



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:19 PM UTC

PDB ID : 4NJB / pdb_00004njb
Title : Crystal structure of the complex of lactoperoxidase from bovine with 3,3-oxydipyridine at 2.31 Å resolution
Authors : Yamini, S.; Sirohi, H.V.; Sinha, M.; Bhushan, A.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2013-11-09
Resolution : 2.31 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

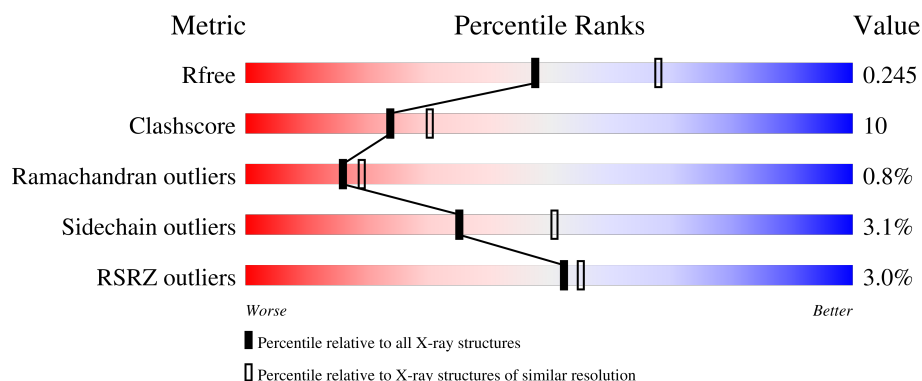
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

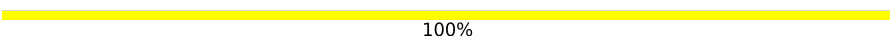
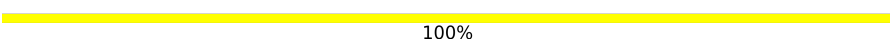
The reported resolution of this entry is 2.31 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	 3% 75% 21% .
2	B	2	 100%
2	C	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	-	-
6	IOD	A	614	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5371 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
			4774	3037	847	863	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			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

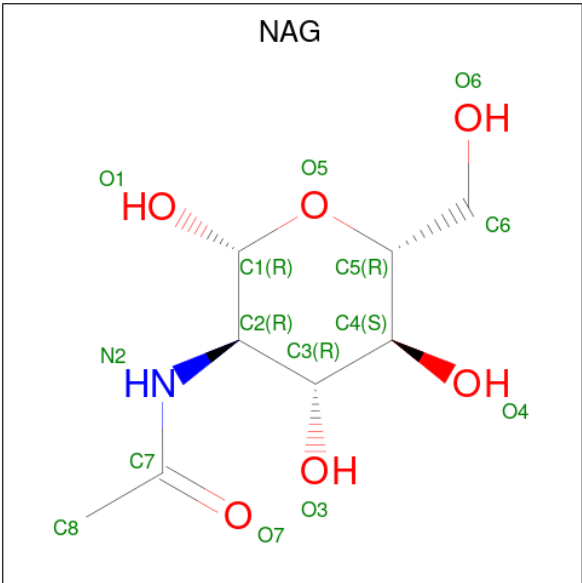
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

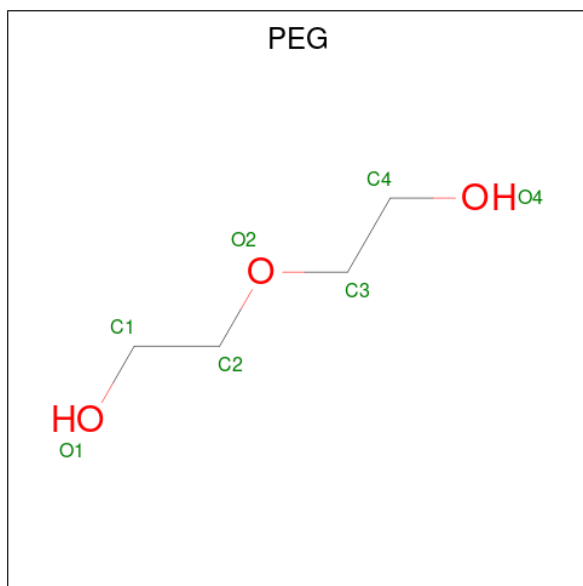


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

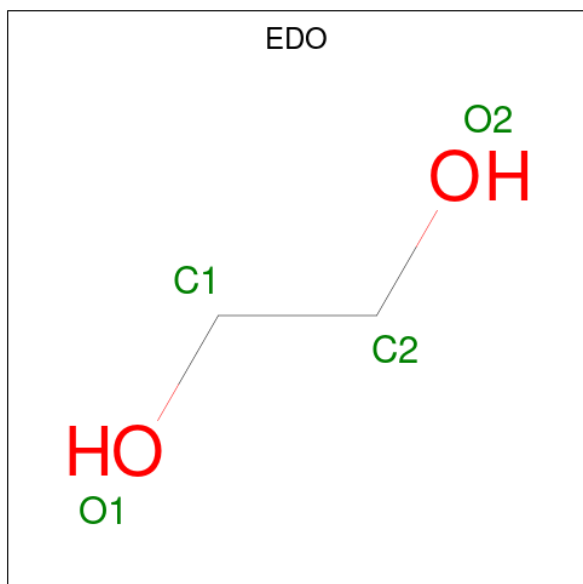
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	11	Total I 11 11	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



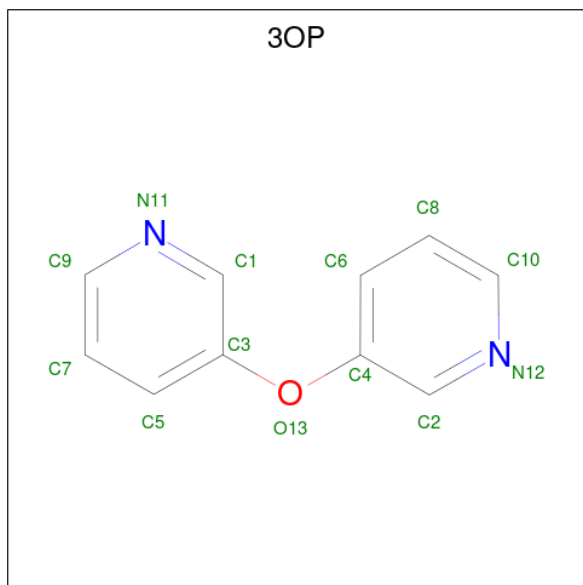
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is 3,3'-oxydipyridine (CCD ID: 3OP) (formula: C₁₀H₈N₂O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O 13 10 2 1	0	0

