



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 07:05 PM BST

PDB ID : 4OEK
Title : Crystal Structure of the Complex of goat Lactoperoxidase with Phenylethylamine at 2.47 Å Resolution
Authors : Kumar, M.; Singh, R.P.; Sinha, M.; Bhushan, A.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2014-01-13
Resolution : 2.47 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 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 : 2.13.1
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) : 2.13.1

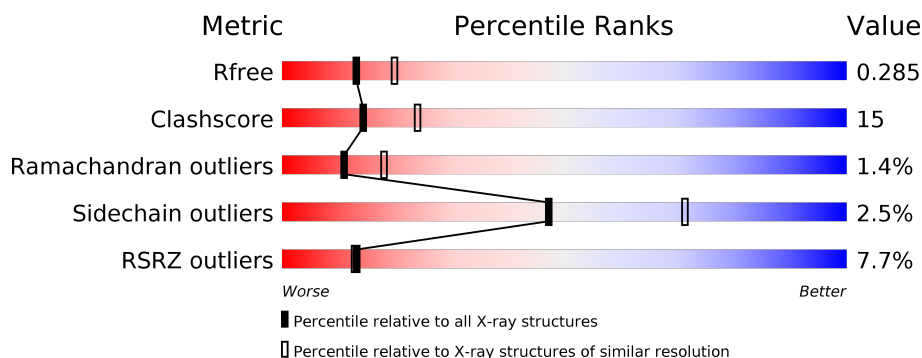
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 on 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
6	IOD	A	615	-	-	X	-
6	IOD	A	620	-	-	X	-
9	PEA	A	627	-	-	X	-

2 Entry composition [i](#)

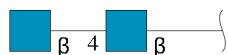
There are 10 unique types of molecules in this entry. The entry contains 5166 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

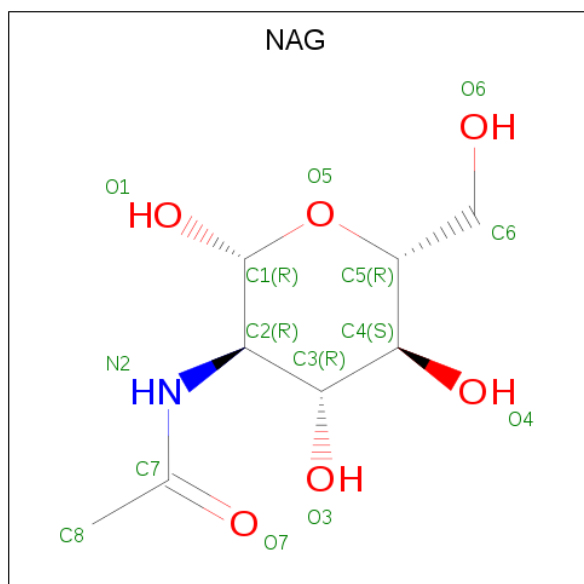
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4757	3021	844	865	1	26			

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



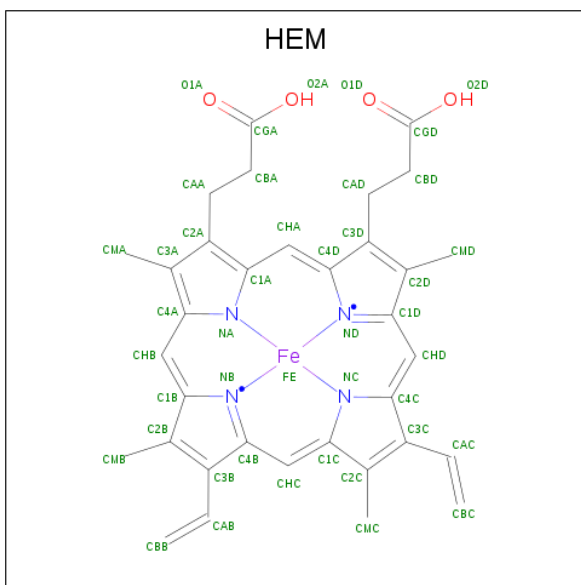
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

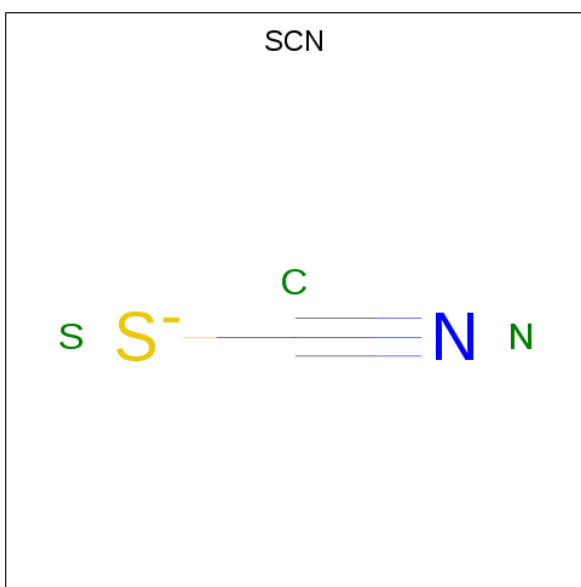
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is IODIDE ION (three-letter code: IOD) (formula: I).

