



Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2025 – 03:43 PM EDT

PDB ID : 3RKE / pdb_00003rke
Title : Crystal Structure of goat Lactoperoxidase complexed with a tightly bound inhibitor, 4-aminophenyl-4H-imidazole-1-yl methanone at 2.3 Å resolution
Authors : Dube, D.; Singh, R.P.; Sinha, M.; Singh, A.K.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2011-04-18
Resolution : 2.30 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

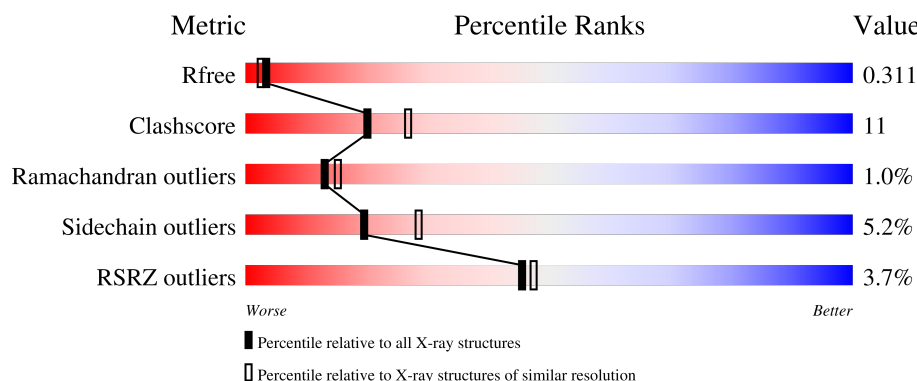
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	 4% 76% 22% .
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
1	SEP	A	198	-	-	X	-
8	MZZ	A	610	-	X	X	-

2 Entry composition [i](#)

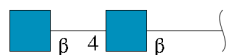
There are 9 unique types of molecules in this entry. The entry contains 5174 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

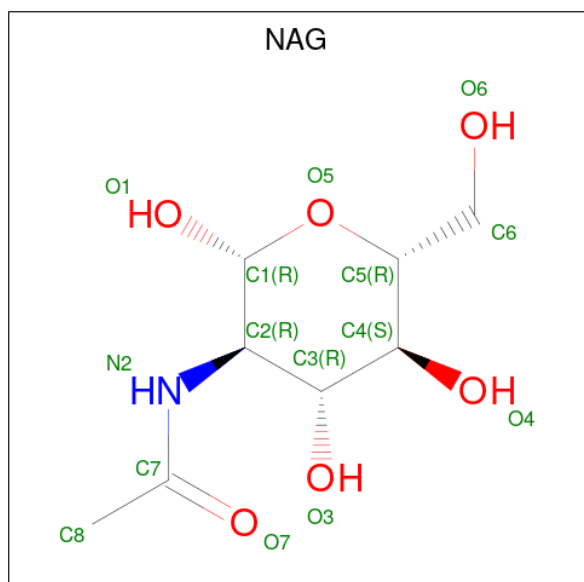
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4757	3021	844	865	1	26			

- 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			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

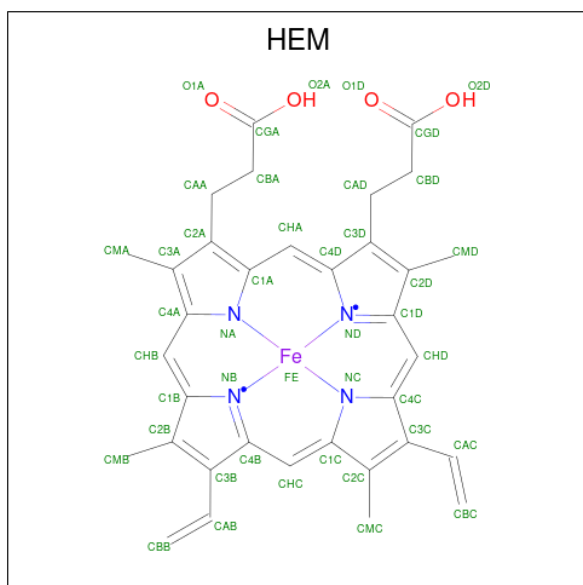


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).