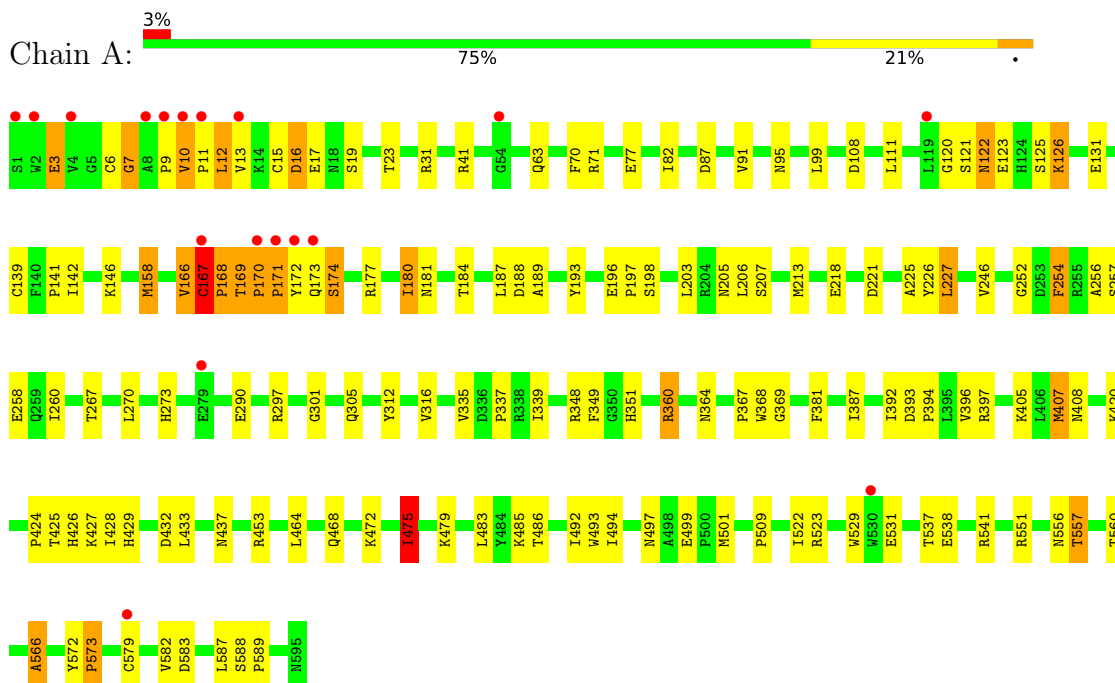
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	430	Total O 430 430	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.

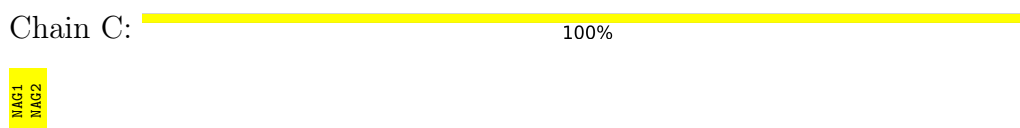
- Molecule 1: Lactoperoxidase



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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	54.36Å 80.40Å 76.28Å 90.00° 103.37° 90.00°	Depositor
Resolution (Å)	39.02 – 2.31 39.02 – 2.31	Depositor EDS
% Data completeness (in resolution range)	95.6 (39.02-2.31) 95.6 (39.02-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.09 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.227 0.203 , 0.245	Depositor DCC
R_{free} test set	1332 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.767	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5371	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: PEG, SEP, 3OP, EDO, HEM, CA, IOD, NAG

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	0.51	0/4891	1.13	47/6634 (0.7%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	PRO	N-CA-C	-14.87	92.56	110.70
1	A	429	HIS	N-CA-C	-8.04	98.37	109.71
1	A	3	GLU	N-CA-C	7.23	126.20	110.80
1	A	426	HIS	N-CA-C	-7.16	101.29	110.53
1	A	158	MET	N-CA-C	-6.91	98.34	109.40
1	A	146	LYS	N-CA-C	6.88	119.65	111.33
1	A	225	ALA	N-CA-C	6.84	119.39	110.43
1	A	95	ASN	N-CA-C	6.83	119.15	110.61
1	A	566	ALA	N-CA-C	6.79	119.51	111.71
1	A	369	GLY	CA-C-N	6.76	126.36	119.19
1	A	369	GLY	C-N-CA	6.76	126.36	119.19
1	A	174	SER	N-CA-C	6.68	121.66	112.04
1	A	316	VAL	N-CA-C	-6.61	105.39	111.67
1	A	15	CYS	N-CA-C	6.49	119.82	109.24
1	A	428	ILE	N-CA-C	6.47	119.23	109.20
1	A	87	ASP	N-CA-C	6.45	118.67	108.67
1	A	556	ASN	N-CA-C	6.11	120.61	112.30
1	A	492	ILE	N-CA-C	6.10	116.84	110.62
1	A	260	ILE	N-CA-C	6.08	119.56	111.17
1	A	131	GLU	N-CA-C	6.06	117.89	111.28
1	A	171	PRO	N-CA-C	6.00	124.83	112.47
1	A	111	LEU	N-CA-C	5.99	120.60	113.12
1	A	312	TYR	N-CA-C	5.89	118.83	111.24
1	A	364	ASN	N-CA-C	-5.81	105.77	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	LYS	N-CA-C	-5.77	101.94	110.48
1	A	173	GLN	N-CA-C	5.69	123.28	114.64
1	A	537	THR	N-CA-C	-5.68	103.43	110.41
1	A	254	PHE	N-CA-C	5.65	119.43	112.54
1	A	166	VAL	N-CA-C	5.59	116.52	110.21
1	A	180	ILE	CB-CA-C	-5.57	103.38	111.68
1	A	407	MET	N-CA-C	-5.44	102.83	110.50
1	A	427	LYS	N-CA-C	5.39	120.86	113.97
1	A	582	VAL	N-CA-C	5.25	116.15	108.53
1	A	453	ARG	N-CA-C	-5.25	105.45	111.07
1	A	167	CYS	CA-C-N	-5.20	113.34	119.84
1	A	167	CYS	C-N-CA	-5.20	113.34	119.84
1	A	23	THR	N-CA-C	-5.17	103.86	110.53
1	A	420	LYS	N-CA-C	5.14	119.09	112.41
1	A	360	ARG	N-CA-C	-5.13	100.81	109.07
1	A	167	CYS	CA-CB-SG	-5.08	102.71	114.40
1	A	158	MET	CA-C-N	-5.07	114.73	119.85
1	A	158	MET	C-N-CA	-5.07	114.73	119.85
1	A	397	ARG	N-CA-C	-5.06	105.86	112.23
1	A	587	LEU	N-CA-C	5.05	119.08	113.02
1	A	256	ALA	N-CA-C	5.04	118.90	112.34
1	A	475	ILE	N-CA-C	5.04	115.76	110.62
1	A	557	THR	N-CA-C	-5.02	102.12	108.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4774	0	4687	94	0
2	B	28	0	25	0	0
2	C	28	0	25	0	0
3	A	1	0	0	0	0
4	A	43	0	30	7	0
5	A	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	11	0	0	4	0
7	A	7	0	9	0	0
8	A	8	0	12	0	0
9	A	13	0	8	4	0
10	A	430	0	0	9	0
All	All	5371	0	4822	99	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 10.

