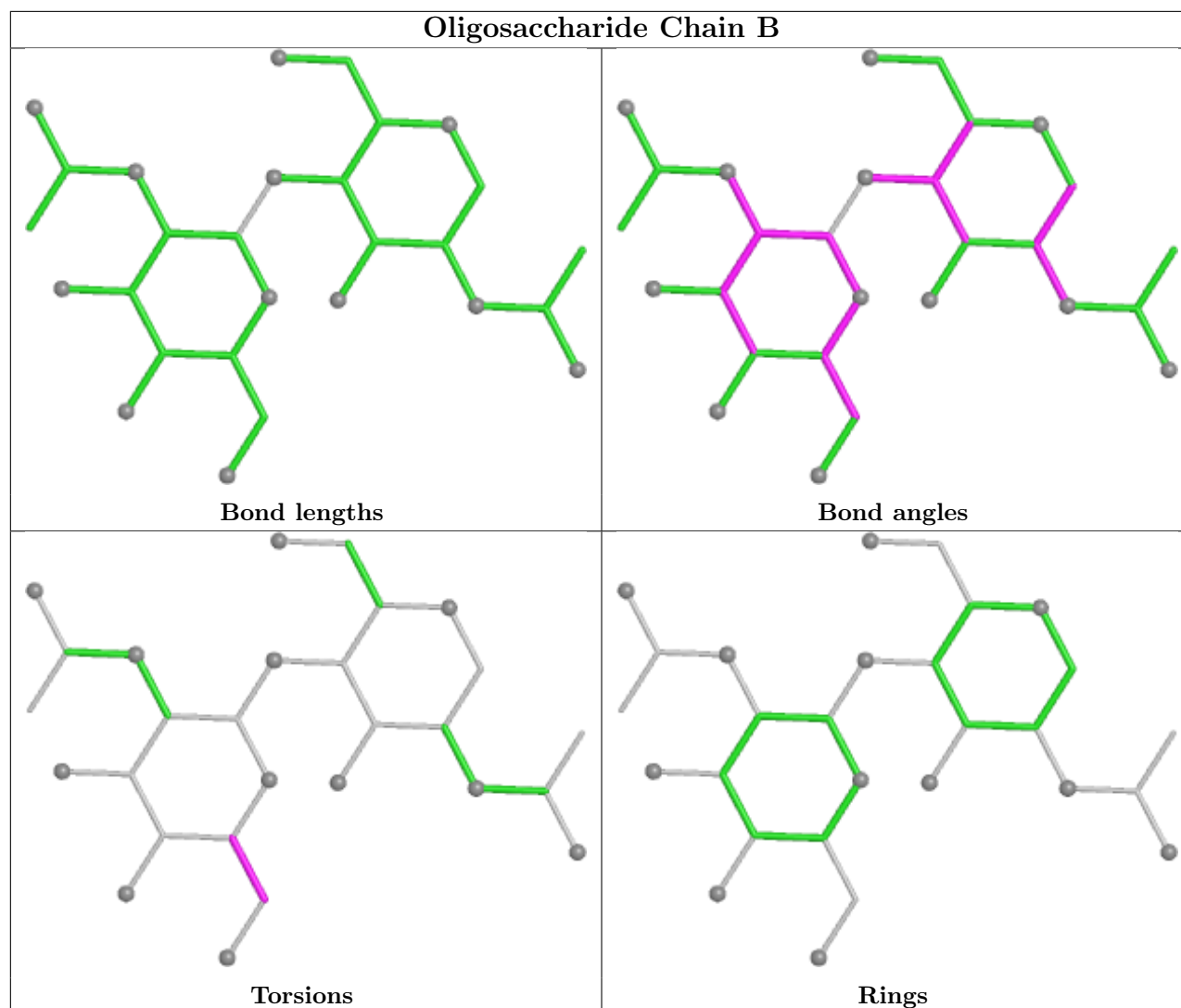
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