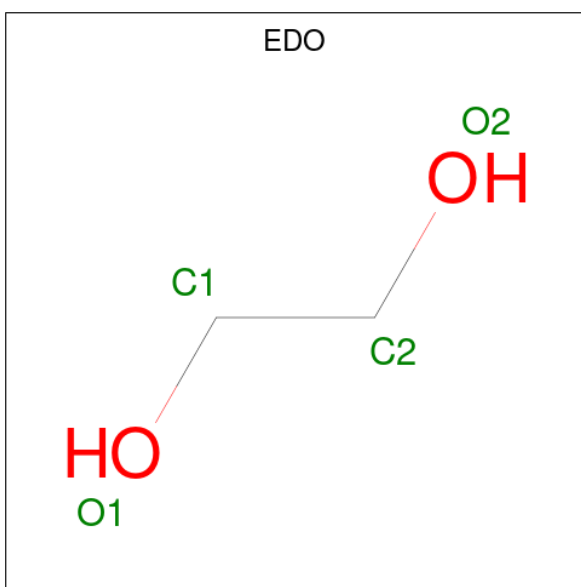


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

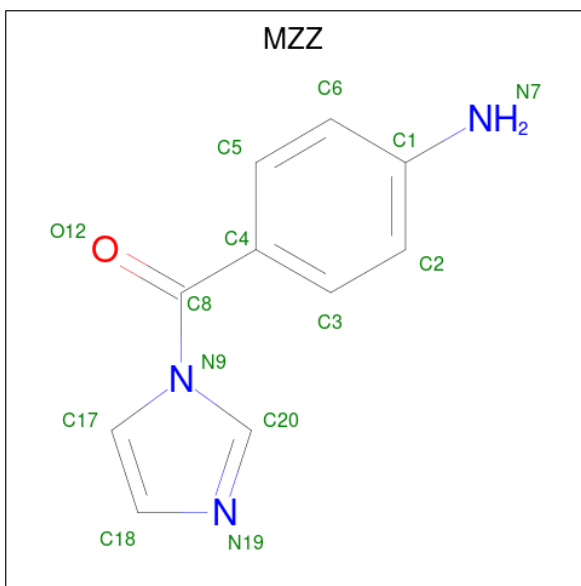
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	I	0	0
			9	9		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 8 is (4-aminophenyl)-imidazol-1-yl-methanone (CCD ID: MZZ) (formula: $C_{10}H_9N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	10	3	1		

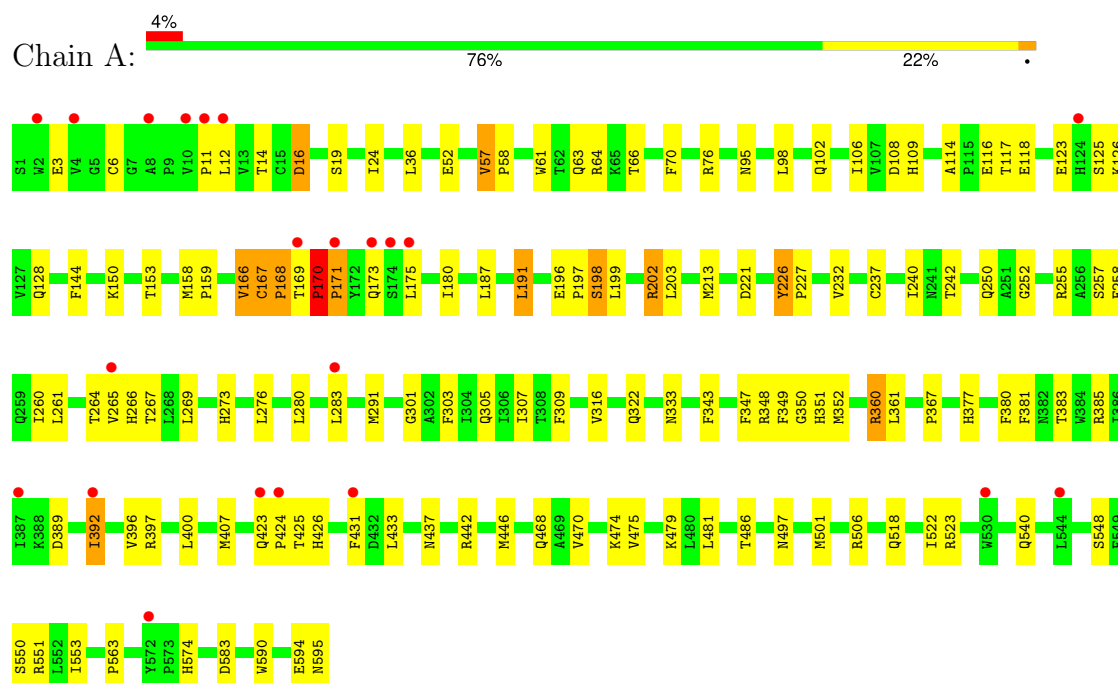
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	290	Total 290	O 290	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: 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	53.98Å 80.53Å 76.16Å 90.00° 103.07° 90.00°	Depositor
Resolution (Å)	44.03 – 2.30 44.03 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (44.03-2.30) 97.7 (44.03-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.245 , 0.263 0.237 , 0.311	Depositor DCC
R_{free} test set	1394 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.894	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5174	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: EDO, CA, NAG, MZZ, HEM, IOD, SEP

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	0.73	2/4875 (0.0%)	0.99	13/6621 (0.2%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	426	HIS	CA-C	-6.42	1.45	1.53
1	A	175	LEU	N-CA	5.12	1.51	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ASP	N-CA-C	10.63	122.95	110.41
1	A	423	GLN	CA-C-N	8.89	128.49	119.24
1	A	423	GLN	C-N-CA	8.89	128.49	119.24
1	A	170	PRO	N-CA-C	6.74	118.92	110.70
1	A	118	GLU	N-CA-C	-6.73	102.48	111.96
1	A	486	THR	N-CA-CB	5.70	120.52	110.37
1	A	173	GLN	N-CA-C	5.57	122.66	110.80
1	A	226	TYR	CA-C-N	-5.27	115.81	119.66
1	A	226	TYR	C-N-CA	-5.27	115.81	119.66
1	A	316	VAL	N-CA-C	-5.27	106.55	111.45
1	A	114	ALA	CA-C-N	5.19	125.11	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	ALA	C-N-CA	5.19	125.11	119.76
1	A	383	THR	N-CA-C	-5.11	107.21	113.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	442	ARG	Sidechain

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	4757	0	4645	102	0
2	B	28	0	25	0	0
3	A	28	0	26	0	0
4	A	1	0	0	0	0
5	A	43	0	30	8	0
6	A	9	0	0	1	0
7	A	4	0	6	2	0
8	A	14	0	9	14	0
9	A	290	0	0	0	0
All	All	5174	0	4741	108	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 11.