All (99) 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:108:ASP:OD1	4:A:602:HEM:HMD1	1.40	1.20
1:A:258:GLU:HG3	9:A:623:3OP:H1	1.15	1.08
1:A:424:PRO:O	1:A:425:THR:HG22	1.56	1.05
1:A:258:GLU:CG	9:A:623:3OP:H1	1.89	1.01
1:A:258:GLU:HG3	9:A:623:3OP:C5	2.07	0.80
1:A:169:THR:H	1:A:170:PRO:CD	1.95	0.79
1:A:408:ASN:HB2	10:A:843:HOH:O	1.82	0.78
1:A:108:ASP:OD1	4:A:602:HEM:CMD	2.28	0.77
1:A:258:GLU:OE1	4:A:602:HEM:HMB3	1.84	0.77
1:A:63:GLN:H	1:A:63:GLN:CD	1.94	0.76
1:A:246:VAL:HG11	1:A:387:ILE:HD12	1.70	0.73
1:A:258:GLU:OE1	4:A:602:HEM:CMB	2.40	0.70
1:A:485:LYS:N	10:A:1127:HOH:O	2.27	0.67
6:A:614:IOD:I	10:A:1100:HOH:O	2.83	0.67
1:A:538:GLU:HG2	1:A:541:ARG:NH2	2.11	0.66
1:A:120:GLY:HA3	1:A:126:LYS:HD2	1.79	0.64
1:A:227:LEU:HD22	1:A:270:LEU:HD22	1.79	0.64
6:A:618:IOD:I	10:A:1105:HOH:O	2.86	0.62
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.35	0.62
1:A:171:PRO:HG2	10:A:1056:HOH:O	2.01	0.60
1:A:168:PRO:HG3	1:A:172:TYR:HB2	1.85	0.59
1:A:475:ILE:HG22	1:A:479:LYS:HE3	1.83	0.59
1:A:572:TYR:CD1	1:A:573:PRO:HA	2.39	0.58
1:A:254:PHE:HB2	10:A:970:HOH:O	2.05	0.56
1:A:169:THR:N	1:A:170:PRO:CD	2.65	0.56
1:A:551:ARG:HD3	1:A:583:ASP:O	2.06	0.56
1:A:424:PRO:O	1:A:425:THR:CG2	2.43	0.55
1:A:71:ARG:HG2	1:A:71:ARG:NH1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HD21	1:A:267:THR:HA	1.87	0.55
1:A:560:THR:HA	1:A:579:CYS:SG	2.46	0.54
1:A:168:PRO:HG3	1:A:172:TYR:CD1	2.42	0.54
1:A:169:THR:H	1:A:170:PRO:HD3	1.72	0.54
1:A:123:GLU:HG3	1:A:125:SER:H	1.72	0.53
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.43	0.53
1:A:12:LEU:HD23	1:A:13:VAL:H	1.74	0.53
1:A:468:GLN:O	1:A:472:LYS:N	2.42	0.53
1:A:572:TYR:CE2	1:A:573:PRO:HB3	2.44	0.53
1:A:139:CYS:SG	1:A:141:PRO:HD3	2.49	0.52
6:A:614:IOD:I	10:A:1075:HOH:O	2.89	0.52
1:A:63:GLN:CD	1:A:63:GLN:N	2.62	0.51
1:A:122:ASN:C	1:A:122:ASN:HD22	2.17	0.51
1:A:167:CYS:CB	1:A:168:PRO:CD	2.89	0.51
1:A:121:SER:O	1:A:122:ASN:ND2	2.44	0.51
1:A:6:CYS:SG	1:A:7:GLY:N	2.84	0.50
1:A:257:SER:O	1:A:381:PHE:HA	2.12	0.50
1:A:16:ASP:OD1	1:A:16:ASP:C	2.55	0.49
1:A:407:MET:HB3	1:A:501:MET:CE	2.42	0.49
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.47	0.49
1:A:71:ARG:HG2	1:A:71:ARG:HH11	1.76	0.48
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.94	0.48
1:A:180:ILE:HG22	1:A:181:ASN:N	2.30	0.47
1:A:99:LEU:HD23	1:A:566:ALA:HB1	1.95	0.47
1:A:158:MET:CE	1:A:432:ASP:H	2.27	0.47
1:A:258:GLU:CD	9:A:623:3OP:H1	2.38	0.47
1:A:348:ARG:NH2	4:A:602:HEM:HAD1	2.30	0.47
1:A:464:LEU:O	1:A:468:GLN:HG3	2.15	0.47
4:A:602:HEM:HMB1	4:A:602:HEM:HBB2	1.96	0.46
1:A:572:TYR:CZ	1:A:573:PRO:HB3	2.50	0.46
1:A:70:PHE:CD2	1:A:485:LYS:HG3	2.51	0.45
1:A:177:ARG:HB2	10:A:915:HOH:O	2.16	0.45
1:A:16:ASP:OD2	1:A:19:SER:HB2	2.15	0.45
1:A:301:GLY:O	1:A:305:GLN:HG3	2.16	0.45
1:A:206:LEU:O	1:A:207:SER:C	2.59	0.45
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.14	0.44
1:A:493:TRP:O	1:A:497:ASN:OD1	2.36	0.44
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.83	0.44
1:A:17:GLU:O	1:A:31:ARG:NH2	2.51	0.44
1:A:142:ILE:HG23	10:A:977:HOH:O	2.18	0.43
1:A:166:VAL:O	1:A:167:CYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLU:HA	1:A:197:PRO:HD3	1.90	0.43
1:A:9:PRO:CG	1:A:167:CYS:H	2.32	0.43
1:A:10:VAL:HG11	1:A:41:ARG:CZ	2.49	0.42
1:A:290:GLU:HA	1:A:290:GLU:OE1	2.20	0.42
1:A:393:ASP:OD1	1:A:557:THR:HB	2.19	0.42
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.93	0.42
1:A:193:TYR:OH	1:A:297:ARG:HA	2.18	0.42
1:A:392:ILE:O	1:A:396:VAL:HG23	2.19	0.42
1:A:407:MET:HB3	1:A:501:MET:HE3	2.02	0.42
1:A:203:LEU:HD11	1:A:252:GLY:HA2	2.02	0.42
1:A:9:PRO:HG2	1:A:167:CYS:H	1.84	0.42
4:A:602:HEM:CMB	4:A:602:HEM:HBB2	2.49	0.42
1:A:82:ILE:HD11	1:A:483:LEU:HD12	2.01	0.42
1:A:184:THR:OG1	1:A:188:ASP:OD2	2.38	0.42
1:A:351:HIS:CE1	1:A:433:LEU:HD21	2.55	0.42
1:A:499:GLU:OE1	1:A:509:PRO:HD2	2.20	0.41
1:A:63:GLN:O	1:A:71:ARG:NH1	2.54	0.41
1:A:588:SER:N	1:A:589:PRO:CD	2.82	0.41
1:A:168:PRO:CG	1:A:172:TYR:HB2	2.49	0.41
1:A:77:GLU:HG3	6:A:610:IOD:I	2.91	0.41
1:A:188:ASP:O	1:A:189:ALA:HB3	2.20	0.41
1:A:339:ILE:CD1	1:A:522:ILE:HD11	2.51	0.41
1:A:82:ILE:CD1	1:A:483:LEU:HD12	2.50	0.41
1:A:120:GLY:HA3	1:A:126:LYS:CD	2.49	0.41
1:A:168:PRO:HG3	1:A:172:TYR:HD1	1.84	0.40
1:A:221:ASP:HB2	1:A:226:TYR:CE2	2.57	0.40
1:A:205:ASN:OD1	1:A:205:ASN:C	2.64	0.40
1:A:335:VAL:O	1:A:337:PRO:HD3	2.21	0.40
1:A:360:ARG:HB3	1:A:368:TRP:HB3	2.04	0.40
1:A:393:ASP:CB	1:A:394:PRO:HD3	2.51	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%)	562 (95%)	25 (4%)	5 (1%)	16	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	167	CYS
1	A	11	PRO
1	A	169	THR
1	A	7	GLY