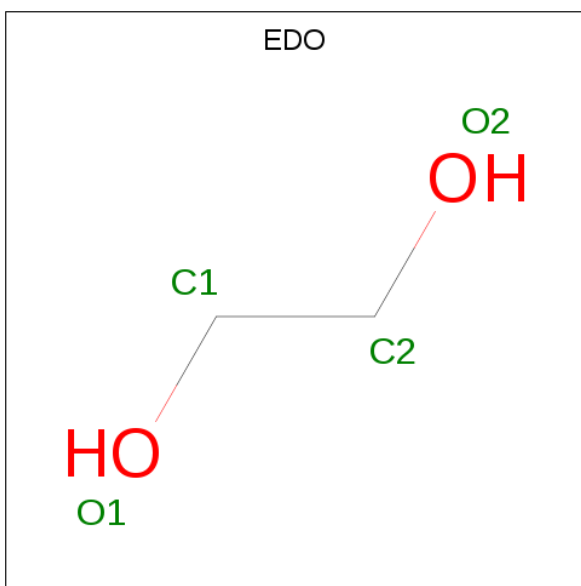
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	13	Total I 13 13	0	0

- Molecule 7 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



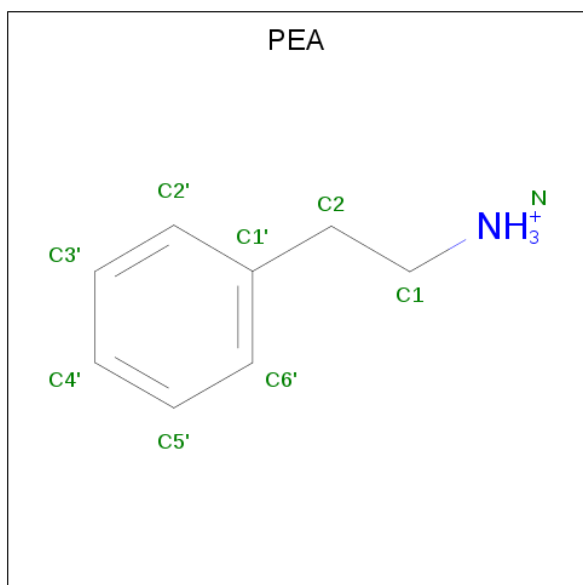
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 9 is 2-PHENYLETHYLAMINE (three-letter code: PEA) (formula: C₈H₁₂N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	N	0	0
			9	8	1		

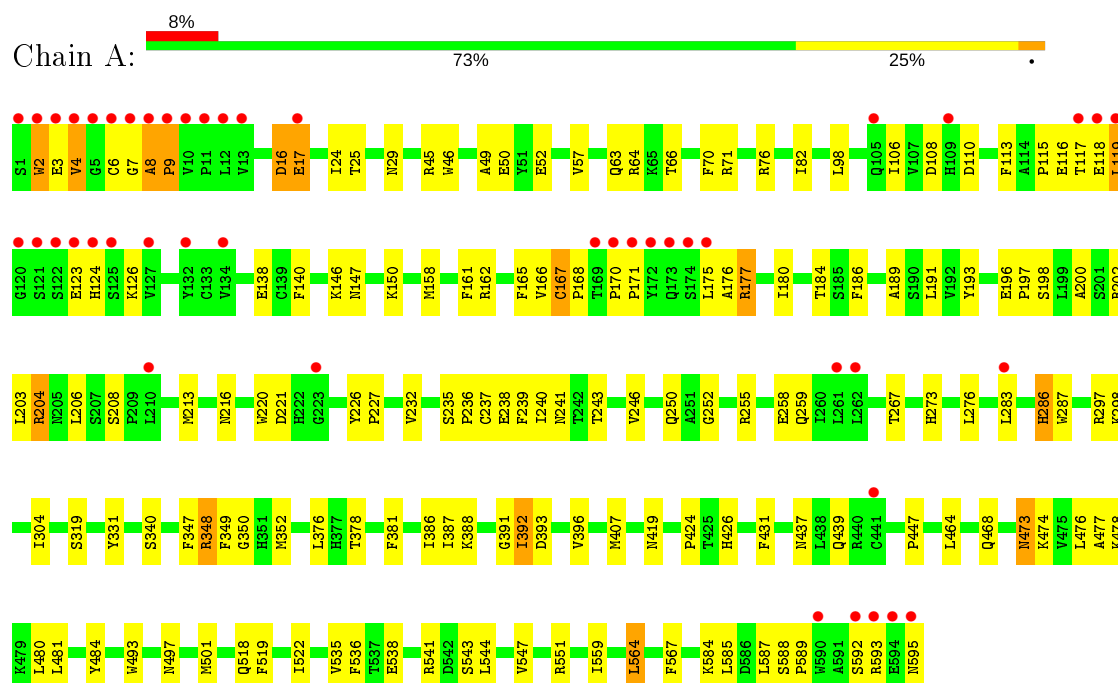
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	250	Total	O	0	0
			250	250		

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	53.17Å 79.89Å 75.28Å 90.00° 101.80° 90.00°	Depositor
Resolution (Å)	73.69 – 2.47 39.95 – 2.47	Depositor EDS
% Data completeness (in resolution range)	88.0 (73.69-2.47) 88.0 (39.95-2.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.43 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.204 , 0.281 0.208 , 0.285	Depositor DCC
R_{free} test set	995 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5166	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: SCN, NAG, SEP, CA, EDO, HEM, IOD, PEA

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	0.71	3/4875 (0.1%)	0.76	3/6621 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	ILE	C-N	8.39	1.53	1.34
1	A	241	ASN	C-N	-5.13	1.22	1.34
1	A	220	TRP	CD2-CE2	5.01	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	204	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	348	ARG	NE-CZ-NH1	5.13	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4643	144	0
2	B	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	42	0	39	0	0
4	A	43	0	30	15	0
5	A	1	0	0	0	0
6	A	13	0	0	7	0
7	A	3	0	0	0	0
8	A	20	0	30	3	0
9	A	9	0	12	13	0
10	A	250	0	0	11	0
All	All	5166	0	4779	150	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 15.