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 18 ligands modelled in this entry, 10 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	$\# Z > 2$
9	HEM	A	820	1,10	50,50,50	1.63	8 (16%)	66,82,82	1.87	14 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	808	1	14,14,15	0.58	0	17,19,21	1.61	4 (23%)
6	PGE	A	806	-	9,9,9	0.50	0	8,8,8	0.82	0
6	PGE	A	807	-	9,9,9	0.59	0	8,8,8	1.01	0
3	SO4	A	801	-	4,4,4	0.37	0	6,6,6	0.68	0
7	NAG	A	809	1	14,14,15	0.59	0	17,19,21	1.37	2 (11%)
7	NAG	A	812	1	14,14,15	0.70	0	17,19,21	1.60	2 (11%)
4	OSM	A	802	-	1,3,3	0.58	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
9	HEM	A	820	1,10	-	4/14/54/54	-
7	NAG	A	808	1	-	0/6/23/26	0/1/1/1
6	PGE	A	806	-	-	2/7/7/7	-
6	PGE	A	807	-	-	5/7/7/7	-
7	NAG	A	809	1	-	2/6/23/26	0/1/1/1
7	NAG	A	812	1	-	2/6/23/26	0/1/1/1
4	OSM	A	802	-	-	0/0/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	820	HEM	FE-NC	4.85	2.11	1.95
9	A	820	HEM	FE-NB	4.82	2.09	1.94
9	A	820	HEM	C1B-NB	-4.02	1.33	1.40
9	A	820	HEM	C4C-NC	-2.86	1.34	1.39
9	A	820	HEM	FE-NA	2.57	2.03	1.95
9	A	820	HEM	C1D-C2D	2.53	1.49	1.44
9	A	820	HEM	C1C-C2C	-2.52	1.40	1.45
9	A	820	HEM	C3B-C4B	2.24	1.49	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	820	HEM	C1B-NB-C4B	7.37	112.68	105.07
9	A	820	HEM	CHC-C4B-NB	5.70	130.61	124.42
9	A	820	HEM	C4C-NC-C1C	4.61	109.87	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	812	NAG	C1-O5-C5	4.32	118.05	112.19
7	A	812	NAG	O5-C1-C2	-3.75	105.37	111.29
7	A	808	NAG	O6-C6-C5	-3.59	98.96	111.29
9	A	820	HEM	CHB-C1B-NB	3.53	128.72	124.37
9	A	820	HEM	CHA-C4D-ND	2.95	128.01	124.37
9	A	820	HEM	CHA-C4D-C3D	-2.93	119.82	125.33
9	A	820	HEM	O2A-CGA-CBA	2.75	122.87	114.03
9	A	820	HEM	CHD-C4C-NC	2.54	127.18	124.44
7	A	808	NAG	C1-O5-C5	2.47	115.55	112.19
9	A	820	HEM	O2A-CGA-O1A	-2.33	117.50	123.30
9	A	820	HEM	CMB-C2B-C1B	2.33	128.58	125.04
9	A	820	HEM	CHD-C1D-ND	2.25	126.86	124.42
9	A	820	HEM	CBD-CAD-C3D	-2.24	106.40	112.63
9	A	820	HEM	CHD-C1D-C2D	-2.22	121.50	124.98
9	A	820	HEM	CBA-CAA-C2A	-2.22	106.46	112.63
7	A	808	NAG	C3-C4-C5	-2.22	106.28	110.24
7	A	809	NAG	O7-C7-N2	2.18	125.96	121.95
7	A	808	NAG	O5-C1-C2	-2.10	107.97	111.29
7	A	809	NAG	O3-C3-C2	-2.10	105.12	109.47

There are no chirality outliers.

All (15) torsion outliers are listed below:

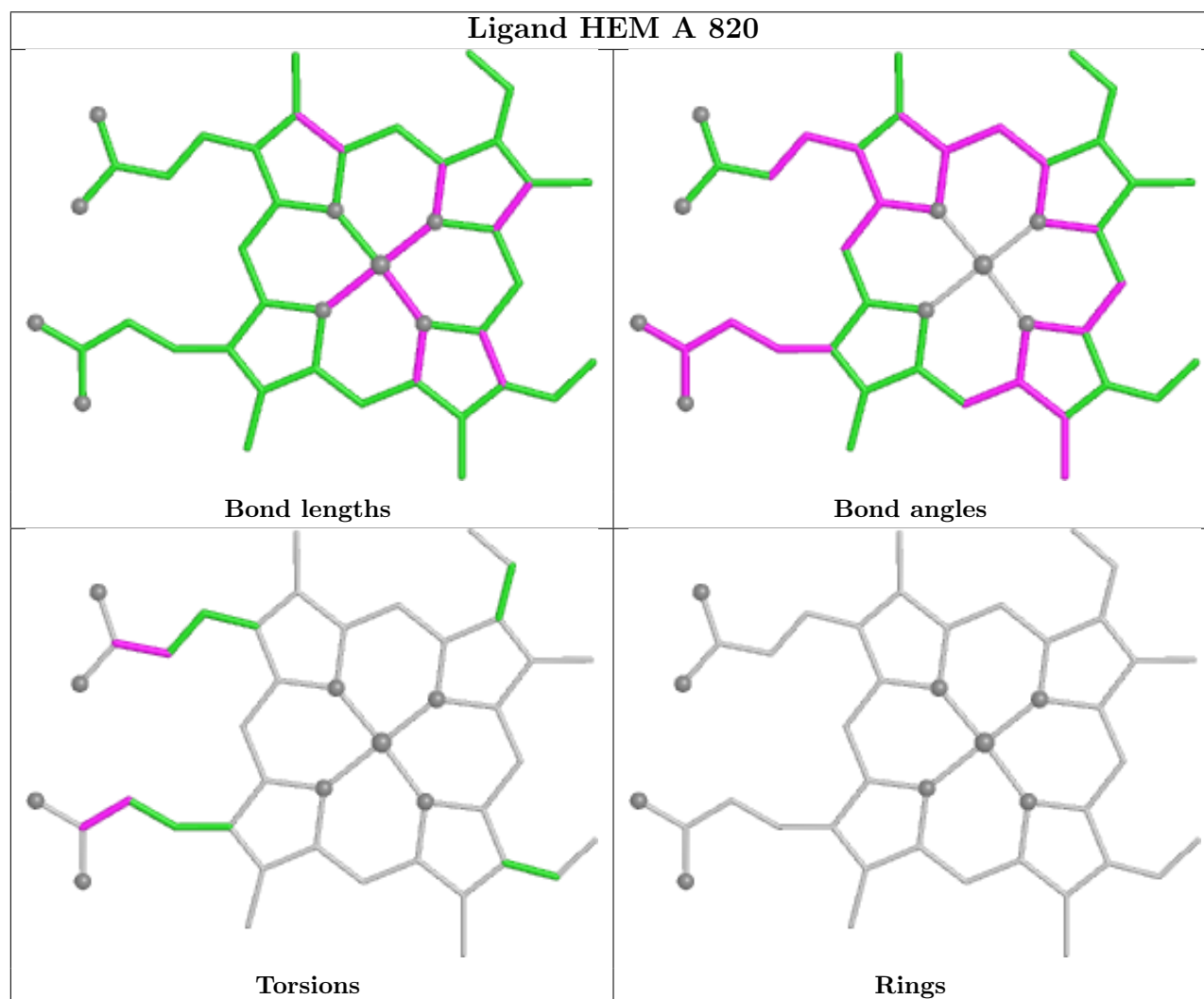
Mol	Chain	Res	Type	Atoms
6	A	806	PGE	O1-C1-C2-O2
6	A	807	PGE	O1-C1-C2-O2
6	A	807	PGE	O3-C5-C6-O4
6	A	807	PGE	O2-C3-C4-O3
7	A	809	NAG	O5-C5-C6-O6
7	A	809	NAG	C4-C5-C6-O6
6	A	807	PGE	C1-C2-O2-C3
6	A	807	PGE	C3-C4-O3-C5
6	A	806	PGE	C3-C4-O3-C5
7	A	812	NAG	O5-C5-C6-O6
9	A	820	HEM	CAA-CBA-CGA-O2A
9	A	820	HEM	CAA-CBA-CGA-O1A
9	A	820	HEM	CAD-CBD-CGD-O1D
9	A	820	HEM	CAD-CBD-CGD-O2D
7	A	812	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	820	HEM	5	0
6	A	807	PGE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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%)	0.52	62 (10%)	11 16	19, 31, 106, 182	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	PRO	7.8
1	A	10	VAL	7.3
1	A	9	PRO	7.2
1	A	168	PRO	6.8
1	A	11	PRO	6.6
1	A	8	ALA	6.6
1	A	13	VAL	5.8
1	A	169	THR	5.6
1	A	428	ILE	5.1
1	A	173	GLN	5.0
1	A	234	PRO	5.0
1	A	119	LEU	4.9
1	A	2	TRP	4.8
1	A	6	CYS	4.7
1	A	5	GLY	4.6
1	A	171	PRO	4.5
1	A	15	CYS	4.4
1	A	12	LEU	4.3
1	A	167	CYS	4.2
1	A	7	GLY	3.9
1	A	117	THR	3.9
1	A	581	THR	3.9
1	A	125	SER	3.7
1	A	175	LEU	3.7
1	A	129	CYS	3.6
1	A	239	PHE	3.6
1	A	4	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	426	HIS	3.5
1	A	172	TYR	3.5
1	A	121	SER	3.4
1	A	232	LYS	3.3
1	A	127	THR	3.3
1	A	120	GLY	3.1
1	A	425	THR	3.1
1	A	134	ILE	3.1
1	A	283	LEU	3.1
1	A	14	LYS	3.0
1	A	423	GLN	2.9
1	A	233	LYS	2.9
1	A	427	LYS	2.9
1	A	132	TYR	2.9
1	A	422	PHE	2.7
1	A	595	ASN	2.7
1	A	126	LYS	2.7
1	A	3	GLU	2.6
1	A	147	ASN	2.6
1	A	124	HIS	2.5
1	A	90	GLY	2.4
1	A	128	GLN	2.4
1	A	287	TRP	2.4
1	A	387	ILE	2.3
1	A	329	GLN	2.3
1	A	219	ALA	2.2
1	A	1	SER	2.1
1	A	209	PRO	2.1
1	A	245	ARG	2.1
1	A	17	GLU	2.1
1	A	594	GLU	2.1
1	A	122	ASN	2.1
1	A	572	TYR	2.1
1	A	64	ARG	2.1
1	A	166	VAL	2.0