All (108) 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:167:CYS:HB3	1:A:168:PRO:HD2	1.29	1.14
1:A:202:ARG:HG3	1:A:202:ARG:HH11	1.10	1.08
1:A:167:CYS:CB	1:A:168:PRO:HD2	1.85	1.06
1:A:360:ARG:NH1	1:A:360:ARG:HG3	1.63	1.05
1:A:360:ARG:HG3	1:A:360:ARG:HH11	0.87	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLU:HB3	1:A:198:SEP:O2P	1.67	0.94
1:A:167:CYS:HB3	1:A:168:PRO:CD	1.98	0.93
1:A:360:ARG:HH11	1:A:360:ARG:CG	1.79	0.92
1:A:202:ARG:HG3	1:A:202:ARG:NH1	1.86	0.87
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.09	0.87
1:A:3:GLU:HB3	1:A:6:CYS:HB2	1.59	0.84
1:A:227:PRO:HD3	1:A:267:THR:HG23	1.60	0.84
1:A:198:SEP:O	1:A:202:ARG:HG2	1.78	0.83
1:A:52:GLU:HB3	1:A:57:VAL:HG12	1.60	0.83
1:A:125:SER:HA	1:A:128:GLN:HB3	1.61	0.82
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.28	0.82
1:A:202:ARG:HH11	1:A:202:ARG:CG	1.94	0.78
1:A:261:LEU:O	1:A:265:VAL:HG23	1.83	0.78
1:A:167:CYS:CB	1:A:168:PRO:CD	2.56	0.76
1:A:407:MET:HB3	1:A:501:MET:CE	2.18	0.73
1:A:102:GLN:HG2	1:A:265:VAL:HG21	1.73	0.71
1:A:301:GLY:O	1:A:305:GLN:HG3	1.88	0.71
1:A:594:GLU:HG3	1:A:595:ASN:HD22	1.56	0.70
5:A:1001:HEM:C2A	8:A:610:MZZ:H2	2.26	0.70
1:A:102:GLN:CG	1:A:265:VAL:HG21	2.22	0.69
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.29	0.67
1:A:187:LEU:HB3	1:A:305:GLN:HE21	1.60	0.66
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.72	0.66
1:A:255:ARG:HA	8:A:610:MZZ:H20	1.78	0.64
1:A:203:LEU:HD23	1:A:250:GLN:HE21	1.63	0.63
1:A:63:GLN:HG3	1:A:64:ARG:H	1.64	0.63
1:A:258:GLU:HB2	8:A:610:MZZ:H5	1.81	0.62
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.84	0.60
1:A:106:ILE:HG23	1:A:191:LEU:HD21	1.84	0.60
1:A:424:PRO:O	6:A:604:IOD:I	2.90	0.59
1:A:237:CYS:HA	1:A:381:PHE:O	2.02	0.59
1:A:52:GLU:CB	1:A:57:VAL:HG12	2.30	0.59
1:A:150:LYS:HD2	1:A:158:MET:HE2	1.84	0.58
1:A:197:PRO:HD2	1:A:198:SEP:O2P	2.04	0.58
1:A:392:ILE:HG23	1:A:396:VAL:CG2	2.34	0.57
1:A:258:GLU:CB	8:A:610:MZZ:H5	2.37	0.54
5:A:1001:HEM:C1A	8:A:610:MZZ:H2	2.42	0.53
5:A:1001:HEM:C2A	8:A:610:MZZ:C2	2.91	0.53
1:A:199:LEU:HA	1:A:202:ARG:HG3	1.92	0.52
1:A:255:ARG:HA	8:A:610:MZZ:C20	2.39	0.52
1:A:117:THR:HG23	1:A:117:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:SEP:O	1:A:202:ARG:CG	2.55	0.51
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.45	0.51
1:A:257:SER:O	1:A:381:PHE:HA	2.11	0.50
1:A:240:ILE:HG12	1:A:381:PHE:O	2.12	0.50
1:A:255:ARG:CB	8:A:610:MZZ:H20	2.42	0.49
1:A:166:VAL:HG13	1:A:167:CYS:N	2.28	0.49
1:A:66:THR:HB	1:A:70:PHE:N	2.28	0.49
1:A:242:THR:O	1:A:242:THR:HG22	2.14	0.48
1:A:424:PRO:HG2	8:A:610:MZZ:H17	1.95	0.48
1:A:169:THR:N	1:A:170:PRO:CD	2.76	0.48
1:A:255:ARG:CA	8:A:610:MZZ:H20	2.43	0.48
1:A:343:PHE:CG	1:A:518:GLN:HG2	2.49	0.48
1:A:106:ILE:HD11	1:A:265:VAL:HB	1.95	0.48
1:A:102:GLN:HG3	1:A:265:VAL:HG21	1.95	0.47
1:A:392:ILE:HG23	1:A:396:VAL:HG23	1.96	0.47
1:A:400:LEU:HD21	1:A:553:ILE:CD1	2.44	0.47
1:A:551:ARG:HD3	1:A:583:ASP:O	2.15	0.47
1:A:123:GLU:HB3	1:A:126:LYS:HG3	1.97	0.47
1:A:159:PRO:HD2	1:A:431:PHE:CE2	2.50	0.47
1:A:255:ARG:HG2	8:A:610:MZZ:H20	1.97	0.46
1:A:360:ARG:NH1	1:A:360:ARG:CG	2.47	0.46
5:A:1001:HEM:C3A	8:A:610:MZZ:C2	2.99	0.46
1:A:350:GLY:HA3	5:A:1001:HEM:CBC	2.45	0.46
5:A:1001:HEM:NA	8:A:610:MZZ:N7	2.64	0.45
1:A:468:GLN:HG2	1:A:474:LYS:HA	1.98	0.45
1:A:446:MET:HA	1:A:446:MET:HE2	1.98	0.45
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.51	0.45
1:A:361:LEU:O	1:A:397:ARG:HD2	2.16	0.45
1:A:276:LEU:O	1:A:280:LEU:HG	2.17	0.45
1:A:574:HIS:CD2	1:A:574:HIS:C	2.94	0.45
1:A:16:ASP:HB3	1:A:19:SER:HB2	1.98	0.44
1:A:166:VAL:HG23	1:A:180:ILE:HG12	1.99	0.44
1:A:170:PRO:CB	1:A:171:PRO:HD3	2.47	0.44
1:A:303:PHE:O	1:A:307:ILE:HG12	2.18	0.44
1:A:506:ARG:NH2	7:A:598:EDO:H22	2.33	0.44
1:A:102:GLN:HG2	1:A:265:VAL:CG2	2.45	0.44
1:A:109:HIS:NE2	8:A:610:MZZ:N7	2.65	0.43
1:A:108:ASP:OD2	1:A:108:ASP:C	2.62	0.43
5:A:1001:HEM:HMC2	5:A:1001:HEM:HBC2	2.00	0.43
1:A:347:PHE:C	1:A:349:PHE:H	2.27	0.43
1:A:199:LEU:HA	1:A:202:ARG:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLN:HG3	1:A:64:ARG:N	2.33	0.42
1:A:203:LEU:HD11	1:A:252:GLY:HA2	2.02	0.42
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.84	0.42
1:A:349:PHE:CD1	1:A:349:PHE:C	2.98	0.42
1:A:351:HIS:CE1	1:A:433:LEU:HD21	2.55	0.42
1:A:58:PRO:HG2	1:A:61:TRP:HB2	2.01	0.42
1:A:196:GLU:CB	1:A:198:SEP:O2P	2.55	0.41
1:A:144:PHE:HE2	1:A:158:MET:HE3	1.84	0.41
1:A:203:LEU:CD2	1:A:250:GLN:HE21	2.31	0.41
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.90	0.41
1:A:221:ASP:HB2	1:A:226:TYR:CE2	2.56	0.41
1:A:540:GLN:HG2	1:A:590:TRP:CE2	2.56	0.41
1:A:98:LEU:HD12	1:A:98:LEU:HA	1.87	0.41
1:A:400:LEU:HD13	1:A:563:PRO:HD3	2.03	0.41
1:A:305:GLN:O	1:A:309:PHE:HB2	2.20	0.40
1:A:95:ASN:HD22	7:A:598:EDO:H21	1.87	0.40
1:A:191:LEU:O	1:A:266:HIS:HE1	2.04	0.40
1:A:348:ARG:NH2	5:A:1001:HEM:HAD1	2.37	0.40
1:A:76:ARG:HH21	1:A:150:LYS:HG3	1.87	0.40
1:A:260:ILE:CD1	1:A:385:ARG:HB2	2.52	0.40
1:A:475:VAL:O	1:A:479:LYS:HG3	2.22	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%)	543 (92%)	43 (7%)	6 (1%)	13 15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	171	PRO
1	A	11	PRO
1	A	170	PRO
1	A	367	PRO
1	A	168	PRO

