



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 06:00 AM EDT

PDB ID : 3RKE
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

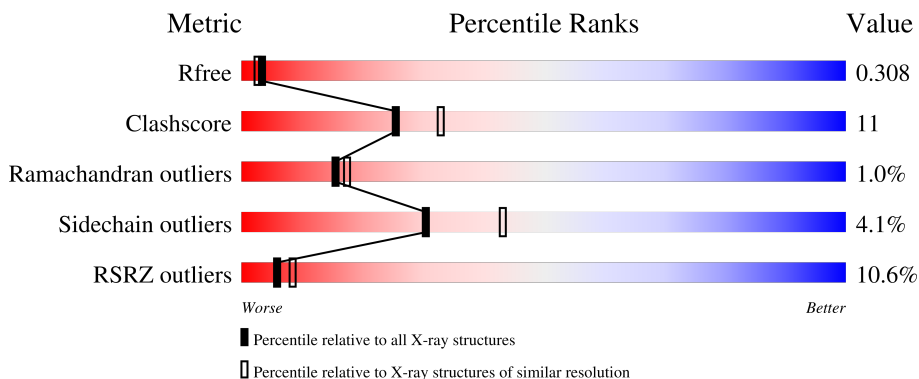
1 Overall quality at a glance

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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	
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	-
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.

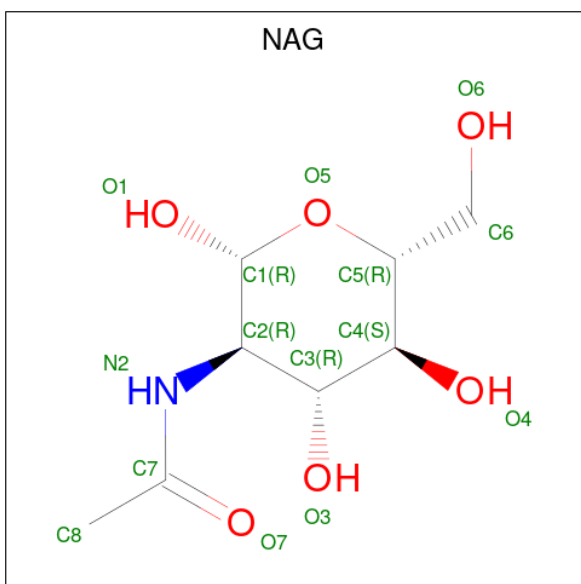
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	595	4757	3021	844	865	1	26	0	0	0

- 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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

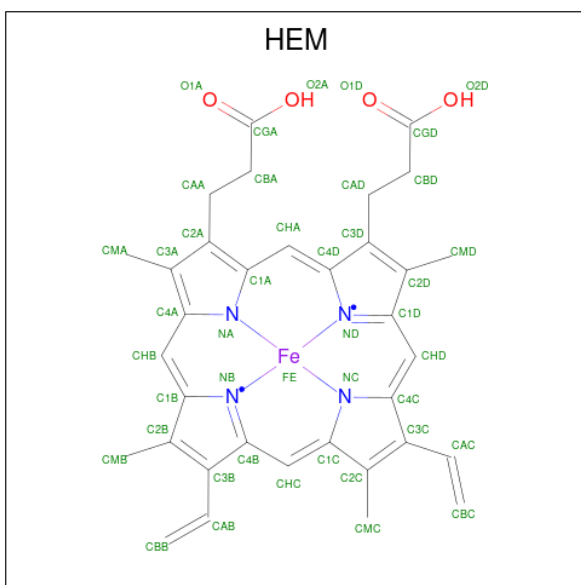


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (three-letter code: 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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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 (three-letter code: IOD) (formula: I).