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

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.

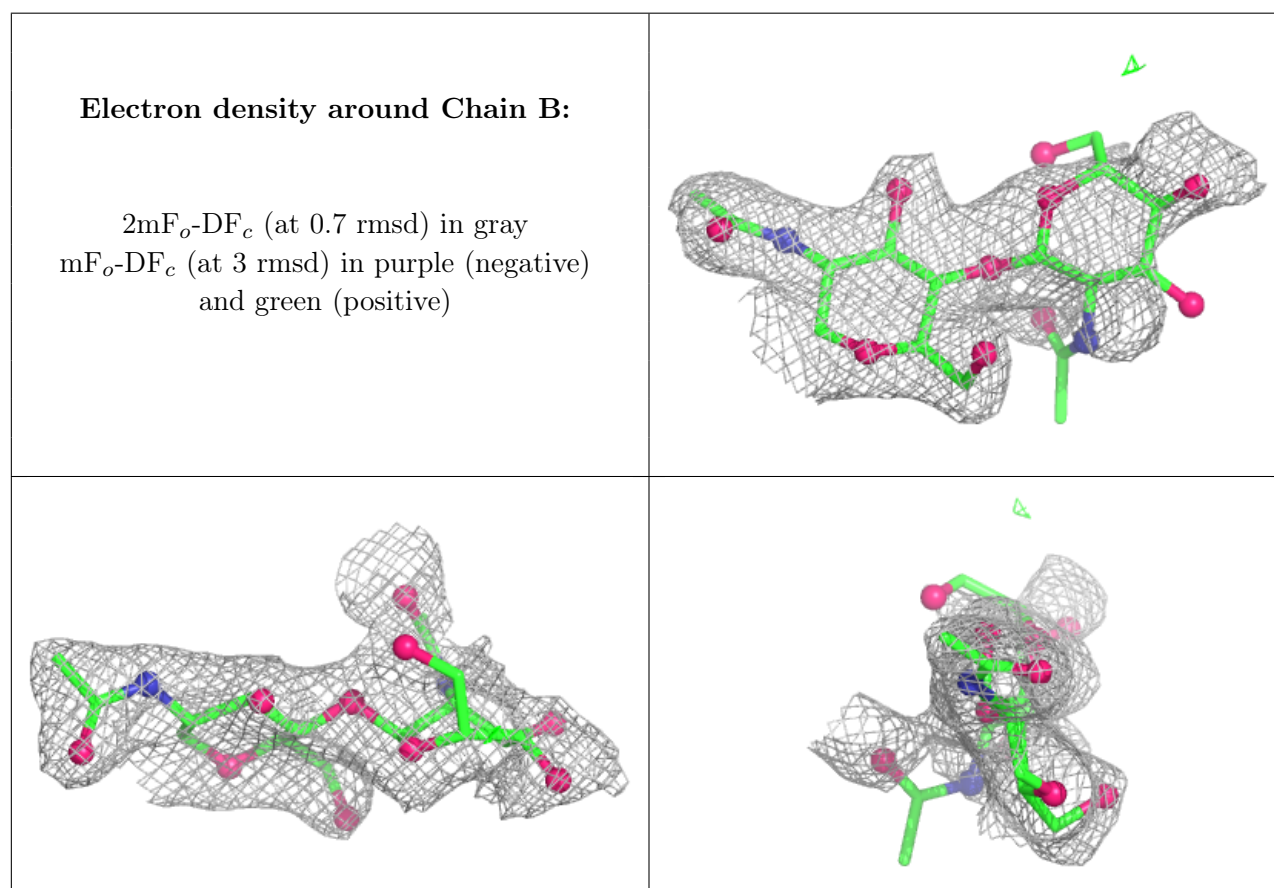
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	SEP	A	198	10/11	0.92	0.14	26,32,51,54	0