All (150) 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:258:GLU:OE2	4:A:606:HEM:CMB	1.73	1.36
1:A:108:ASP:OD2	4:A:606:HEM:CMD	1.76	1.32
6:A:616:IOD:I	10:A:719:HOH:O	2.36	1.13
1:A:258:GLU:OE2	4:A:606:HEM:HMB1	0.91	1.07
1:A:108:ASP:OD2	4:A:606:HEM:HMD1	0.82	0.99
1:A:108:ASP:CG	4:A:606:HEM:HMD1	1.86	0.94
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.57	0.87
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.09	0.82
10:A:761:HOH:O	2:B:2:NAG:O6	1.99	0.80
1:A:538:GLU:HG2	1:A:541:ARG:NH2	1.98	0.79
6:A:615:IOD:I	10:A:813:HOH:O	2.73	0.76
1:A:258:GLU:HG3	9:A:627:PEA:H6'	1.69	0.73
4:A:606:HEM:C4A	9:A:627:PEA:H12	2.25	0.72
1:A:255:ARG:HG2	9:A:627:PEA:H2'	1.70	0.72
1:A:258:GLU:CD	4:A:606:HEM:CMB	2.59	0.69
1:A:258:GLU:CD	4:A:606:HEM:HMB1	2.03	0.69
4:A:606:HEM:C3A	9:A:627:PEA:H12	2.28	0.68
1:A:473:ASN:ND2	1:A:476:LEU:H	1.92	0.68
1:A:538:GLU:HG2	1:A:541:ARG:HH22	1.57	0.67
1:A:258:GLU:HG3	9:A:627:PEA:H21	1.77	0.65
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.79	0.64
1:A:63:GLN:O	1:A:71:ARG:NH1	2.32	0.62
1:A:52:GLU:CG	1:A:57:VAL:HG12	2.29	0.62
1:A:123:GLU:HB3	1:A:126:LYS:HB2	1.81	0.62
1:A:167:CYS:CB	1:A:168:PRO:CD	2.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:CG	9:A:627:PEA:H22	2.31	0.61
1:A:203:LEU:HB3	1:A:213:MET:CE	2.30	0.61
1:A:255:ARG:HB3	9:A:627:PEA:H22	1.82	0.60
1:A:2:TRP:CD1	1:A:175:LEU:HD13	2.36	0.60
1:A:567:PHE:HB2	6:A:615:IOD:I	2.72	0.60
1:A:203:LEU:HB3	1:A:213:MET:HE1	1.84	0.60
1:A:158:MET:HE1	1:A:431:PHE:HA	1.84	0.59
1:A:146:LYS:O	1:A:147:ASN:HB2	2.03	0.59
1:A:175:LEU:HD12	1:A:176:ALA:H	1.67	0.59
1:A:108:ASP:CG	4:A:606:HEM:CMD	2.60	0.59
1:A:258:GLU:CG	9:A:627:PEA:H6'	2.33	0.58
1:A:298:LYS:NZ	1:A:535:VAL:O	2.28	0.58
1:A:239:PHE:HB2	10:A:852:HOH:O	2.03	0.57
1:A:387:ILE:HG22	1:A:388:LYS:HG3	1.86	0.57
1:A:8:ALA:H	1:A:9:PRO:HD3	1.70	0.56
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.86	0.56
1:A:2:TRP:HB3	10:A:875:HOH:O	2.06	0.56
1:A:258:GLU:HG3	9:A:627:PEA:C6'	2.35	0.56
1:A:9:PRO:HG2	10:A:924:HOH:O	2.06	0.56
1:A:167:CYS:CB	1:A:168:PRO:HD3	2.36	0.56
1:A:348:ARG:HH11	1:A:437:ASN:HD22	1.53	0.55
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.88	0.55
1:A:197:PRO:HA	8:A:624:EDO:H12	1.89	0.55
1:A:200:ALA:O	1:A:204:ARG:HG3	2.05	0.55
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.42	0.55
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.88	0.54
1:A:170:PRO:HB2	1:A:171:PRO:HD2	1.89	0.53
1:A:119:LEU:HD12	1:A:138:GLU:HG3	1.90	0.53
1:A:407:MET:HG3	10:A:723:HOH:O	2.08	0.53
1:A:237:CYS:HA	1:A:381:PHE:O	2.08	0.53
1:A:206:LEU:C	10:A:861:HOH:O	2.47	0.53
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.91	0.53
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.44	0.52
1:A:16:ASP:OD1	1:A:16:ASP:C	2.47	0.52
1:A:66:THR:HB	1:A:70:PHE:N	2.25	0.51
1:A:63:GLN:HG3	1:A:71:ARG:HH12	1.74	0.51
1:A:7:GLY:O	1:A:8:ALA:HB2	2.10	0.51
1:A:386:ILE:CG2	1:A:392:ILE:HD13	2.40	0.50
1:A:518:GLN:O	1:A:522:ILE:HG23	2.11	0.50
1:A:25:THR:O	1:A:184:THR:HG22	2.10	0.50
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:CE2	1:A:115:PRO:HB3	2.48	0.49
4:A:606:HEM:HBC2	4:A:606:HEM:HMC1	1.93	0.49
1:A:45:ARG:CZ	1:A:49:ALA:HB2	2.42	0.49
1:A:287:TRP:CZ2	1:A:592:SER:HB2	2.48	0.49
1:A:255:ARG:CB	9:A:627:PEA:H22	2.42	0.49
1:A:165:PHE:CG	1:A:177:ARG:HD2	2.48	0.49
1:A:544:LEU:O	1:A:547:VAL:HG22	2.12	0.49
1:A:64:ARG:NH2	10:A:920:HOH:O	2.39	0.48
1:A:255:ARG:HG2	9:A:627:PEA:H22	1.95	0.48