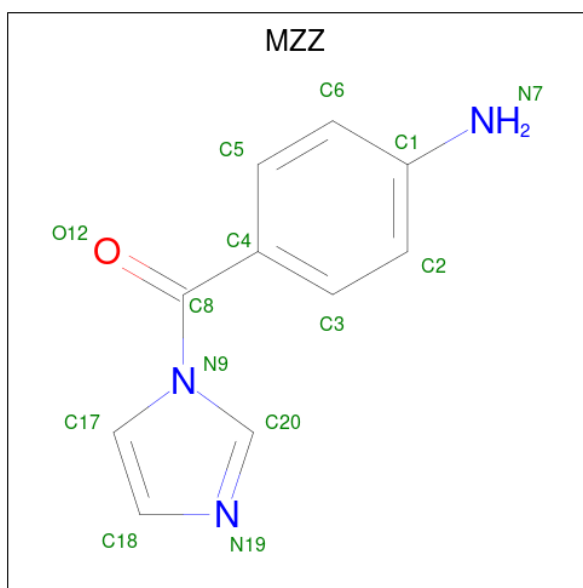
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	I	0	0
			9	9		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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 (three-letter code: 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		

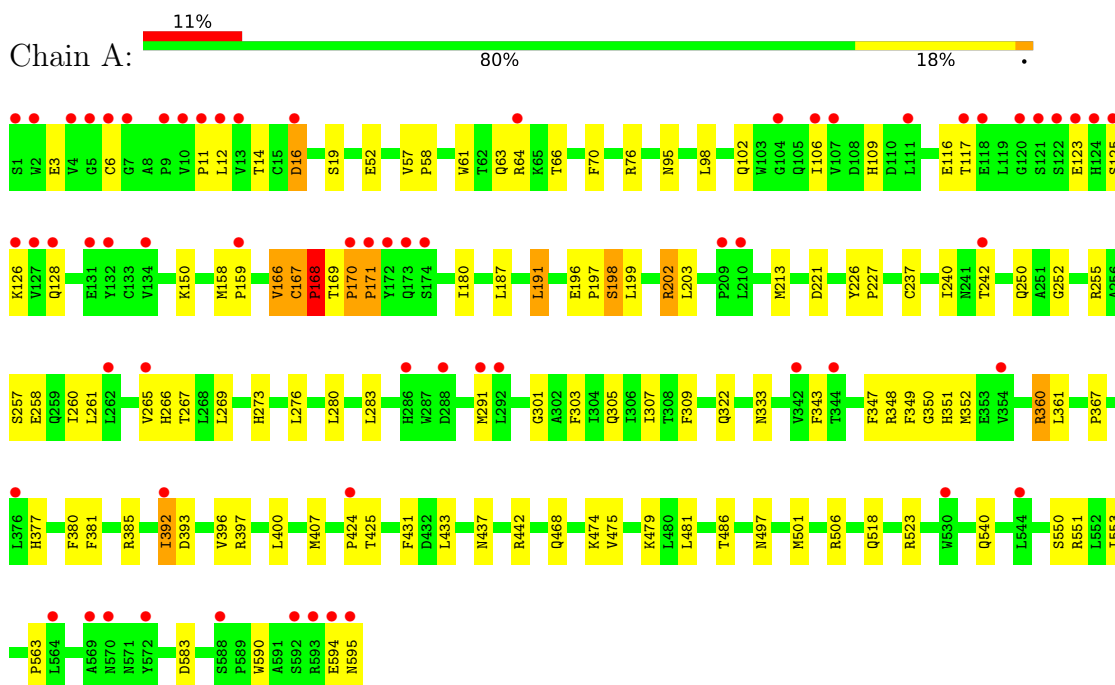
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	290	Total 290	O 290	0	0

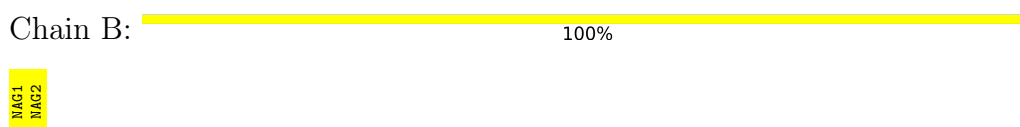
3 Residue-property plots i

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	53.98Å 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) 97.4 (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)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.245 , 0.263 0.236 , 0.308	Depositor DCC
R_{free} test set	1394 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtrriage
Anisotropy	0.894	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.58	0/4875	0.68	1/6621 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	486	THR	N-CA-CB	5.38	120.52	110.30

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 [i](#)

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	96	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	102	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 (102) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
5:A:1001:HEM:HMC2	5:A:1001:HEM:HBC2	2.00	0.43
1:A:199:LEU:HA	1:A:202:ARG:CG	2.48	0.43
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: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: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
1:A:150:LYS:HD2	1:A:158:MET:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	592/595 (100%)	543 (92%)	43 (7%)	6 (1%)	15 17