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	516/516 (100%)	489 (95%)	27 (5%)	19	28

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	14	THR
1	A	16	ASP
1	A	24	ILE
1	A	36	LEU
1	A	57	VAL
1	A	116	GLU
1	A	153	THR
1	A	166	VAL
1	A	191	LEU
1	A	202	ARG
1	A	232	VAL
1	A	264	THR
1	A	283	LEU
1	A	291	MET
1	A	322	GLN
1	A	333	ASN
1	A	352	MET
1	A	360	ARG
1	A	392	ILE
1	A	425	THR

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Mol	Chain	Res	Type
1	A	470	VAL
1	A	481	LEU
1	A	522	ILE
1	A	523	ARG
1	A	548	SER
1	A	550	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	250	GLN
1	A	266	HIS
1	A	305	GLN
1	A	322	GLN
1	A	333	ASN
1	A	403	ASN
1	A	429	HIS
1	A	460	GLN
1	A	497	ASN
1	A	545	GLN
1	A	595	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	1.42	1 (12%)	7,12,14	2.49	5 (71%)

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	-	0/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O1P	2.71	1.58	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O3P-P-OG	4.60	118.67	106.67
1	A	198	SEP	O3P-P-O1P	-2.48	101.19	110.83
1	A	198	SEP	OG-CB-CA	2.24	110.32	108.14
1	A	198	SEP	O2P-P-OG	-2.23	100.85	106.67
1	A	198	SEP	OG-P-O1P	2.22	112.43	106.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	5	0

5.5 Carbohydrates [i](#)

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	0.68	0	17,19,21	1.01	1 (5%)
2	NAG	B	2	2	14,14,15	0.69	0	17,19,21	1.53	3 (17%)

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	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	3.07	116.30	112.19
2	B	2	NAG	C3-C4-C5	2.52	114.79	110.23
2	B	2	NAG	O5-C1-C2	-2.47	107.46	111.29
2	B	1	NAG	O5-C1-C2	-2.40	107.58	111.29

There are no chirality outliers.