1:A:216:ASN:HB2	1:A:227:PRO:O	2.14	0.47
1:A:376:LEU:HD13	10:A:942:HOH:O	2.13	0.47
1:A:393:ASP:HB3	1:A:559:ILE:HD11	1.94	0.47
1:A:246:VAL:HG22	8:A:625:EDO:H11	1.95	0.47
1:A:349:PHE:CD1	1:A:349:PHE:C	2.87	0.47
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.50	0.47
1:A:52:GLU:HG2	1:A:57:VAL:HG12	1.96	0.46
1:A:82:ILE:HD13	1:A:480:LEU:HD23	1.97	0.46
1:A:258:GLU:OE2	4:A:606:HEM:HMB2	1.98	0.46
1:A:140:PHE:CE2	1:A:439:GLN:HG3	2.50	0.46
1:A:276:LEU:HD21	1:A:585:LEU:HD23	1.96	0.46
1:A:170:PRO:CB	1:A:171:PRO:HD2	2.45	0.46
1:A:464:LEU:HA	1:A:481:LEU:HD12	1.98	0.46
1:A:473:ASN:HD22	1:A:473:ASN:C	2.18	0.46
1:A:349:PHE:CB	1:A:497:ASN:HD21	2.29	0.46
1:A:286:HIS:N	1:A:286:HIS:ND1	2.60	0.46
1:A:593:ARG:HA	1:A:593:ARG:NH1	2.31	0.46
1:A:8:ALA:HB3	1:A:167:CYS:O	2.16	0.45
1:A:162:ARG:CZ	1:A:177:ARG:NH2	2.80	0.45
1:A:197:PRO:HD2	6:A:620:IOD:I	2.86	0.45
1:A:113:PHE:CE1	1:A:255:ARG:HD3	2.51	0.45
1:A:350:GLY:HA3	4:A:606:HEM:CBC	2.45	0.45
1:A:119:LEU:HD12	1:A:138:GLU:CG	2.47	0.45
1:A:193:TYR:OH	1:A:297:ARG:HA	2.16	0.45
1:A:117:THR:HG22	1:A:119:LEU:H	1.82	0.45
1:A:468:GLN:HG2	1:A:477:ALA:HB3	1.98	0.45
1:A:474:LYS:O	1:A:478:LYS:HG3	2.17	0.45
1:A:352:MET:CB	1:A:407:MET:HG2	2.46	0.44
1:A:98:LEU:HD22	10:A:745:HOH:O	2.17	0.44
1:A:407:MET:HB3	1:A:501:MET:CE	2.48	0.44
1:A:76:ARG:HH22	1:A:419:ASN:ND2	2.16	0.44
1:A:378:THR:HG22	8:A:622:EDO:H12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:CD2	1:A:587:LEU:HD11	2.47	0.44
1:A:481:LEU:HA	1:A:484:TYR:O	2.17	0.44
1:A:165:PHE:CD2	1:A:177:ARG:HD2	2.52	0.44
1:A:203:LEU:HD11	1:A:252:GLY:HA2	1.99	0.44
1:A:519:PHE:HA	1:A:522:ILE:HG12	2.00	0.44
1:A:259:GLN:HG2	4:A:606:HEM:CBB	2.48	0.44
1:A:8:ALA:N	1:A:9:PRO:HD3	2.32	0.44
1:A:29:ASN:CB	1:A:186:PHE:CZ	3.01	0.44
1:A:7:GLY:O	1:A:8:ALA:CB	2.66	0.43
1:A:236:PRO:HB3	6:A:618:IOD:I	2.89	0.43
1:A:258:GLU:HG3	9:A:627:PEA:C2	2.45	0.43
1:A:117:THR:HG22	1:A:119:LEU:N	2.34	0.43
1:A:202:ARG:HE	1:A:250:GLN:CD	2.22	0.43
1:A:227:PRO:HD3	1:A:267:THR:HG23	2.01	0.43
1:A:258:GLU:OE2	4:A:606:HEM:C2B	2.62	0.42
1:A:392:ILE:O	1:A:396:VAL:HG23	2.19	0.42
1:A:221:ASP:OD1	1:A:391:GLY:HA3	2.20	0.42
1:A:3:GLU:O	1:A:4:VAL:C	2.58	0.42
1:A:232:VAL:O	1:A:232:VAL:HG23	2.19	0.42
1:A:407:MET:HB3	1:A:501:MET:HE3	2.02	0.42
1:A:146:LYS:O	1:A:147:ASN:CB	2.66	0.42
1:A:24:ILE:HA	1:A:24:ILE:HD13	1.80	0.42
1:A:352:MET:CE	1:A:493:TRP:CZ2	3.02	0.42
1:A:202:ARG:HG2	1:A:250:GLN:OE1	2.20	0.42
1:A:116:GLU:HG2	1:A:161:PHE:O	2.19	0.41
1:A:235:SER:HB3	1:A:238:GLU:OE2	2.20	0.41
1:A:158:MET:HE1	1:A:431:PHE:CA	2.49	0.41
1:A:196:GLU:HB3	6:A:620:IOD:I	2.90	0.41
1:A:16:ASP:O	1:A:17:GLU:CB	2.69	0.41
1:A:50:GLU:OE2	1:A:447:PRO:HB3	2.20	0.41
1:A:150:LYS:HE2	1:A:419:ASN:HD22	1.85	0.41
1:A:424:PRO:C	1:A:426:HIS:H	2.24	0.41
1:A:283:LEU:HD13	1:A:587:LEU:O	2.20	0.41
1:A:331:TYR:HE2	6:A:619:IOD:I	2.74	0.41
1:A:29:ASN:HB3	1:A:186:PHE:CZ	2.56	0.41
1:A:298:LYS:HG2	1:A:536:PHE:CZ	2.56	0.41
1:A:595:ASN:HD22	1:A:595:ASN:N	2.19	0.41
1:A:239:PHE:C	1:A:239:PHE:CD2	2.93	0.41
1:A:564:LEU:HA	1:A:564:LEU:HD12	1.90	0.41
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.86	0.40
1:A:193:TYR:O	1:A:200:ALA:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:CG1	1:A:180:ILE:HG12	2.52	0.40
1:A:255:ARG:HB3	9:A:627:PEA:C2	2.49	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%)	546 (92%)	38 (6%)	8 (1%)	11	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	119	LEU
1	A	167	CYS
1	A	2	TRP
1	A	17	GLU
1	A	9	PRO
1	A	319	SER
1	A	4	VAL