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	516/516 (100%)	495 (96%)	21 (4%)	30 43

All (21) 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	116	GLU
1	A	166	VAL

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Mol	Chain	Res	Type
1	A	168	PRO
1	A	191	LEU
1	A	202	ARG
1	A	283	LEU
1	A	291	MET
1	A	322	GLN
1	A	333	ASN
1	A	347	PHE
1	A	352	MET
1	A	360	ARG
1	A	392	ILE
1	A	393	ASP
1	A	425	THR
1	A	481	LEU
1	A	523	ARG
1	A	550	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	217	GLN
1	A	250	GLN
1	A	305	GLN
1	A	333	ASN
1	A	403	ASN
1	A	497	ASN
1	A	570	ASN
1	A	574	HIS
1	A	595	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	1.36	1 (12%)	8,12,14	2.36	5 (62%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	198	1	-	0/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O1P	2.59	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	4.48	118.67	106.73
1	A	198	SEP	O3P-P-O1P	-2.42	101.19	110.68
1	A	198	SEP	OG-CB-CA	2.24	110.32	108.14
1	A	198	SEP	O2P-P-OG	-2.21	100.85	106.73
1	A	198	SEP	OG-P-O1P	2.12	112.43	106.47

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	0.70	0	17,19,21	1.01	1 (5%)
2	NAG	B	2	2	14,14,15	0.71	1 (7%)	17,19,21	1.52	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	-2.10	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	3.03	116.30	112.19
2	B	2	NAG	C3-C4-C5	2.55	114.79	110.24
2	B	2	NAG	O5-C1-C2	-2.42	107.46	111.29
2	B	1	NAG	O5-C1-C2	-2.35	107.58	111.29

There are no chirality outliers.

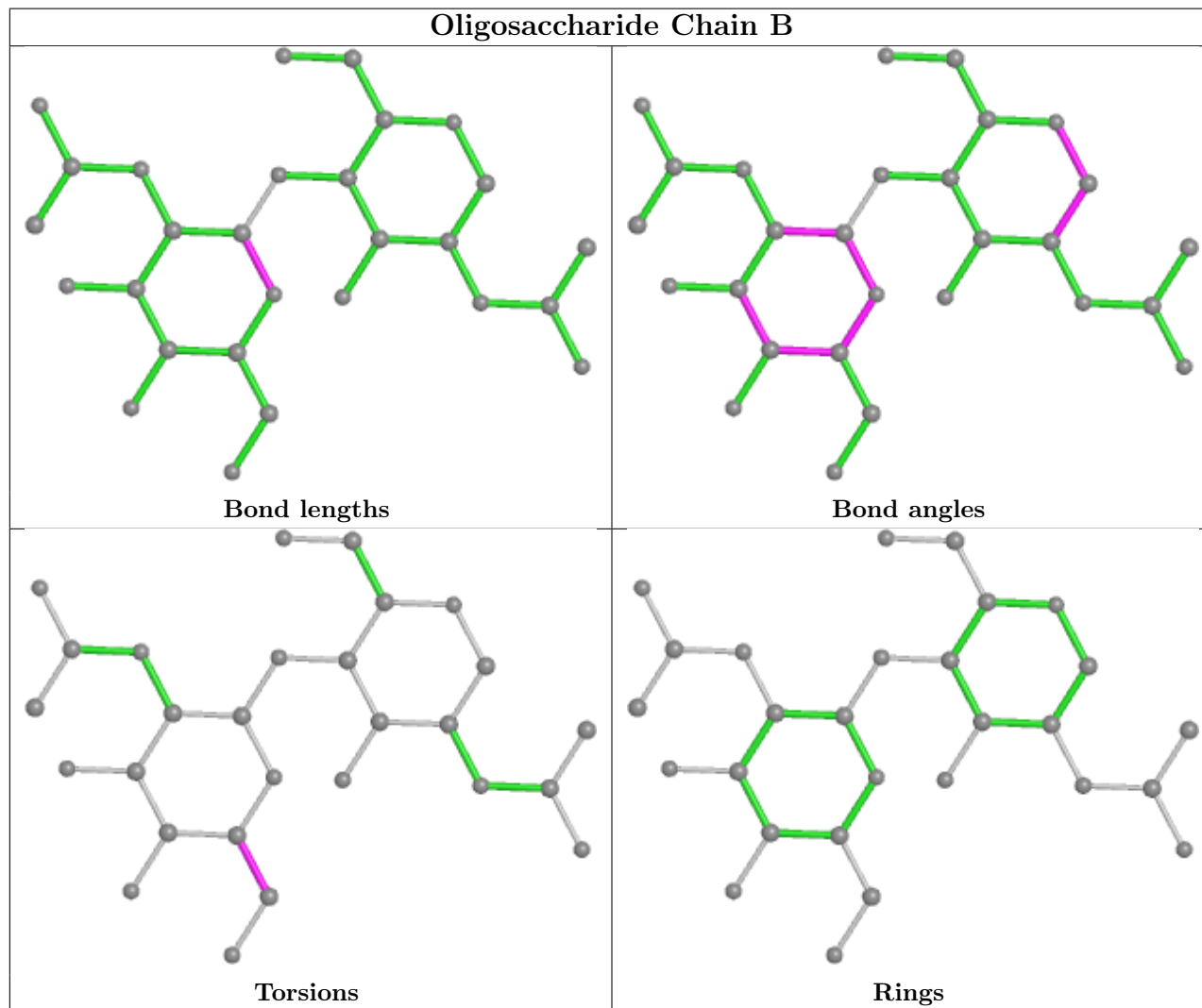
All (2) torsion outliers are listed below:

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	0.53	0	17,19,21	2.71	5 (29%)
7	EDO	A	598	-	3,3,3	0.21	0	2,2,2	1.17	0
5	HEM	A	1001	1	41,50,50	1.88	6 (14%)	45,82,82	1.74	15 (33%)
3	NAG	A	599	1	14,14,15	0.57	0	17,19,21	1.12	1 (5%)
8	MZZ	A	610	-	14,15,15	6.31	11 (78%)	16,20,20	5.10	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
7	EDO	A	598	-	-	0/1/1/1	-
5	HEM	A	1001	1	-	2/12/54/54	-
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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	610	MZZ	O12-C8	14.31	1.41	1.22
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	-7.20	1.24	1.40
5	A	1001	HEM	C3D-C2D	7.14	1.51	1.36
8	A	610	MZZ	C1-N7	6.09	1.59	1.38
8	A	610	MZZ	C3-C4	-5.38	1.30	1.39
8	A	610	MZZ	C3-C2	-4.29	1.31	1.38
8	A	610	MZZ	C2-C1	-3.65	1.32	1.40
5	A	1001	HEM	C3C-C2C	-3.59	1.35	1.40
5	A	1001	HEM	C3C-CAC	3.40	1.54	1.47
8	A	610	MZZ	C5-C4	-3.40	1.33	1.39
8	A	610	MZZ	C6-C5	-3.37	1.32	1.38
5	A	1001	HEM	CAB-C3B	3.15	1.56	1.47
5	A	1001	HEM	FE-NB	2.40	2.08	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	HEM	FE-ND	2.16	2.07	1.96
8	A	610	MZZ	C20-N19	2.10	1.39	1.34