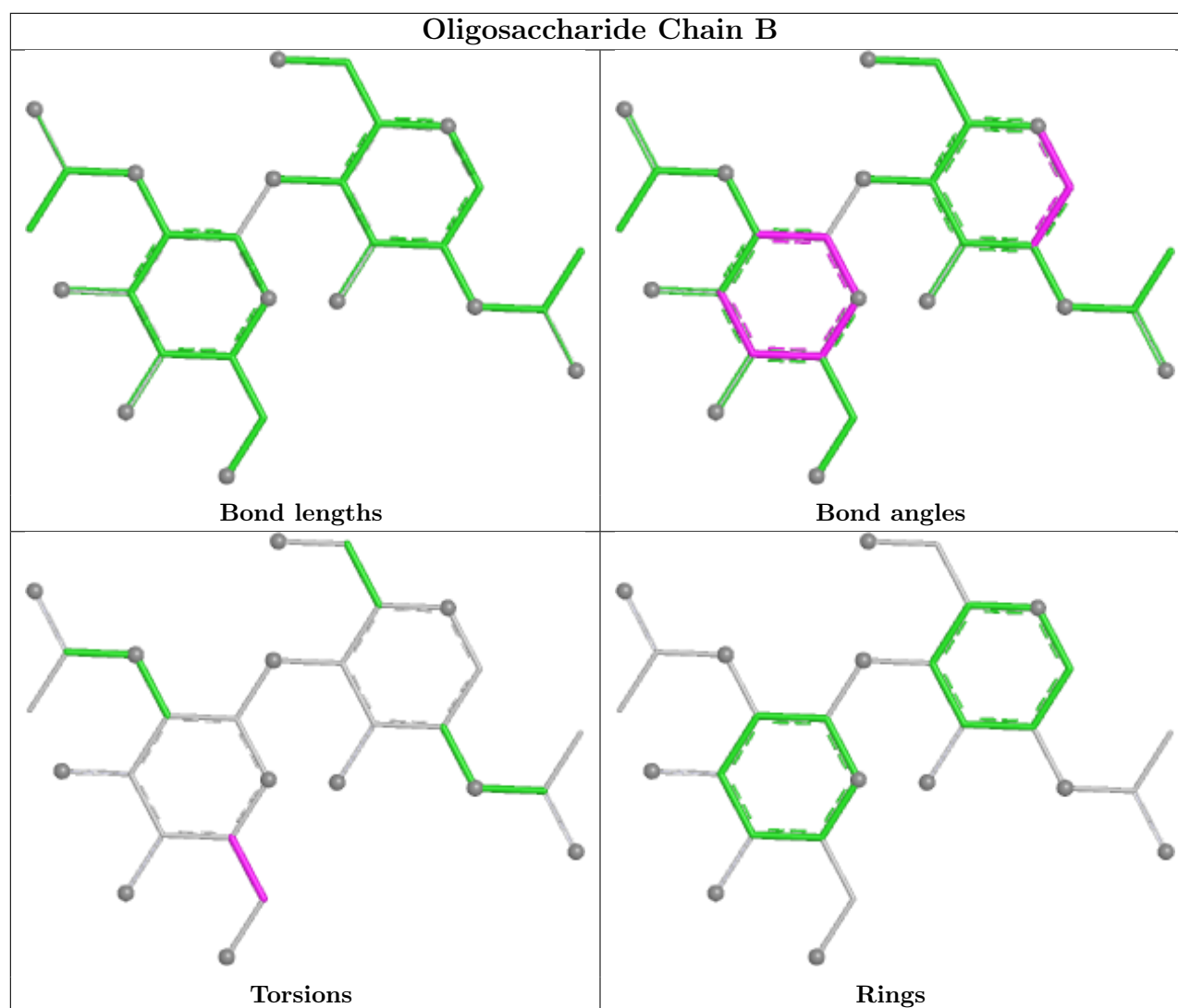
All (2) torsion outliers are listed below:

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

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 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 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	NAG	A	596	1	14,14,15	0.52	0	17,19,21	2.74	5 (29%)
5	HEM	A	1001	1	42,50,50	1.85	5 (11%)	46,82,82	1.67	15 (32%)
7	EDO	A	598	-	3,3,3	0.20	0	2,2,2	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	599	1	14,14,15	0.59	0	17,19,21	1.13	1 (5%)
8	MZZ	A	610	-	14,15,15	5.55	11 (78%)	16,20,20	5.19	11 (68%)