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%)	503 (98%)	13 (2%)	47 71

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	CYS
1	A	16	ASP
1	A	118	GLU
1	A	124	HIS
1	A	177	ARG
1	A	208	SER
1	A	243	THR
1	A	286	HIS
1	A	347	PHE
1	A	392	ILE
1	A	473	ASN
1	A	543	SER
1	A	564	LEU

Some 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	147	ASN
1	A	245	HIS
1	A	377	HIS
1	A	419	ASN
1	A	437	ASN
1	A	468	GLN
1	A	473	ASN
1	A	497	ASN
1	A	570	ASN
1	A	574	HIS
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	0.83	0	8,12,14	2.55	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	-	4/5/8/10	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	OG-CB-CA	3.80	111.84	108.14
1	A	198	SEP	O2P-P-OG	3.71	116.61	106.73
1	A	198	SEP	O3P-P-O1P	3.00	122.42	110.68
1	A	198	SEP	O3P-P-OG	-2.74	99.45	106.73
1	A	198	SEP	OG-P-O1P	-2.11	100.55	106.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	N-CA-CB-OG
1	A	198	SEP	CB-OG-P-O2P
1	A	198	SEP	CB-OG-P-O1P
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	1.11	1 (7%)	17,19,21	2.68	6 (35%)
2	NAG	B	2	2	14,14,15	0.91	1 (7%)	17,19,21	1.36	2 (11%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	O5-C1	-2.80	1.39	1.43
2	B	2	NAG	C1-C2	2.67	1.56	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	O5-C1-C2	-6.76	100.62	111.29
2	B	1	NAG	C2-N2-C7	4.43	129.21	122.90
2	B	1	NAG	C3-C4-C5	-4.28	102.60	110.24
2	B	1	NAG	C4-C3-C2	3.63	116.33	111.02
2	B	1	NAG	O7-C7-N2	2.78	127.06	121.95
2	B	1	NAG	O3-C3-C2	-2.51	104.27	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	O5-C1-C2	-2.46	107.41	111.29
2	B	2	NAG	O5-C5-C6	2.17	110.61	107.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

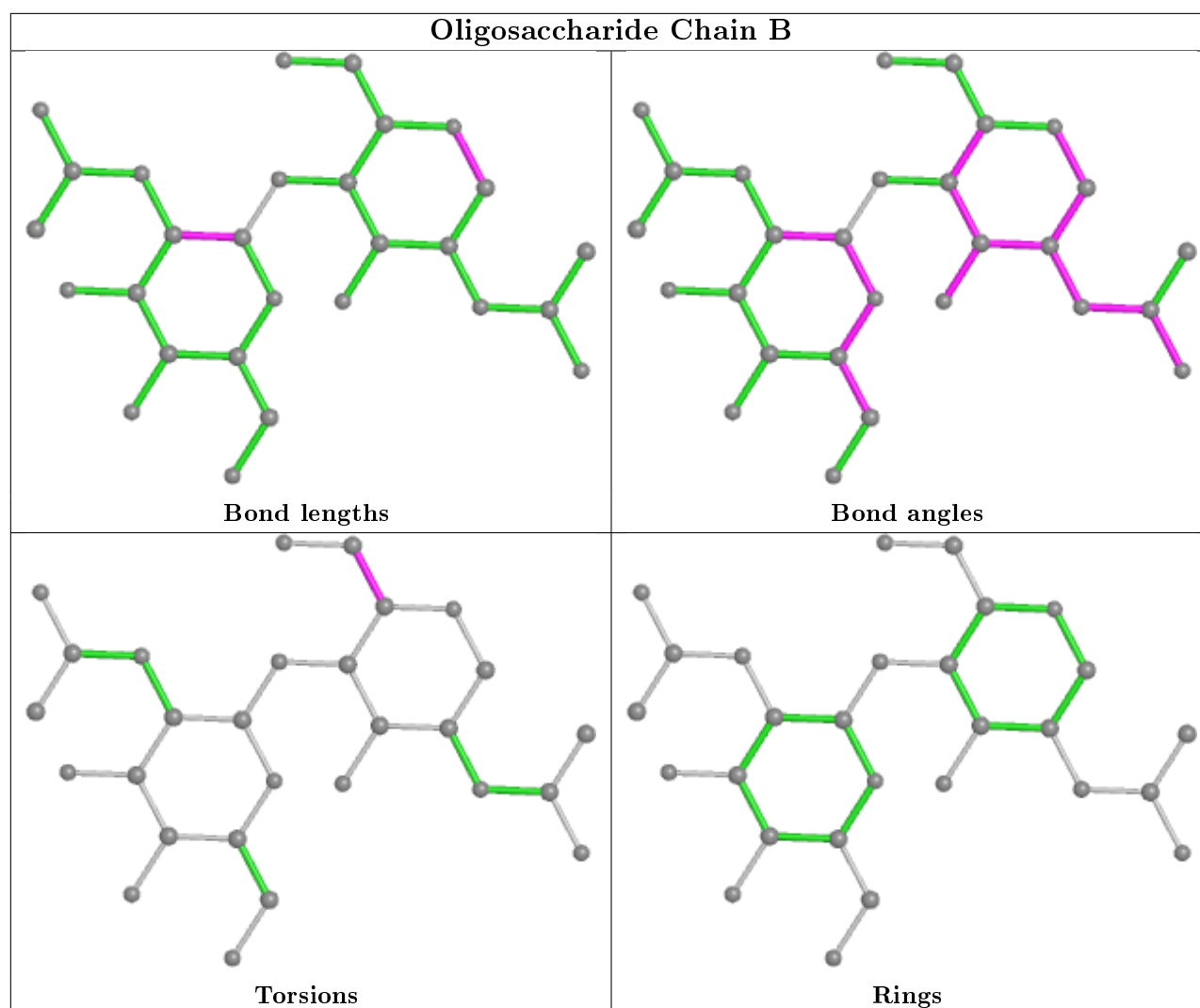
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 14 are monoatomic - leaving 11 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	605	1	14,14,15	0.46	0	17,19,21	2.45	6 (35%)
7	SCN	A	621	-	1,2,2	0.28	0	0,1,1	0.00	-
8	EDO	A	624	-	3,3,3	0.58	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	A	623	-	3,3,3	0.63	0	2,2,2	0.43	0
8	EDO	A	622	-	3,3,3	0.15	0	2,2,2	0.91	0
8	EDO	A	626	-	3,3,3	0.59	0	2,2,2	0.06	0
4	HEM	A	606	1,10	27,50,50	2.40	9 (33%)	17,82,82	2.95	8 (47%)
3	NAG	A	601	1	14,14,15	1.16	2 (14%)	17,19,21	1.72	2 (11%)
8	EDO	A	625	-	3,3,3	0.27	0	2,2,2	0.97	0
9	PEA	A	627	-	8,9,9	1.02	1 (12%)	9,10,10	0.98	0
3	NAG	A	602	1	14,14,15	1.19	0	17,19,21	1.80	7 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	605	1	-	2/6/23/26	0/1/1/1
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
8	EDO	A	624	-	-	1/1/1/1	-
8	EDO	A	623	-	-	0/1/1/1	-
8	EDO	A	622	-	-	0/1/1/1	-
8	EDO	A	626	-	-	0/1/1/1	-
4	HEM	A	606	1,10	-	0/6/54/54	-
8	EDO	A	625	-	-	0/1/1/1	-
9	PEA	A	627	-	-	0/3/3/3	0/1/1/1
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	606	HEM	C4A-NA	5.34	1.47	1.36
4	A	606	HEM	C3C-C2C	5.12	1.47	1.40
4	A	606	HEM	C1A-NA	4.96	1.46	1.36
4	A	606	HEM	C3B-C2B	4.33	1.46	1.40
4	A	606	HEM	C2A-C3A	3.22	1.47	1.37
4	A	606	HEM	C1C-C2C	3.19	1.49	1.42
4	A	606	HEM	C1B-C2B	2.89	1.49	1.42
3	A	601	NAG	O5-C1	-2.79	1.39	1.43
4	A	606	HEM	C4D-C3D	2.46	1.48	1.42
4	A	606	HEM	C3D-C2D	2.32	1.44	1.37
9	A	627	PEA	C2'-C1'	-2.26	1.34	1.38
3	A	601	NAG	C2-N2	-2.12	1.42	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	606	HEM	C1D-C2D-C3D	-6.61	102.39	107.00
3	A	605	NAG	C2-N2-C7	6.57	132.26	122.90
3	A	601	NAG	C2-N2-C7	-5.30	115.36	122.90
4	A	606	HEM	C3B-C4B-NB	5.30	116.06	109.21
3	A	605	NAG	O5-C5-C6	4.28	113.92	107.20
4	A	606	HEM	CBD-CAD-C3D	-3.66	105.73	112.48
3	A	605	NAG	C1-C2-N2	-3.65	104.26	110.49
4	A	606	HEM	C4A-C3A-C2A	-3.59	104.50	107.00
3	A	601	NAG	O5-C1-C2	-3.54	105.69	111.29
3	A	602	NAG	C2-N2-C7	-3.46	117.97	122.90
4	A	606	HEM	CMC-C2C-C3C	3.46	131.15	124.68
4	A	606	HEM	CMB-C2B-C3B	3.43	131.10	124.68
4	A	606	HEM	CAD-CBD-CGD	-3.05	107.56	112.67
3	A	602	NAG	O3-C3-C2	-2.65	103.98	109.47
4	A	606	HEM	CBA-CAA-C2A	-2.63	107.63	112.49
3	A	602	NAG	C3-C4-C5	-2.52	105.75	110.24
3	A	602	NAG	O5-C1-C2	-2.41	107.48	111.29
3	A	602	NAG	C8-C7-N2	2.18	119.79	116.10
3	A	602	NAG	O5-C5-C6	2.15	110.57	107.20
3	A	605	NAG	O4-C4-C5	-2.09	104.10	109.30
3	A	602	NAG	C1-O5-C5	2.07	115.00	112.19
3	A	605	NAG	C4-C3-C2	2.02	113.97	111.02
3	A	605	NAG	O5-C1-C2	2.01	114.46	111.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