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($\text{\AA}^2$)	Q<0.9
2	NAG	B	2	14/15	0.57	0.16	68,80,97,101	0
2	NAG	B	1	14/15	0.93	0.08	38,44,51,58	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,

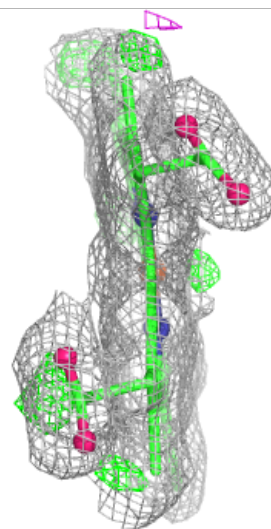
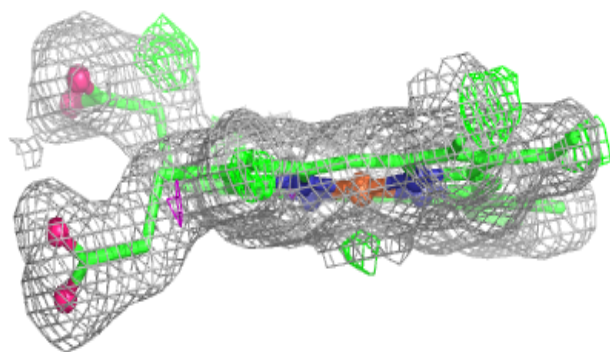
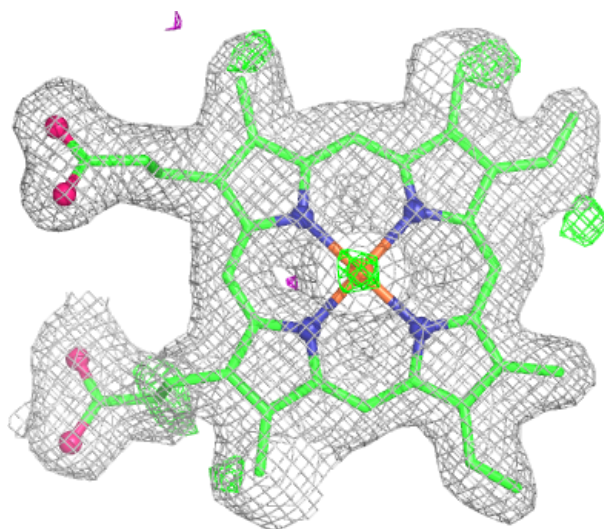
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	812	14/15	0.77	0.14	51,66,72,78	0
7	NAG	A	808	14/15	0.79	0.12	48,53,59,66	0
7	NAG	A	809	14/15	0.84	0.10	38,49,56,66	0
6	PGE	A	806	10/10	0.91	0.10	38,41,43,45	0
6	PGE	A	807	10/10	0.92	0.10	33,48,51,52	0
5	IOD	A	805	1/1	0.94	0.11	72,72,72,72	1
5	IOD	A	819	1/1	0.95	0.15	74,74,74,74	1
5	IOD	A	818	1/1	0.96	0.17	73,73,73,73	1
9	HEM	A	820	43/43	0.96	0.08	20,25,30,37	0
4	OSM	A	802	4/4	0.97	0.09	15,19,22,29	0
3	SO4	A	801	5/5	0.98	0.05	32,32,35,35	0
5	IOD	A	814	1/1	0.98	0.04	47,47,47,47	1
5	IOD	A	816	1/1	0.99	0.03	30,30,30,30	0
5	IOD	A	817	1/1	0.99	0.03	33,33,33,33	1
5	IOD	A	803	1/1	0.99	0.02	23,23,23,23	1
5	IOD	A	804	1/1	0.99	0.05	41,41,41,41	1
8	CA	A	813	1/1	0.99	0.02	24,24,24,24	0
5	IOD	A	815	1/1	0.99	0.03	34,34,34,34	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 820:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.