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	NAG	A	596	1	-	2/6/23/26	0/1/1/1
5	HEM	A	1001	1	-	2/12/54/54	-
7	EDO	A	598	-	-	0/1/1/1	-
3	NAG	A	599	1	-	0/6/23/26	0/1/1/1
8	MZZ	A	610	-	-	0/4/8/8	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	610	MZZ	C20-N9	-10.25	1.25	1.36
8	A	610	MZZ	C17-N9	-8.26	1.27	1.39
8	A	610	MZZ	C6-C1	-7.43	1.24	1.40
8	A	610	MZZ	O12-C8	7.23	1.41	1.23
5	A	1001	HEM	C3D-C2D	7.02	1.51	1.36
8	A	610	MZZ	C3-C4	-6.16	1.30	1.39
8	A	610	MZZ	C1-N7	6.04	1.59	1.38
8	A	610	MZZ	C3-C2	-4.86	1.31	1.38
8	A	610	MZZ	C5-C4	-3.92	1.33	1.39
8	A	610	MZZ	C6-C5	-3.83	1.32	1.38
8	A	610	MZZ	C2-C1	-3.77	1.32	1.40
5	A	1001	HEM	C3C-C2C	-3.68	1.35	1.40
5	A	1001	HEM	CAB-C3B	3.23	1.56	1.47
5	A	1001	HEM	C3C-CAC	3.17	1.54	1.47
8	A	610	MZZ	C20-N19	2.12	1.39	1.34
5	A	1001	HEM	C3C-C4C	2.07	1.44	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	610	MZZ	C4-C8-N9	14.42	133.00	118.50
3	A	596	NAG	C1-O5-C5	8.54	123.64	112.19
8	A	610	MZZ	C3-C2-C1	7.90	130.31	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	610	MZZ	C6-C1-C2	-6.11	108.97	118.16
8	A	610	MZZ	O12-C8-C4	-5.06	110.25	120.29
8	A	610	MZZ	C5-C4-C3	-4.84	112.41	118.57
8	A	610	MZZ	C5-C4-C8	4.76	131.01	120.28
8	A	610	MZZ	C5-C6-C1	3.66	125.13	120.66
5	A	1001	HEM	C4B-CHC-C1C	3.63	127.35	122.56
5	A	1001	HEM	C4D-ND-C1D	3.58	109.45	105.21
3	A	596	NAG	O5-C1-C2	3.49	116.69	111.29
3	A	596	NAG	C3-C4-C5	3.42	116.42	110.23
8	A	610	MZZ	C6-C5-C4	3.22	124.24	120.80
5	A	1001	HEM	CMB-C2B-C1B	3.06	129.82	125.03
3	A	596	NAG	O5-C5-C4	3.04	118.23	110.83
8	A	610	MZZ	C20-N9-C17	2.90	113.76	108.50
5	A	1001	HEM	CMD-C2D-C1D	2.84	129.48	125.03
8	A	610	MZZ	C6-C1-N7	2.65	125.78	120.90
5	A	1001	HEM	CMB-C2B-C3B	-2.61	122.10	128.43
5	A	1001	HEM	CBA-CAA-C2A	-2.53	108.29	112.54
3	A	596	NAG	C1-C2-N2	-2.50	106.49	110.43
5	A	1001	HEM	CBD-CAD-C3D	-2.44	105.80	112.53
3	A	599	NAG	C1-O5-C5	2.34	115.32	112.19
8	A	610	MZZ	C2-C1-N7	2.32	125.18	120.90
5	A	1001	HEM	C4A-C3A-C2A	2.31	108.60	107.00
5	A	1001	HEM	C4C-CHD-C1D	2.24	125.52	122.56
5	A	1001	HEM	C3B-C2B-C1B	2.22	108.08	106.41
5	A	1001	HEM	CMC-C2C-C3C	2.20	129.07	124.68
5	A	1001	HEM	CAD-CBD-CGD	-2.13	108.03	113.67
5	A	1001	HEM	C1D-C2D-C3D	-2.06	104.81	106.98
5	A	1001	HEM	CAD-C3D-C4D	2.03	128.24	124.70
5	A	1001	HEM	C2B-C1B-NB	-2.03	107.50	109.84

There are no chirality outliers.

All (4) torsion outliers are listed below:

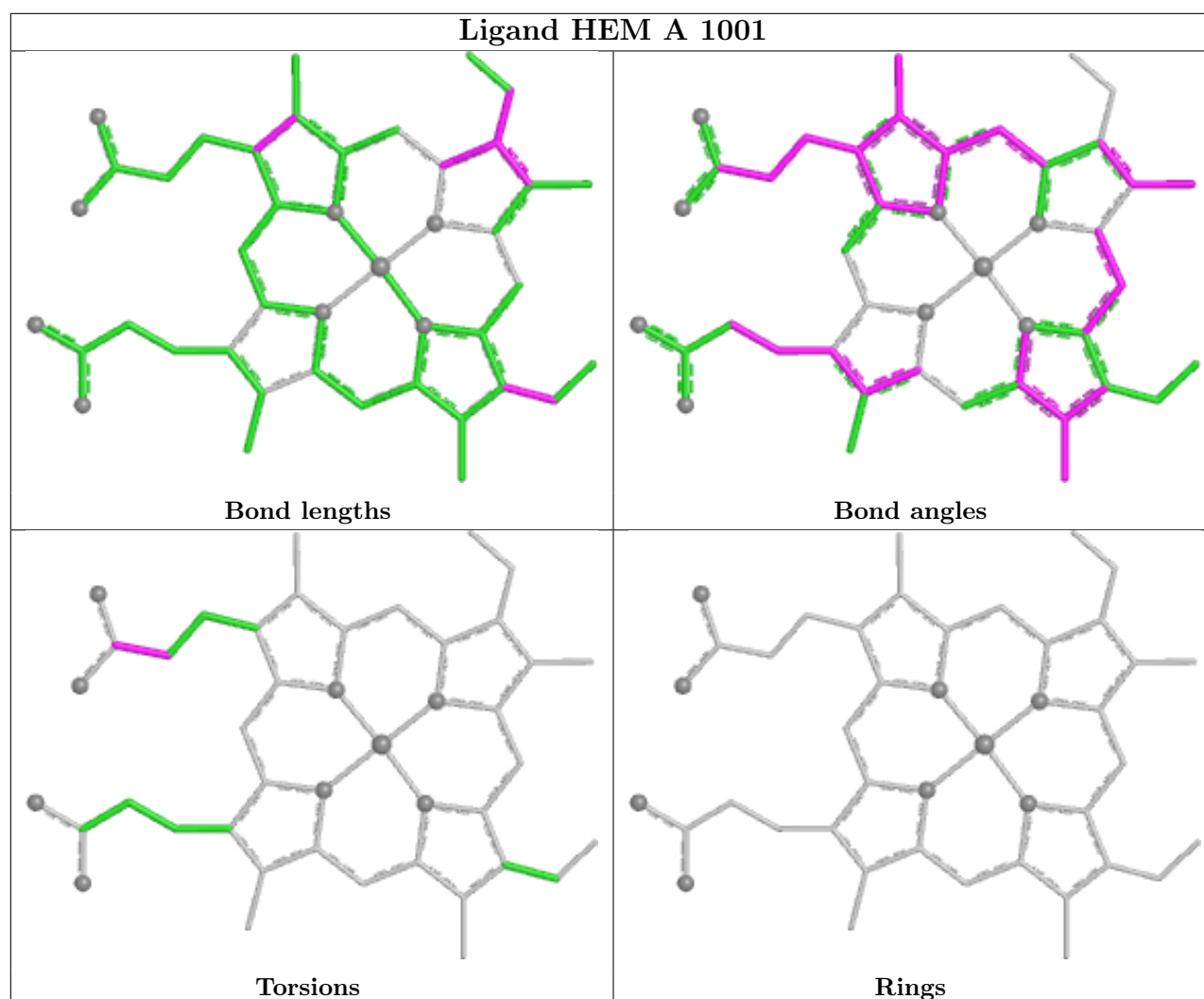
Mol	Chain	Res	Type	Atoms
3	A	596	NAG	O5-C5-C6-O6
3	A	596	NAG	C4-C5-C6-O6
5	A	1001	HEM	CAD-CBD-CGD-O1D
5	A	1001	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1001	HEM	8	0
7	A	598	EDO	2	0
8	A	610	MZZ	14	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%)	0.25	22 (3%)	45 47	24, 45, 81, 106	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	LEU	4.6
1	A	8	ALA	4.1
1	A	2	TRP	4.1
1	A	10	VAL	4.0
1	A	265	VAL	3.8
1	A	174	SER	3.4
1	A	544	LEU	3.4
1	A	11	PRO	2.8
1	A	4	VAL	2.6
1	A	169	THR	2.6
1	A	283	LEU	2.5
1	A	392	ILE	2.4
1	A	171	PRO	2.4
1	A	530	TRP	2.4
1	A	424	PRO	2.3
1	A	572	TYR	2.3
1	A	423	GLN	2.3
1	A	175	LEU	2.3
1	A	173	GLN	2.1
1	A	431	PHE	2.0
1	A	124	HIS	2.0
1	A	387	ILE	2.0

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

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

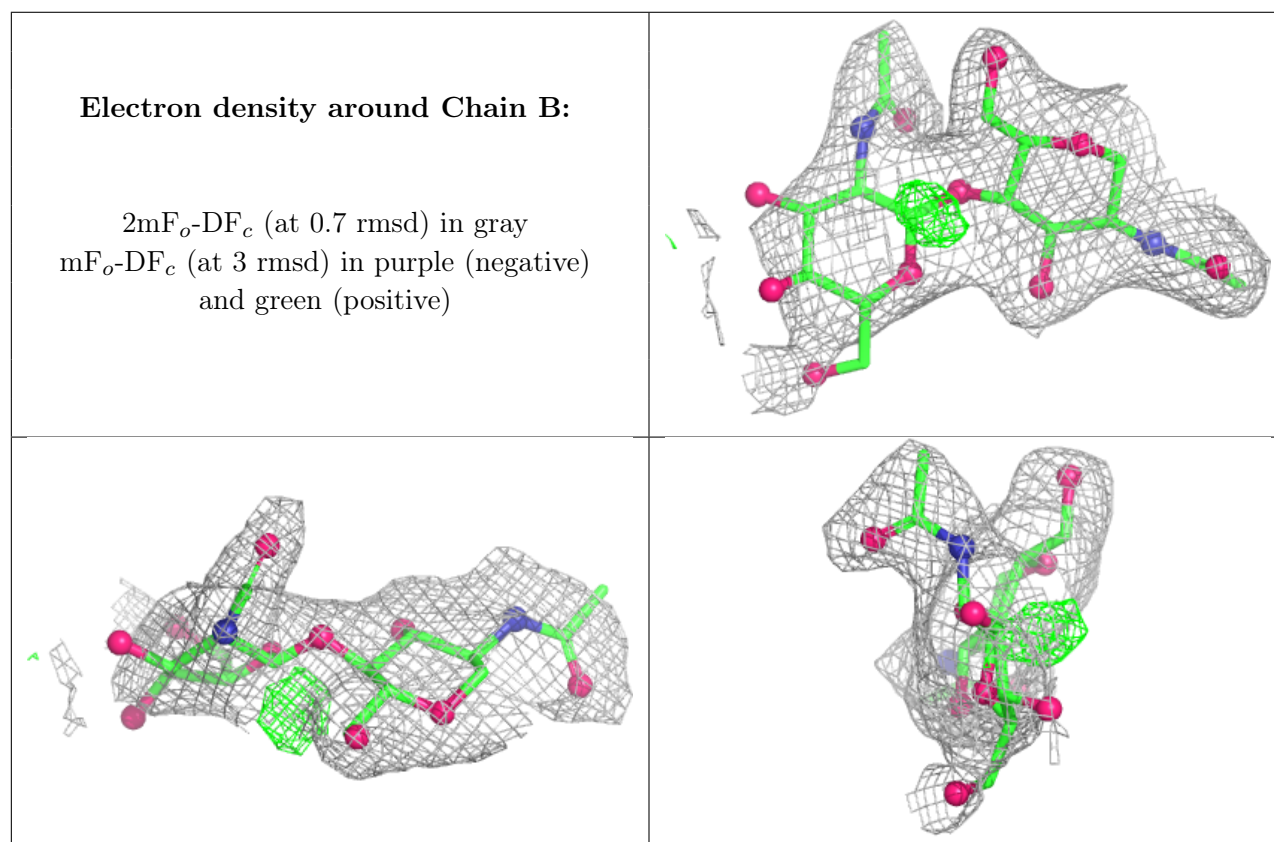
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	SEP	A	198	10/11	0.89	0.11	36,45,48,48	0