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	8.45	123.64	112.19
8	A	610	MZZ	C3-C2-C1	7.49	130.31	120.67
8	A	610	MZZ	C6-C1-C2	-5.91	108.97	118.15
8	A	610	MZZ	O12-C8-C4	-5.12	110.25	120.23
8	A	610	MZZ	C5-C4-C8	4.98	131.01	120.26
8	A	610	MZZ	C5-C4-C3	-4.34	112.41	118.59
5	A	1001	HEM	C4D-ND-C1D	4.24	109.45	105.07
5	A	1001	HEM	C4B-CHC-C1C	3.63	127.35	122.56
8	A	610	MZZ	C5-C6-C1	3.47	125.13	120.67
3	A	596	NAG	C3-C4-C5	3.47	116.42	110.24
3	A	596	NAG	O5-C1-C2	3.42	116.69	111.29
5	A	1001	HEM	CMB-C2B-C1B	3.14	129.82	125.04
3	A	596	NAG	O5-C5-C4	3.04	118.23	110.83
8	A	610	MZZ	C6-C5-C4	2.97	124.24	120.78
5	A	1001	HEM	CMD-C2D-C1D	2.91	129.48	125.04
8	A	610	MZZ	C20-N9-C17	2.90	113.76	108.50
8	A	610	MZZ	C6-C1-N7	2.61	125.78	120.91
5	A	1001	HEM	CAD-CBD-CGD	-2.59	108.03	113.60
5	A	1001	HEM	CBA-CAA-C2A	-2.54	108.29	112.62
5	A	1001	HEM	CMB-C2B-C3B	-2.53	122.10	128.30
5	A	1001	HEM	CBD-CAD-C3D	-2.46	105.80	112.63
5	A	1001	HEM	CMC-C2C-C3C	2.35	129.07	124.68
3	A	596	NAG	C1-C2-N2	-2.34	106.49	110.49
3	A	599	NAG	C1-O5-C5	2.31	115.32	112.19
5	A	1001	HEM	C4A-C3A-C2A	2.31	108.60	107.00
8	A	610	MZZ	C2-C1-N7	2.29	125.18	120.91
5	A	1001	HEM	C4C-CHD-C1D	2.24	125.52	122.56
5	A	1001	HEM	C3B-C2B-C1B	2.14	108.08	106.49
5	A	1001	HEM	C1B-NB-C4B	2.13	107.27	105.07
5	A	1001	HEM	CAD-C3D-C4D	2.05	128.24	124.66
5	A	1001	HEM	C1D-C2D-C3D	-2.04	104.81	106.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