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	517/517 (100%)	501 (97%)	16 (3%)	35	51

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	12	LEU
1	A	16	ASP
1	A	91	VAL
1	A	122	ASN
1	A	126	LYS
1	A	168	PRO
1	A	174	SER
1	A	218	GLU
1	A	227	LEU
1	A	367	PRO
1	A	475	ILE
1	A	486	THR
1	A	494	ILE

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Mol	Chain	Res	Type
1	A	531	GLU
1	A	573	PRO

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

Mol	Chain	Res	Type
1	A	122	ASN
1	A	135	GLN
1	A	147	ASN
1	A	230	ASN
1	A	497	ASN
1	A	521	GLN
1	A	570	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	A	198	1	8,9,10	2.68	4 (50%)	7,12,14	2.59	6 (85%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	198	1	-	5/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O3P	-4.41	1.38	1.54
1	A	198	SEP	P-O1P	-4.37	1.36	1.50
1	A	198	SEP	P-O2P	-3.59	1.41	1.54
1	A	198	SEP	CA-N	-2.13	1.42	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O2P-P-OG	3.42	115.59	106.67
1	A	198	SEP	O2P-P-O1P	2.88	122.04	110.83
1	A	198	SEP	OG-CB-CA	-2.82	105.40	108.14
1	A	198	SEP	O3P-P-OG	2.71	113.74	106.67
1	A	198	SEP	O3P-P-O2P	-2.35	98.97	107.80
1	A	198	SEP	OG-P-O1P	-2.09	100.78	106.44

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

4 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	0.56	0	17,19,21	1.30	2 (11%)
2	NAG	B	2	2	14,14,15	0.77	0	17,19,21	1.69	3 (17%)
2	NAG	C	1	2,1	14,14,15	0.76	0	17,19,21	1.53	3 (17%)
2	NAG	C	2	2	14,14,15	0.65	0	17,19,21	2.90	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
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	7.67	122.46	112.19
2	C	2	NAG	C4-C3-C2	-5.59	102.82	111.02
2	C	2	NAG	C1-C2-N2	4.37	117.31	110.43
2	B	2	NAG	C1-C2-N2	-3.92	104.25	110.43
2	B	2	NAG	C4-C3-C2	3.58	116.26	111.02
2	B	2	NAG	C1-O5-C5	-3.16	107.95	112.19
2	C	2	NAG	O3-C3-C2	2.90	115.42	109.40
2	C	1	NAG	C1-O5-C5	-2.81	108.42	112.19
2	C	1	NAG	O5-C1-C2	-2.76	107.02	111.29
2	C	2	NAG	O5-C5-C6	2.65	112.81	107.66
2	C	2	NAG	O5-C1-C2	-2.53	107.37	111.29
2	B	1	NAG	C1-C2-N2	2.40	114.21	110.43
2	C	1	NAG	C3-C4-C5	-2.18	106.29	110.23
2	C	2	NAG	O5-C5-C4	2.06	115.85	110.83
2	B	1	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

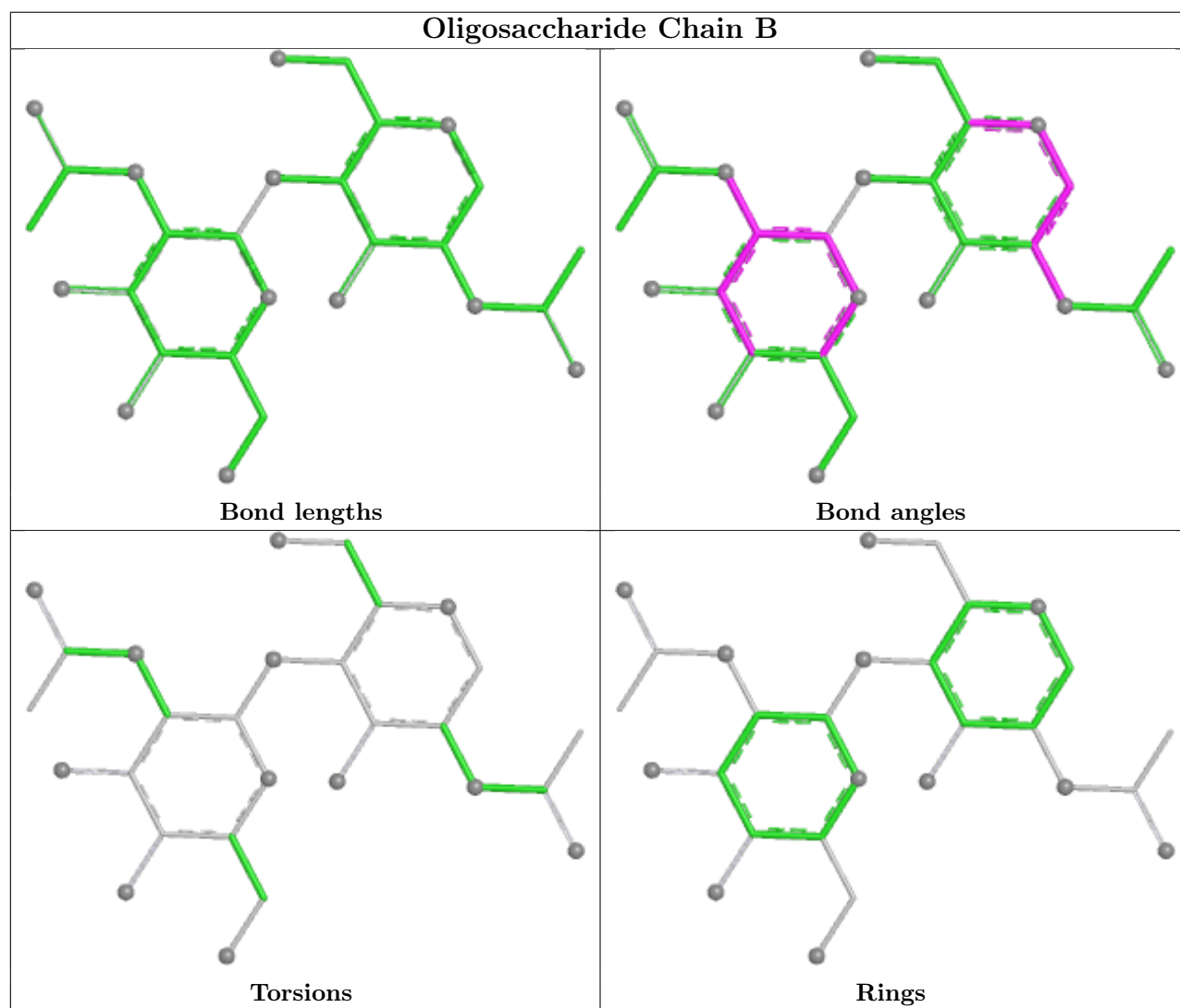
All (1) torsion outliers are listed below:

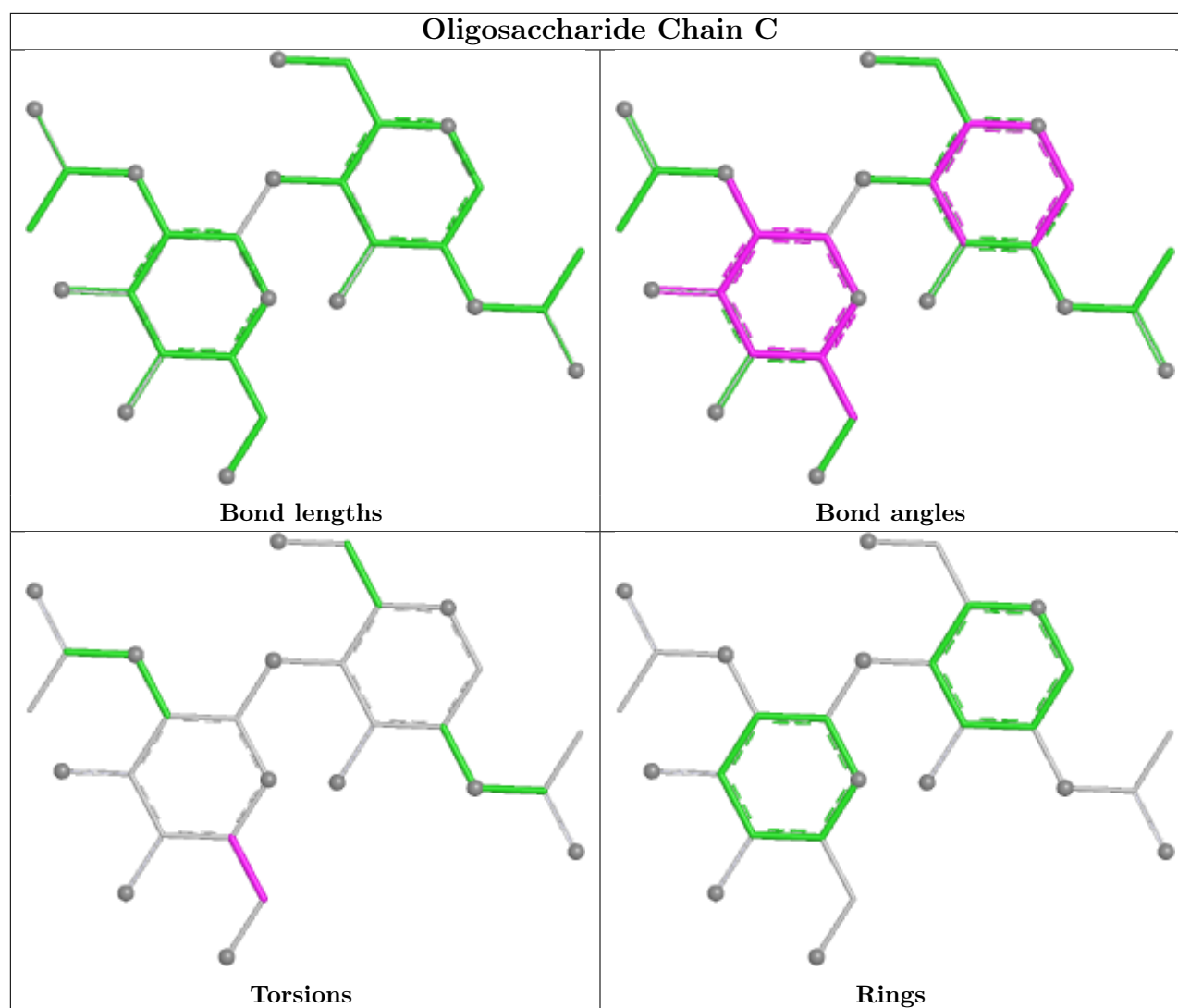
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6

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 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 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	$\# Z > 2$
4	HEM	A	602	10,1	50,50,50	3.21	25 (50%)	67,82,82	2.48	28 (41%)
7	PEG	A	620	-	6,6,6	1.90	2 (33%)	5,5,5	0.97	0
5	NAG	A	603	1	14,14,15	0.66	0	17,19,21	1.29	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	3OP	A	623	-	14,14,14	2.45	5 (35%)	17,17,17	1.18	2 (11%)
8	EDO	A	622	-	3,3,3	0.68	0	2,2,2	0.72	0
8	EDO	A	621	-	3,3,3	0.75	0	2,2,2	0.68	0
5	NAG	A	608	1	14,14,15	0.52	0	17,19,21	1.31	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
4	HEM	A	602	10,1	-	4/14/54/54	-
7	PEG	A	620	-	-	3/4/4/4	-
5	NAG	A	603	1	-	1/6/23/26	0/1/1/1
9	3OP	A	623	-	-	1/4/4/4	0/2/2/2
8	EDO	A	622	-	-	1/1/1/1	-
8	EDO	A	621	-	-	0/1/1/1	-
5	NAG	A	608	1	-	0/6/23/26	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	HEM	FE-NB	7.98	2.19	1.94
4	A	602	HEM	CMA-C3A	-7.71	1.35	1.50
4	A	602	HEM	FE-NA	7.18	2.18	1.95
4	A	602	HEM	CHB-C4A	6.59	1.54	1.39
4	A	602	HEM	C1A-C2A	6.07	1.56	1.44
4	A	602	HEM	CMC-C2C	5.83	1.62	1.50
4	A	602	HEM	CBA-CGA	-5.56	1.37	1.50
9	A	623	3OP	C1-C3	-5.15	1.30	1.38
4	A	602	HEM	C3D-C2D	4.64	1.46	1.36
4	A	602	HEM	CMB-C2B	4.23	1.59	1.50
4	A	602	HEM	FE-ND	4.17	2.07	1.94
9	A	623	3OP	C2-C4	-3.98	1.32	1.38
9	A	623	3OP	C7-C5	-3.84	1.32	1.38
7	A	620	PEG	O1-C1	-3.56	1.24	1.42
4	A	602	HEM	CHD-C1D	3.33	1.46	1.39
4	A	602	HEM	CBD-CGD	3.18	1.57	1.50
4	A	602	HEM	C1A-NA	-3.14	1.33	1.39
4	A	602	HEM	FE-NC	3.13	2.05	1.95
4	A	602	HEM	C4A-C3A	3.09	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	HEM	C1B-NB	-2.93	1.35	1.40
4	A	602	HEM	O1D-CGD	2.89	1.31	1.22
9	A	623	3OP	O13-C4	-2.86	1.33	1.39
4	A	602	HEM	C2A-C3A	-2.74	1.31	1.38
7	A	620	PEG	C2-C1	-2.66	1.35	1.49
4	A	602	HEM	CHB-C1B	2.55	1.43	1.38
4	A	602	HEM	CAC-C3C	2.50	1.54	1.47
9	A	623	3OP	C5-C3	-2.27	1.34	1.38
4	A	602	HEM	CHA-C1A	-2.23	1.34	1.39
4	A	602	HEM	CBC-CAC	2.21	1.41	1.30
4	A	602	HEM	C4A-NA	-2.18	1.35	1.39
4	A	602	HEM	C3B-C2B	2.10	1.41	1.37
4	A	602	HEM	C4D-C3D	-2.07	1.41	1.45