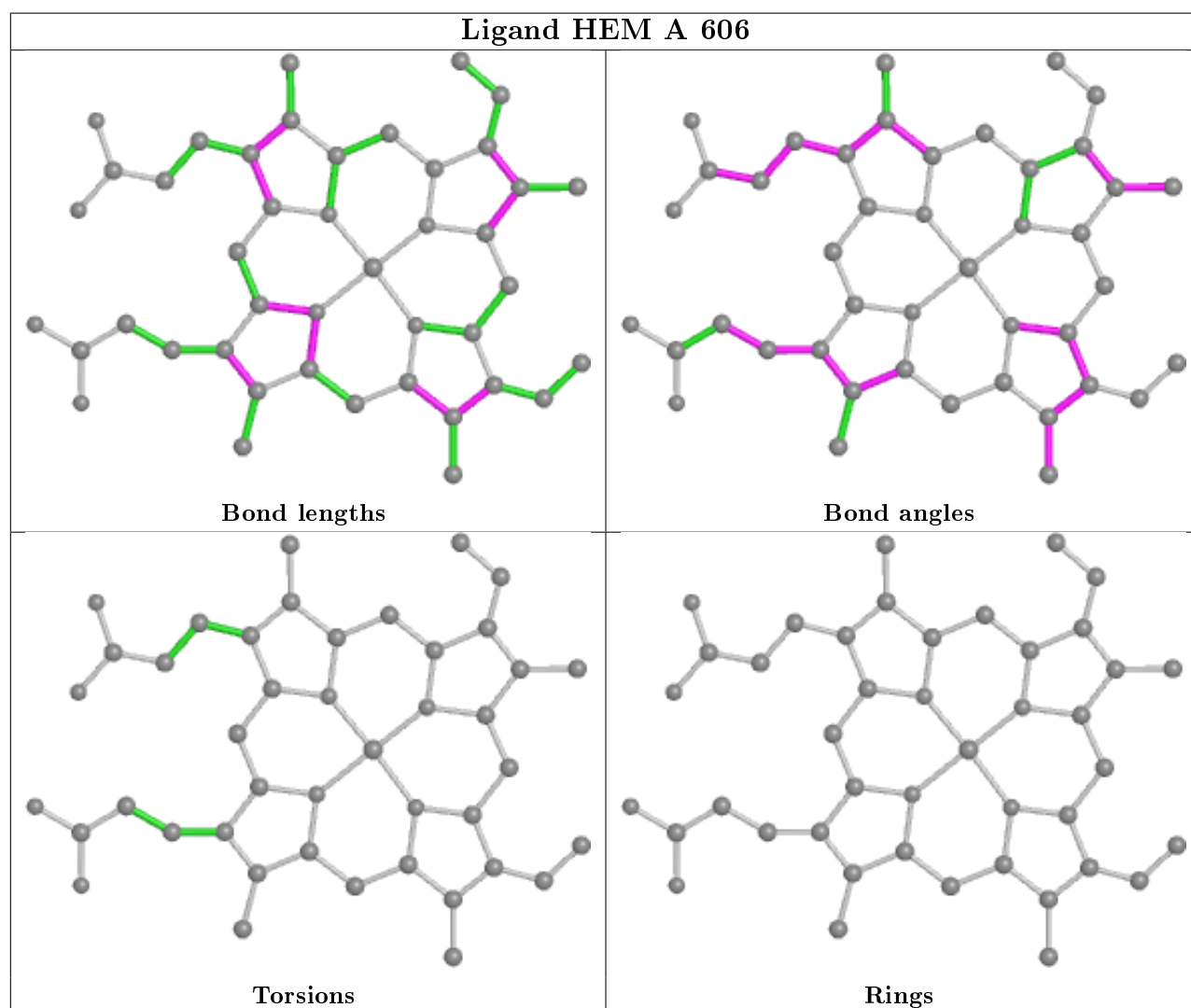
Mol	Chain	Res	Type	Atoms
3	A	605	NAG	C4-C5-C6-O6
3	A	605	NAG	O5-C5-C6-O6
8	A	624	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	624	EDO	1	0
8	A	622	EDO	1	0
4	A	606	HEM	15	0
8	A	625	EDO	1	0
9	A	627	PEA	13	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.29	46 (7%) 13 13	24, 40, 83, 111	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	TRP	10.0
1	A	1	SER	9.6
1	A	174	SER	8.1
1	A	121	SER	7.4
1	A	13	VAL	7.2
1	A	12	LEU	7.0
1	A	120	GLY	6.6
1	A	173	GLN	6.6
1	A	8	ALA	6.2
1	A	172	TYR	6.2
1	A	122	SER	6.2
1	A	595	ASN	6.1
1	A	125	SER	5.6
1	A	9	PRO	5.2
1	A	119	LEU	4.9
1	A	7	GLY	4.9
1	A	11	PRO	4.8
1	A	593	ARG	4.7
1	A	5	GLY	4.6
1	A	124	HIS	4.3
1	A	4	VAL	4.2
1	A	127	VAL	4.2
1	A	592	SER	4.2
1	A	118	GLU	4.0
1	A	6	CYS	3.8
1	A	223	GLY	3.6
1	A	10	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	3.6
1	A	283	LEU	3.2
1	A	117	THR	3.2
1	A	262	LEU	3.1
1	A	170	PRO	3.0
1	A	175	LEU	2.9
1	A	169	THR	2.5
1	A	594	GLU	2.5
1	A	261	LEU	2.5
1	A	109	HIS	2.4
1	A	132	TYR	2.4
1	A	210	LEU	2.4
1	A	105	GLN	2.2
1	A	3	GLU	2.2
1	A	123	GLU	2.2
1	A	590	TRP	2.1
1	A	134	VAL	2.1
1	A	17	GLU	2.1
1	A	441	CYS	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.