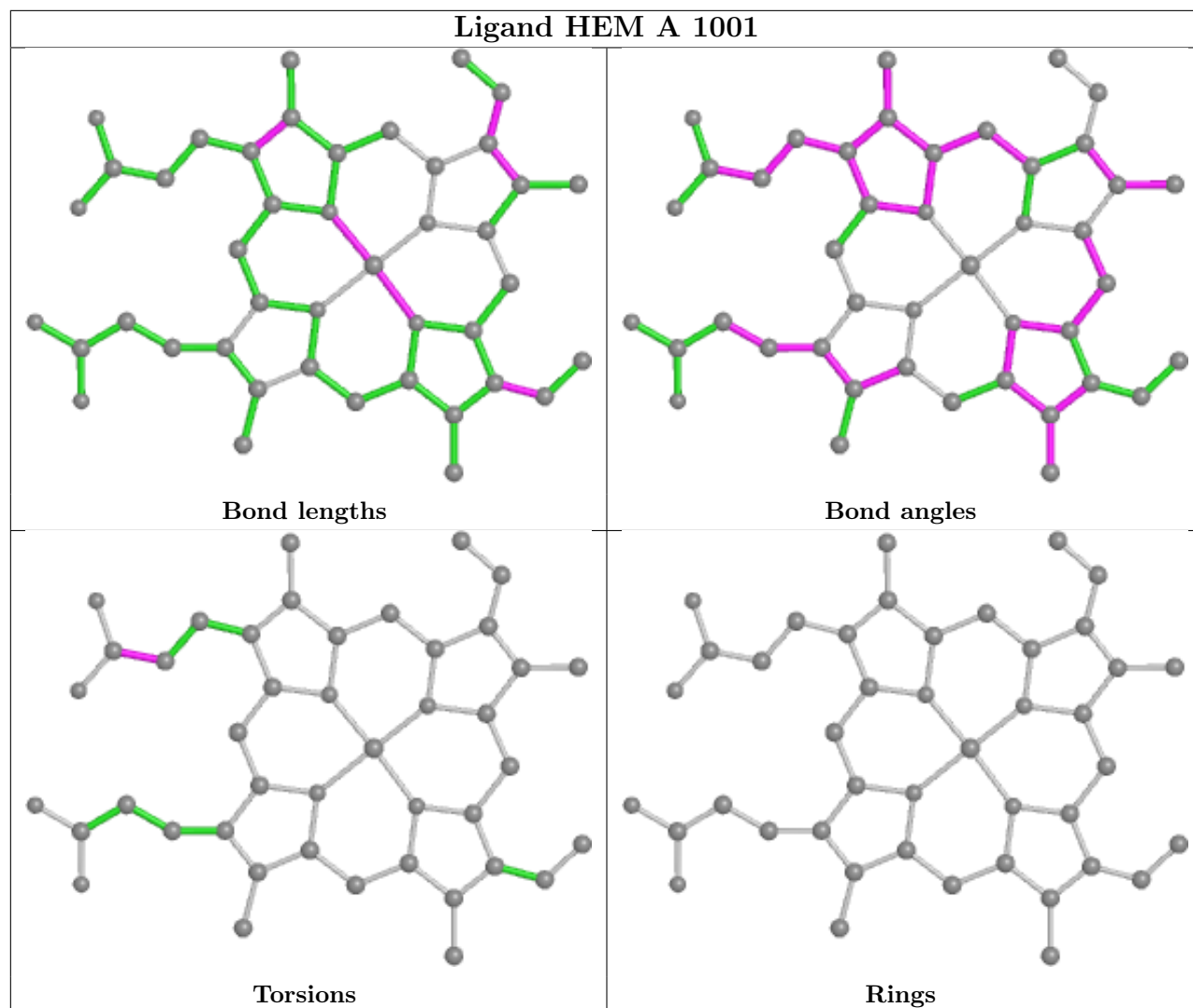
Mol	Chain	Res	Type	Atoms
3	A	596	NAG	O5-C5-C6-O6
3	A	596	NAG	C4-C5-C6-O6
5	A	1001	HEM	CAD-CBD-CGD-O2D
5	A	1001	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	598	EDO	2	0
5	A	1001	HEM	8	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%)	0.59	63 (10%) 6 8	24, 45, 81, 106	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	LEU	12.2
1	A	7	GLY	10.2
1	A	120	GLY	8.9
1	A	593	ARG	8.1
1	A	595	ASN	8.0
1	A	10	VAL	7.4
1	A	2	TRP	7.3
1	A	174	SER	6.7
1	A	4	VAL	6.1
1	A	594	GLU	5.9
1	A	121	SER	5.9
1	A	124	HIS	5.8
1	A	544	LEU	5.5
1	A	13	VAL	5.3
1	A	173	GLN	4.9
1	A	172	TYR	4.7
1	A	5	GLY	4.5
1	A	1	SER	4.4
1	A	170	PRO	4.3
1	A	122	SER	4.2
1	A	171	PRO	4.2
1	A	11	PRO	4.1
1	A	6	CYS	3.9
1	A	111	LEU	3.8
1	A	292	LEU	3.5
1	A	131	GLU	3.3
1	A	125	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	132	TYR	3.1
1	A	64	ARG	3.1
1	A	354	VAL	3.0
1	A	209	PRO	3.0
1	A	288	ASP	3.0
1	A	123	GLU	2.9
1	A	592	SER	2.9
1	A	9	PRO	2.9
1	A	569	ALA	2.8
1	A	265	VAL	2.8
1	A	118	GLU	2.7
1	A	376	LEU	2.6
1	A	107	VAL	2.6
1	A	242	THR	2.5
1	A	262	LEU	2.5
1	A	564	LEU	2.5
1	A	127	VAL	2.5
1	A	106	ILE	2.5
1	A	588	SER	2.4
1	A	134	VAL	2.4
1	A	286	HIS	2.4
1	A	159	PRO	2.3
1	A	128	GLN	2.3
1	A	117	THR	2.2
1	A	572	TYR	2.2
1	A	530	TRP	2.2
1	A	342	VAL	2.2
1	A	210	LEU	2.2
1	A	392	ILE	2.2
1	A	104	GLY	2.2
1	A	344	THR	2.1
1	A	16	ASP	2.1
1	A	570	ASN	2.1
1	A	291	MET	2.1
1	A	126	LYS	2.1
1	A	424	PRO	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.