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	HEM	C4A-NA-C1A	5.90	115.44	105.82
4	A	602	HEM	CMD-C2D-C1D	5.12	133.04	125.03
4	A	602	HEM	C2A-C1A-NA	-4.99	104.62	110.15
4	A	602	HEM	CHC-C1C-NC	4.89	129.78	124.45
4	A	602	HEM	CHA-C1A-NA	4.80	132.56	123.86
4	A	602	HEM	CHD-C4C-NC	4.54	129.40	124.45
4	A	602	HEM	C1B-NB-C4B	4.41	110.43	105.21
4	A	602	HEM	CBD-CAD-C3D	-4.30	100.64	112.53
4	A	602	HEM	C3A-C4A-NA	-4.17	103.46	110.14
4	A	602	HEM	C4A-C3A-C2A	4.00	111.39	106.82
4	A	602	HEM	CHD-C1D-ND	3.77	128.48	124.42
4	A	602	HEM	C3C-C2C-C1C	3.73	110.58	107.05
4	A	602	HEM	CMC-C2C-C1C	-3.48	118.59	124.73
4	A	602	HEM	CHC-C4B-NB	3.36	128.04	124.42
4	A	602	HEM	CAD-C3D-C4D	3.21	130.30	124.70
4	A	602	HEM	CAC-C3C-C4C	-2.93	117.81	124.82
4	A	602	HEM	C4C-NC-C1C	2.84	110.44	105.82
4	A	602	HEM	O1A-CGA-CBA	-2.75	114.36	123.09
5	A	603	NAG	O4-C4-C5	2.75	116.09	109.32
5	A	608	NAG	C3-C4-C5	-2.71	105.32	110.23
4	A	602	HEM	C4C-C3C-C2C	2.69	109.14	106.81
4	A	602	HEM	O1D-CGD-CBD	-2.56	114.98	123.09
9	A	623	3OP	C7-C5-C3	2.48	122.73	118.98
4	A	602	HEM	C4D-ND-C1D	2.48	108.14	105.21
4	A	602	HEM	CAA-C2A-C3A	2.48	132.62	127.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	HEM	CHB-C4A-NA	2.44	128.29	123.86
5	A	603	NAG	C1-O5-C5	2.37	115.36	112.19
4	A	602	HEM	C2C-C1C-NC	-2.26	105.45	109.64
4	A	602	HEM	C2B-C1B-NB	-2.20	107.31	109.84
4	A	602	HEM	C4C-CHD-C1D	-2.19	121.36	126.02
4	A	602	HEM	CMD-C2D-C3D	-2.18	120.26	126.15
4	A	602	HEM	CHB-C1B-NB	2.10	126.97	124.37
5	A	608	NAG	O5-C5-C6	2.09	111.74	107.66
9	A	623	3OP	C9-N11-C1	2.04	120.42	116.85

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	620	PEG	O2-C3-C4-O4
8	A	622	EDO	O1-C1-C2-O2
7	A	620	PEG	O1-C1-C2-O2
5	A	603	NAG	C4-C5-C6-O6
9	A	623	3OP	C2-C4-O13-C3
4	A	602	HEM	CAA-CBA-CGA-O1A
4	A	602	HEM	CAA-CBA-CGA-O2A
4	A	602	HEM	CAD-CBD-CGD-O1D
4	A	602	HEM	CAD-CBD-CGD-O2D
7	A	620	PEG	C4-C3-O2-C2

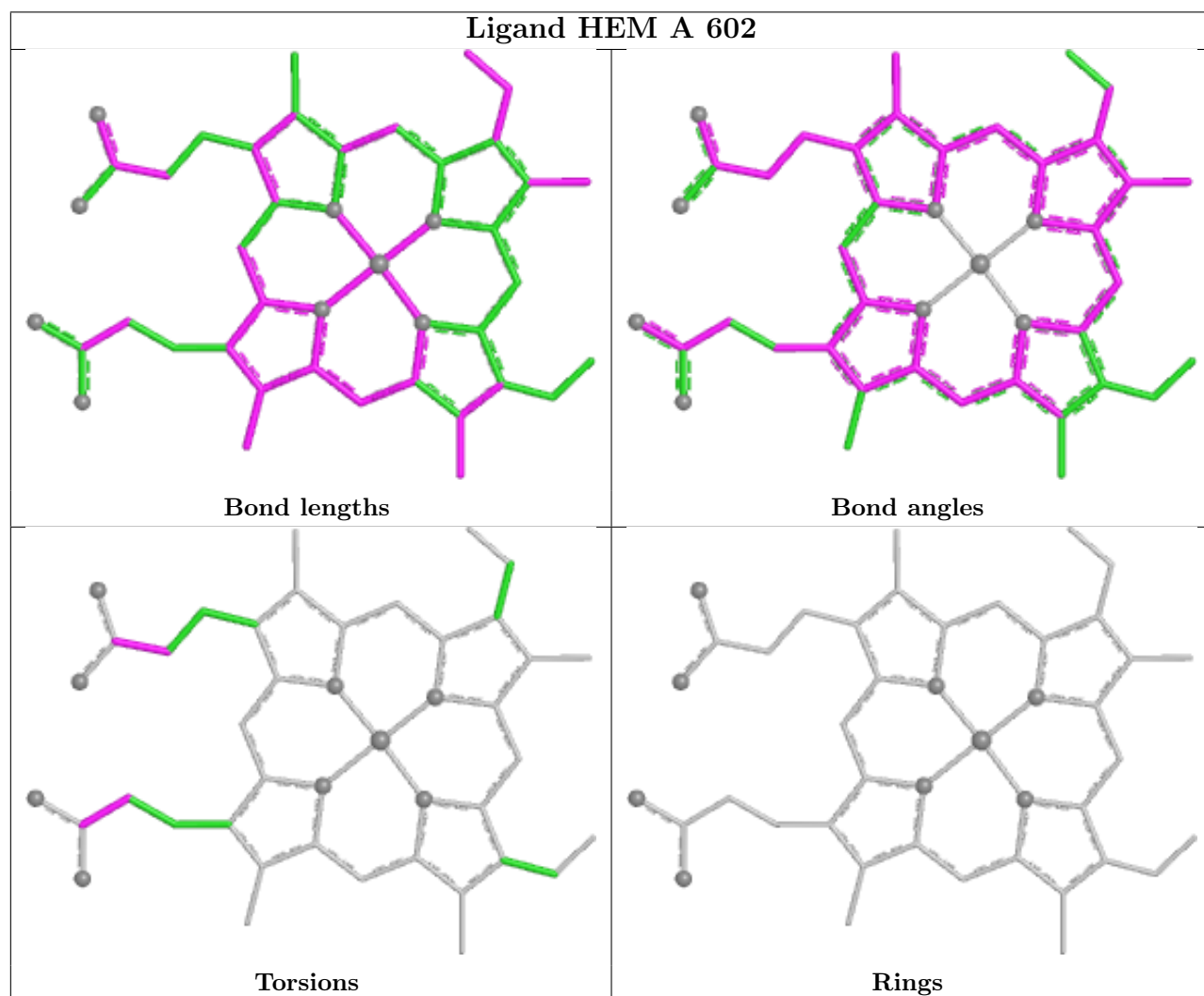
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	HEM	7	0
9	A	623	3OP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	594/595 (99%)	0.18	18 (3%) 52 55	29, 49, 98, 100	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	ALA	4.6
1	A	2	TRP	4.0
1	A	172	TYR	3.8
1	A	9	PRO	3.8
1	A	119	LEU	3.8
1	A	173	GLN	3.0
1	A	530	TRP	3.0
1	A	13	VAL	2.9
1	A	4	VAL	2.8
1	A	11	PRO	2.8
1	A	10	VAL	2.4
1	A	579	CYS	2.2
1	A	54	GLY	2.2
1	A	167	CYS	2.1
1	A	1	SER	2.1
1	A	170	PRO	2.1
1	A	171	PRO	2.1
1	A	279	GLU	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.