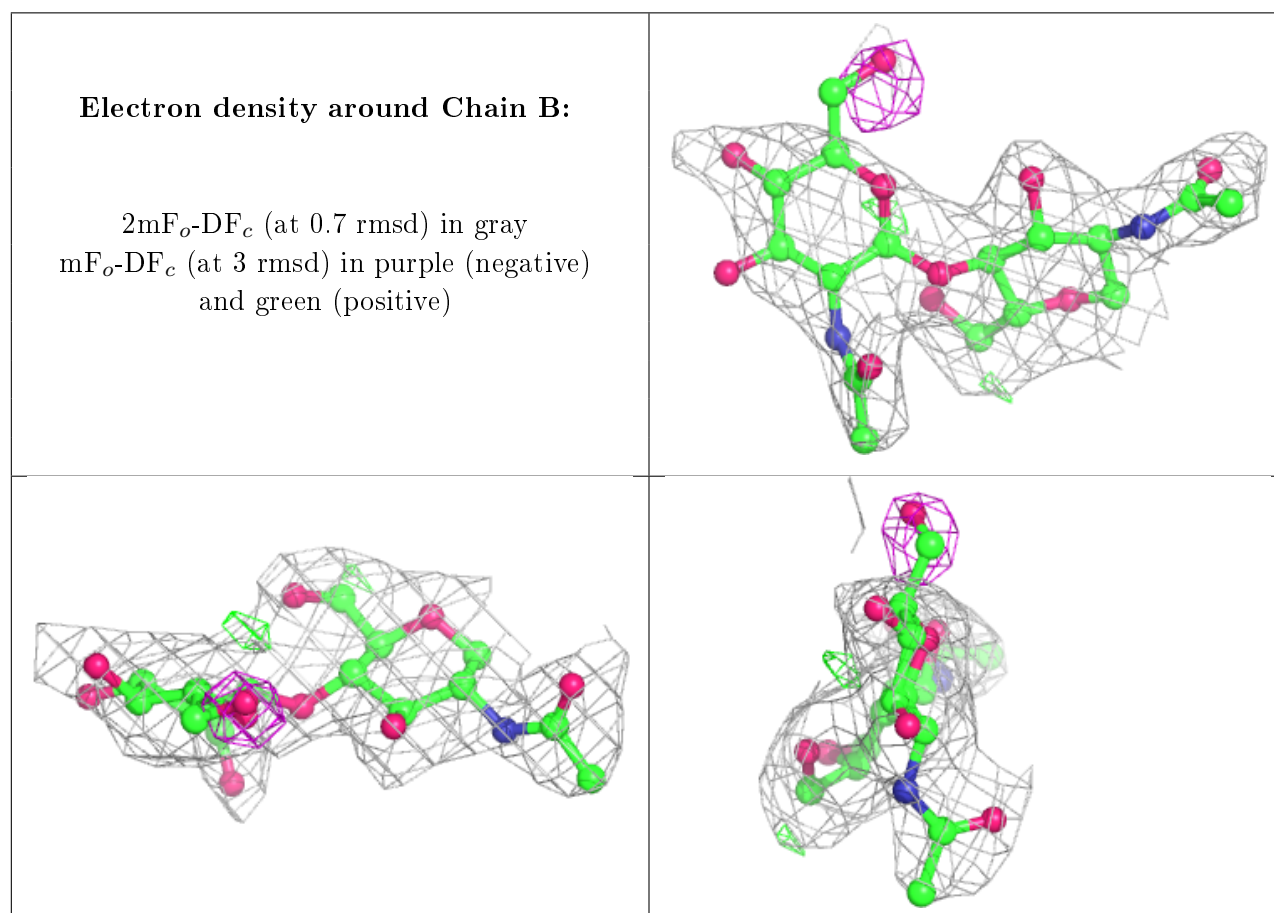
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	A	198	10/11	0.79	0.25	44,50,54,61	0