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(\AA^2)	Q<0.9
2	NAG	B	2	14/15	0.69	0.13	63,65,71,72	0
2	NAG	B	1	14/15	0.92	0.07	48,52,54,59	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

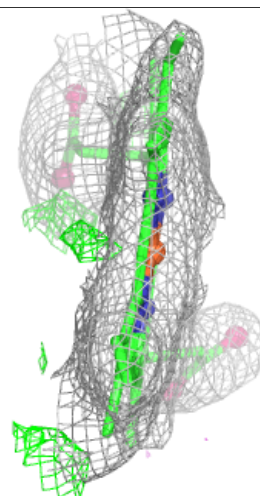
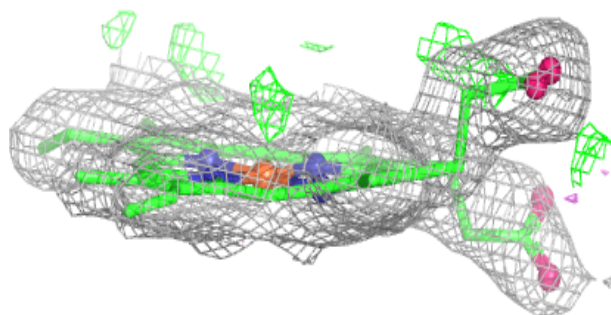
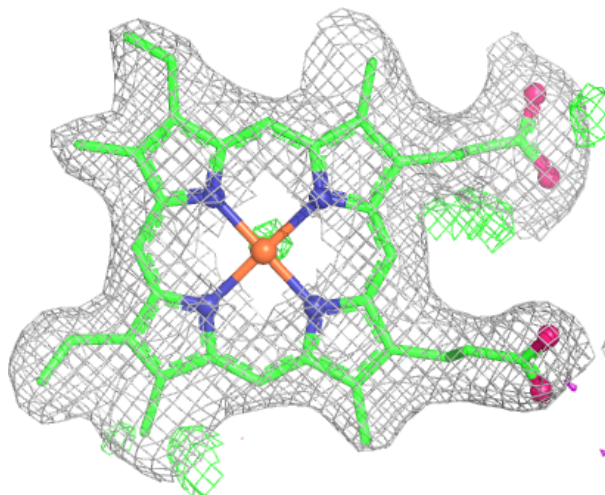
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	596	14/15	0.62	0.14	59,64,69,70	0
6	IOD	A	604	1/1	0.67	0.19	40,40,40,40	1
7	EDO	A	598	4/4	0.68	0.17	32,34,39,39	0
3	NAG	A	599	14/15	0.75	0.12	65,66,69,72	0
8	MZZ	A	610	14/14	0.83	0.15	29,43,46,46	0
6	IOD	A	606	1/1	0.88	0.21	63,63,63,63	1
6	IOD	A	607	1/1	0.90	0.14	61,61,61,61	1
6	IOD	A	601	1/1	0.91	0.09	63,63,63,63	1
6	IOD	A	608	1/1	0.94	0.08	73,73,73,73	1
6	IOD	A	609	1/1	0.95	0.07	63,63,63,63	1
5	HEM	A	1001	43/43	0.97	0.08	21,26,32,38	0
6	IOD	A	600	1/1	0.97	0.22	40,40,40,40	1
6	IOD	A	605	1/1	0.97	0.20	49,49,49,49	1
4	CA	A	1000	1/1	0.99	0.02	34,34,34,34	0
6	IOD	A	597	1/1	0.99	0.14	17,17,17,17	1

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 1001:

$2mF_o-DF_c$ (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.