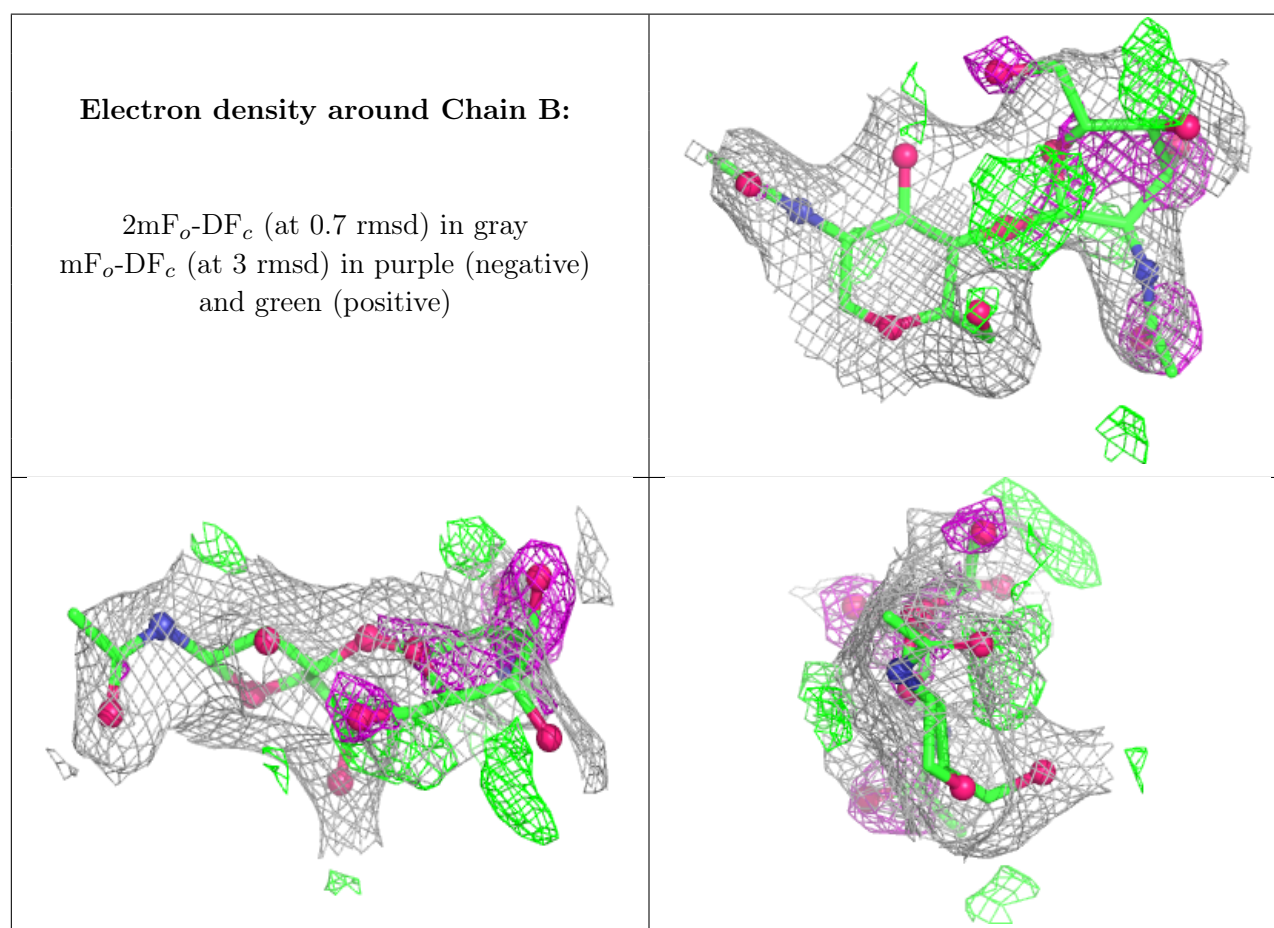
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	SEP	A	198	10/11	0.95	0.09	25,46,51,54	0

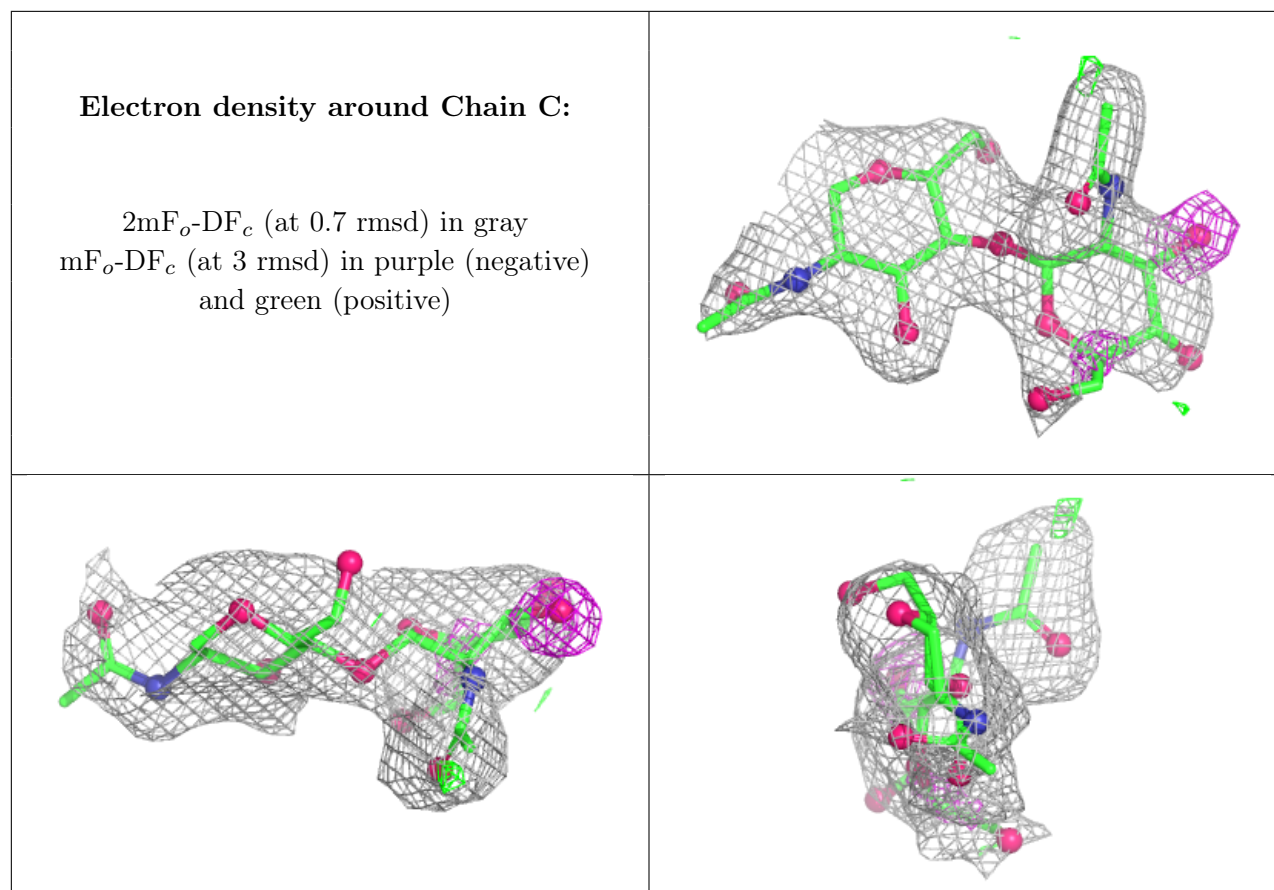
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	2	14/15	0.53	0.14	42,49,57,57	0
2	NAG	C	2	14/15	0.63	0.13	50,54,58,68	0
2	NAG	B	1	14/15	0.74	0.11	40,48,52,55	0
2	NAG	C	1	14/15	0.92	0.09	49,56,68,70	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.