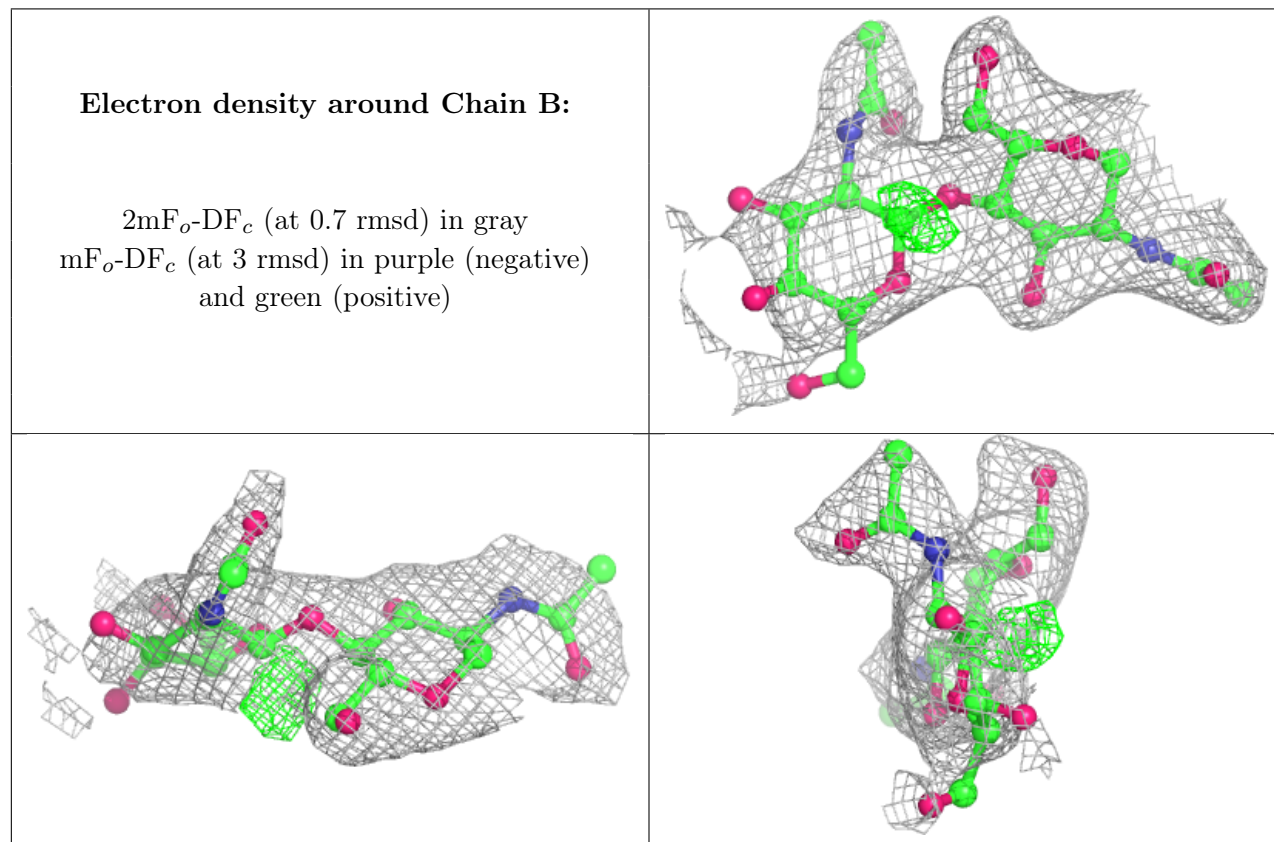
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	SEP	A	198	10/11	0.93	0.18	36,45,48,48	0

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	0.77	0.29	63,65,71,72	0
2	NAG	B	1	14/15	0.95	0.09	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.