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	2	14/15	0.74	0.35	52,56,59,60	14
2	NAG	B	1	14/15	0.91	0.14	49,52,55,56	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
3	NAG	A	605	14/15	0.66	0.26	51,55,57,57	14
8	EDO	A	623	4/4	0.76	0.24	34,39,42,43	0
9	PEA	A	627	9/9	0.80	0.39	27,32,37,37	0
3	NAG	A	601	14/15	0.84	0.32	45,48,51,51	0
8	EDO	A	626	4/4	0.84	0.28	34,35,38,38	0
7	SCN	A	621	3/3	0.86	0.21	42,42,43,49	0
8	EDO	A	622	4/4	0.90	0.40	22,22,24,28	0
8	EDO	A	625	4/4	0.90	0.26	32,34,36,37	0
8	EDO	A	624	4/4	0.92	0.18	35,36,36,37	0
3	NAG	A	602	14/15	0.93	0.15	46,49,51,52	0

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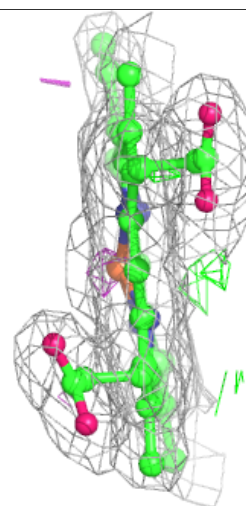
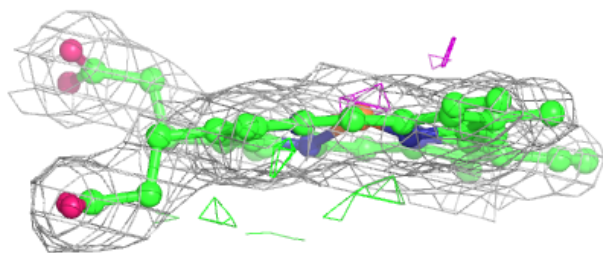
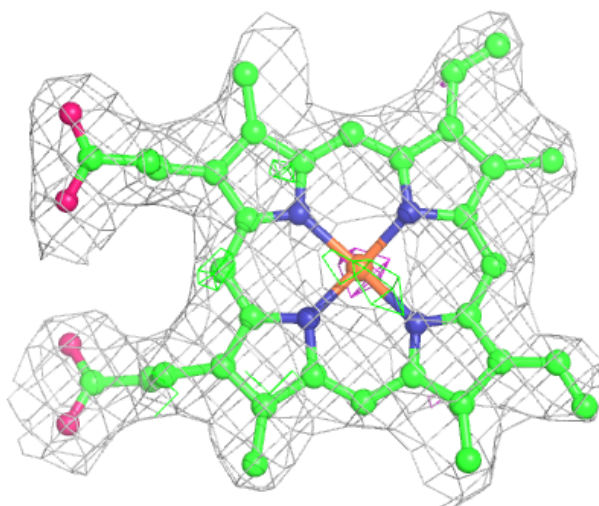
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	IOD	A	612	1/1	0.95	0.17	53,53,53,53	1
6	IOD	A	619	1/1	0.96	0.17	54,54,54,54	1
4	HEM	A	606	43/43	0.96	0.21	21,24,25,27	0
6	IOD	A	610	1/1	0.98	0.06	44,44,44,44	0
6	IOD	A	617	1/1	0.98	0.04	40,40,40,40	1
6	IOD	A	616	1/1	0.98	0.12	48,48,48,48	1
6	IOD	A	615	1/1	0.98	0.15	51,51,51,51	1
6	IOD	A	613	1/1	0.99	0.02	38,38,38,38	0
6	IOD	A	620	1/1	0.99	0.05	45,45,45,45	0
6	IOD	A	609	1/1	0.99	0.04	43,43,43,43	1
6	IOD	A	614	1/1	0.99	0.09	47,47,47,47	1
6	IOD	A	618	1/1	1.00	0.03	45,45,45,45	1
5	CA	A	607	1/1	1.00	0.07	27,27,27,27	0
6	IOD	A	611	1/1	1.00	0.04	43,43,43,43	0
6	IOD	A	608	1/1	1.00	0.05	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 606:

$2mF_o-DF_c$ (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.