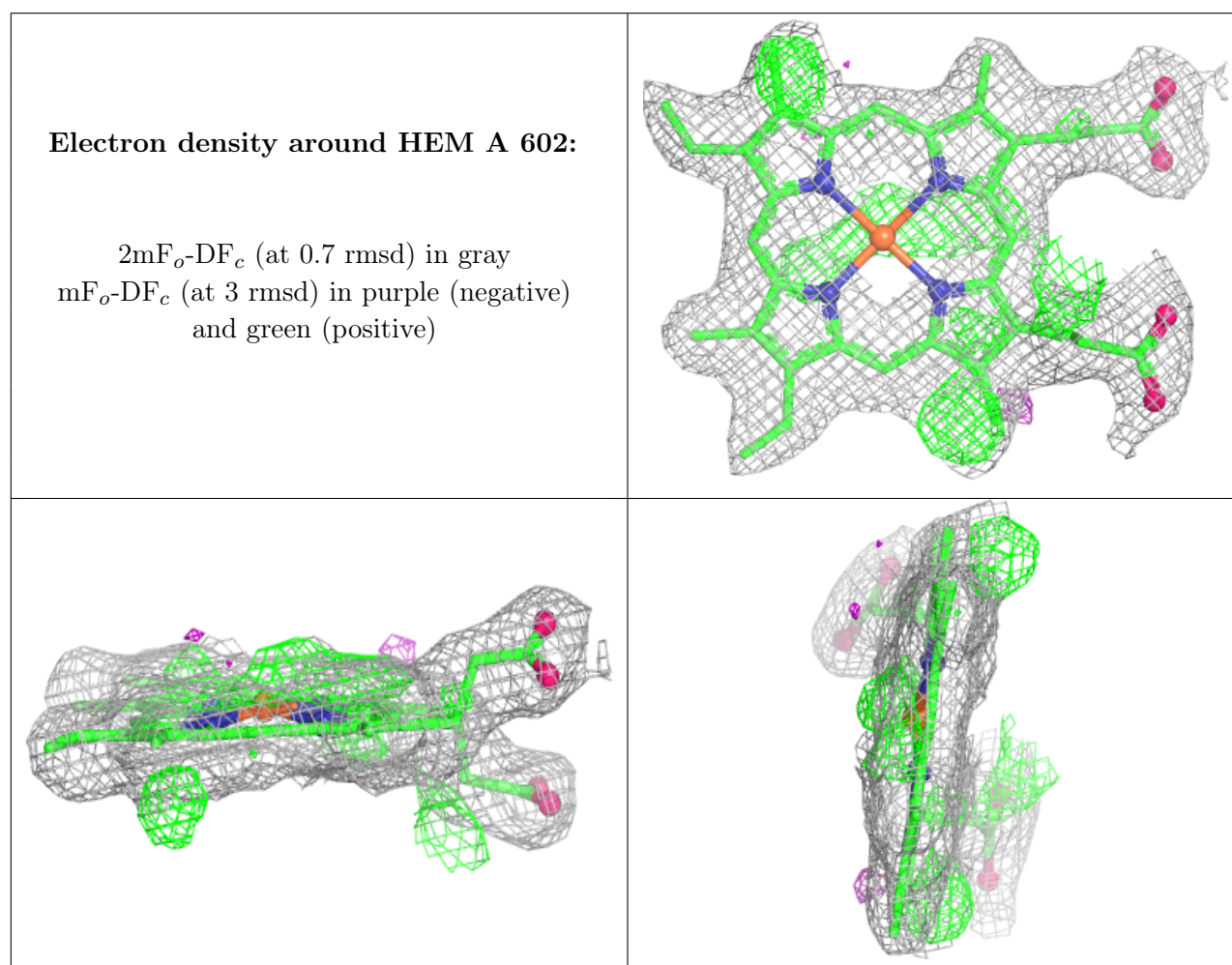
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	603	14/15	0.64	0.14	46,54,59,66	0
5	NAG	A	608	14/15	0.75	0.11	50,52,58,59	0
9	3OP	A	623	13/13	0.81	0.18	44,61,69,69	0
7	PEG	A	620	7/7	0.82	0.14	36,44,48,49	0
8	EDO	A	622	4/4	0.87	0.13	55,55,57,57	0
8	EDO	A	621	4/4	0.89	0.13	46,48,51,53	0
6	IOD	A	612	1/1	0.95	0.16	66,66,66,66	0
6	IOD	A	614	1/1	0.95	0.07	67,67,67,67	1
4	HEM	A	602	43/43	0.96	0.10	27,33,40,41	0
6	IOD	A	609	1/1	0.96	0.11	63,63,63,63	0
6	IOD	A	613	1/1	0.97	0.16	63,63,63,63	0
6	IOD	A	615	1/1	0.97	0.31	60,60,60,60	1
6	IOD	A	611	1/1	0.98	0.04	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	IOD	A	619	1/1	0.98	0.31	61,61,61,61	0
6	IOD	A	610	1/1	0.99	0.08	62,62,62,62	0
3	CA	A	601	1/1	0.99	0.04	39,39,39,39	0
6	IOD	A	616	1/1	0.99	0.05	44,44,44,44	0
6	IOD	A	617	1/1	0.99	0.02	56,56,56,56	0
6	IOD	A	618	1/1	0.99	0.09	65,65,65,65	0

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



6.5 Other polymers ⓘ

There are no such residues in this entry.