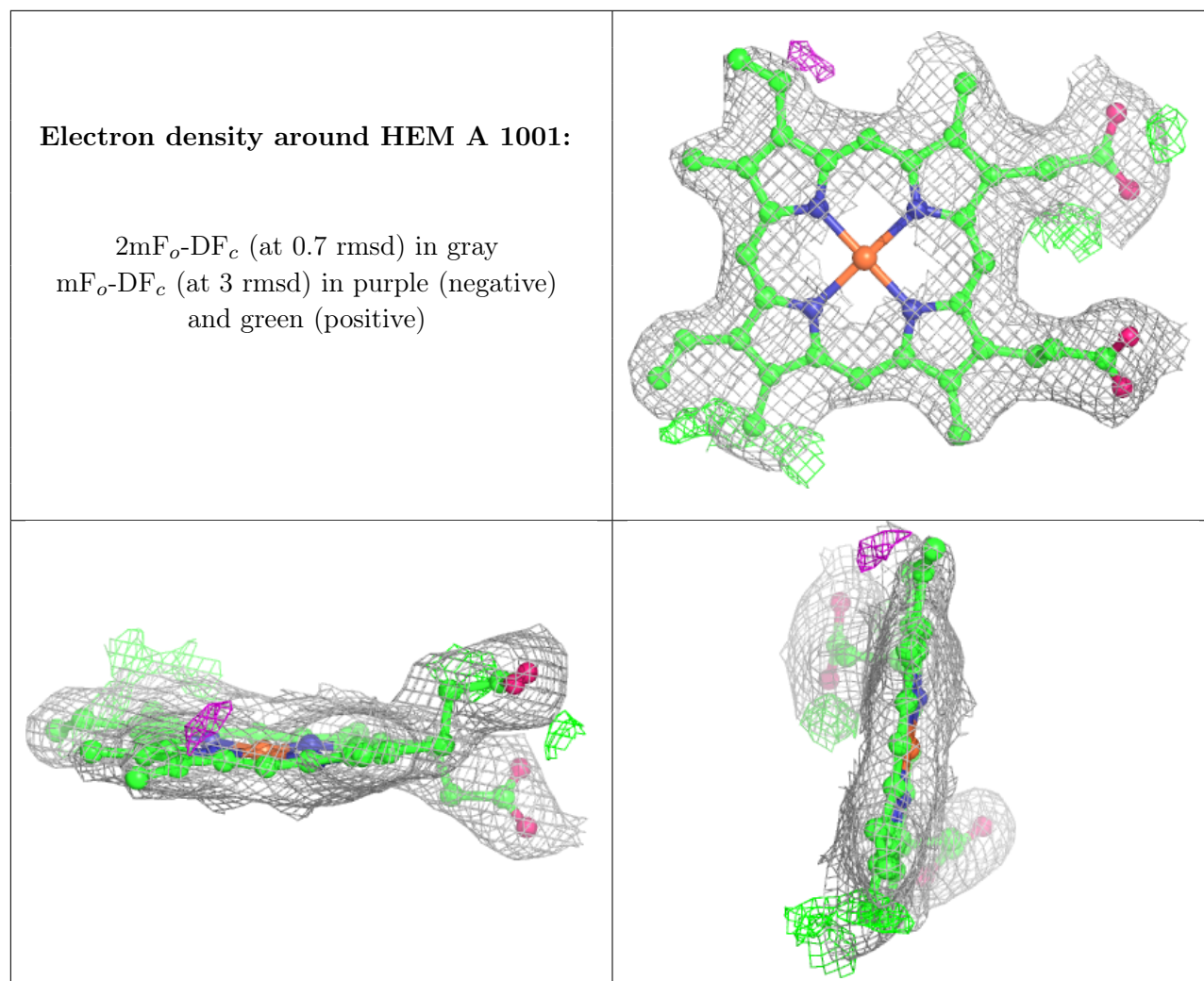


6.4 Ligands

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(Å ²)	Q<0.9
6	IOD	A	604	1/1	0.57	0.24	40,40,40,40	1
7	EDO	A	598	4/4	0.71	0.27	32,34,39,39	0
3	NAG	A	596	14/15	0.75	0.35	59,64,69,70	0
8	MZZ	A	610	14/14	0.82	0.28	29,43,46,46	0
6	IOD	A	606	1/1	0.83	0.23	63,63,63,63	1
3	NAG	A	599	14/15	0.89	0.12	65,66,69,72	0
6	IOD	A	608	1/1	0.92	0.12	73,73,73,73	1
6	IOD	A	607	1/1	0.93	0.19	61,61,61,61	1
6	IOD	A	601	1/1	0.94	0.13	63,63,63,63	1
6	IOD	A	609	1/1	0.96	0.12	63,63,63,63	1
6	IOD	A	605	1/1	0.96	0.28	49,49,49,49	1
5	HEM	A	1001	43/43	0.96	0.22	21,26,32,38	0
6	IOD	A	600	1/1	0.97	0.30	40,40,40,40	1
4	CA	A	1000	1/1	0.99	0.09	34,34,34,34	0
6	IOD	A	597	1/1	0.99	0.23	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.