Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 12:51 PM EDT

PDB ID	:	2OYU
Title	:	Indomethacin-(S)-alpha-ethyl-ethanolamide bound to Cyclooxygenase-1
Authors	:	Harman, C.A.; Garavito, R.M.
Deposited on	:	2007-02-23
Resolution	:	2.70 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:

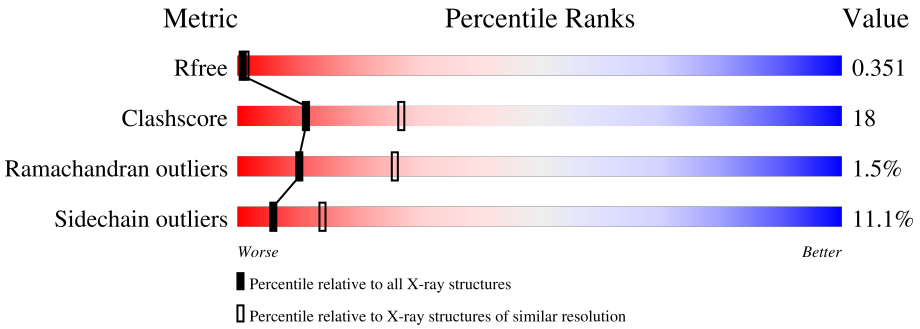
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 <=5%

Mol	Chain	Length	Quality of chain
1	P	600	61% 27% · 8%
2	A	2	100%
2	C	2	100%
3	B	3	33% 67%

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
5	IMS	P	700	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4652 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 Prostaglandin G/H synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	553	Total	C	N	O	S	0	0	0
			4408	2864	741	775	28			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	92	LEU	MET	SEE REMARK 999	UNP P05979

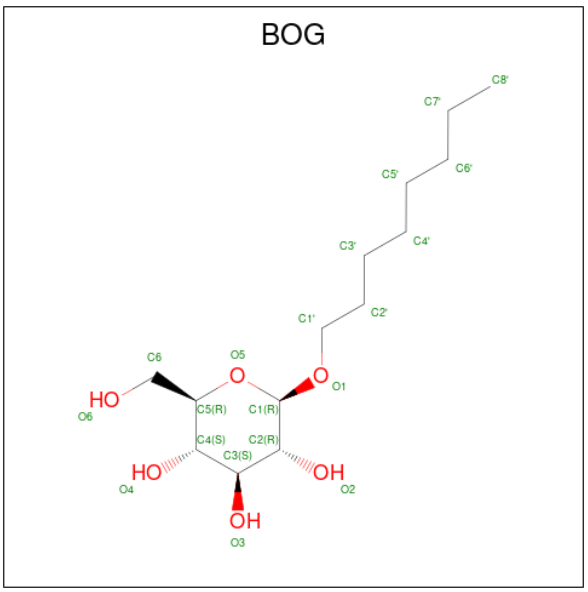
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	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 an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

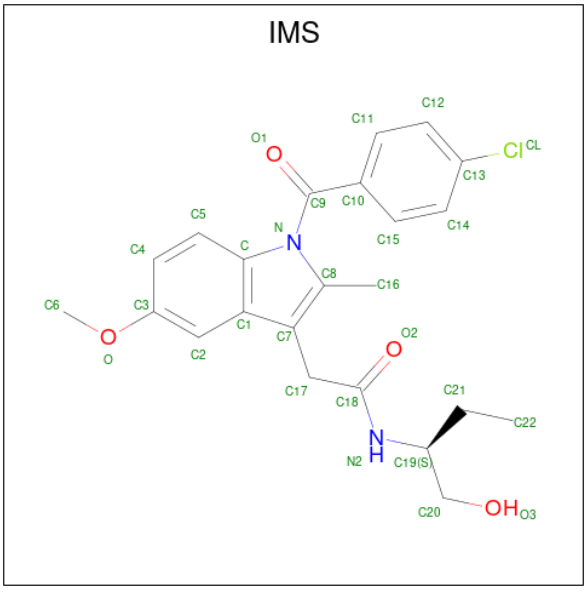
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



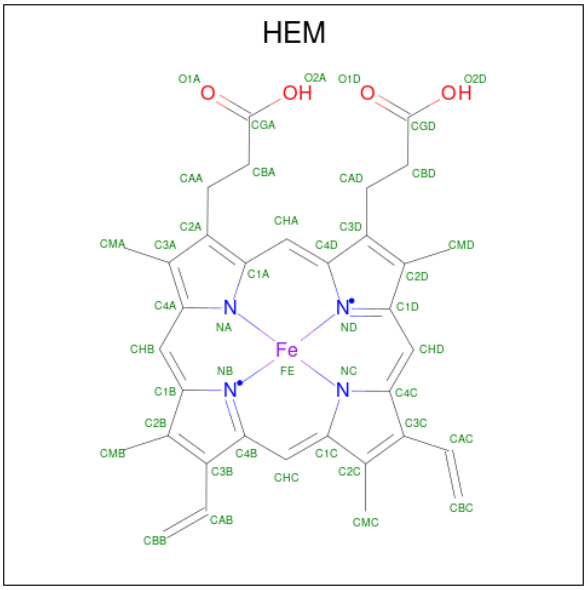
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total C O 12 6 6	0	0
4	P	1	Total C O 12 6 6	0	0

- Molecule 5 is 2-[1-(4-CHLOROBENZOYL)-5-METHOXY-2-METHYL-1H-INDOL-3-YL]-N-[(1S)-1-(HYDROXYMETHYL)PROPYL]ACETAMIDE (three-letter code: IMS) (formula: $C_{23}H_{25}ClN_2O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	P	1	Total	C	Cl	N	O	0	0
			30	23	1	2	4		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 7 is water.

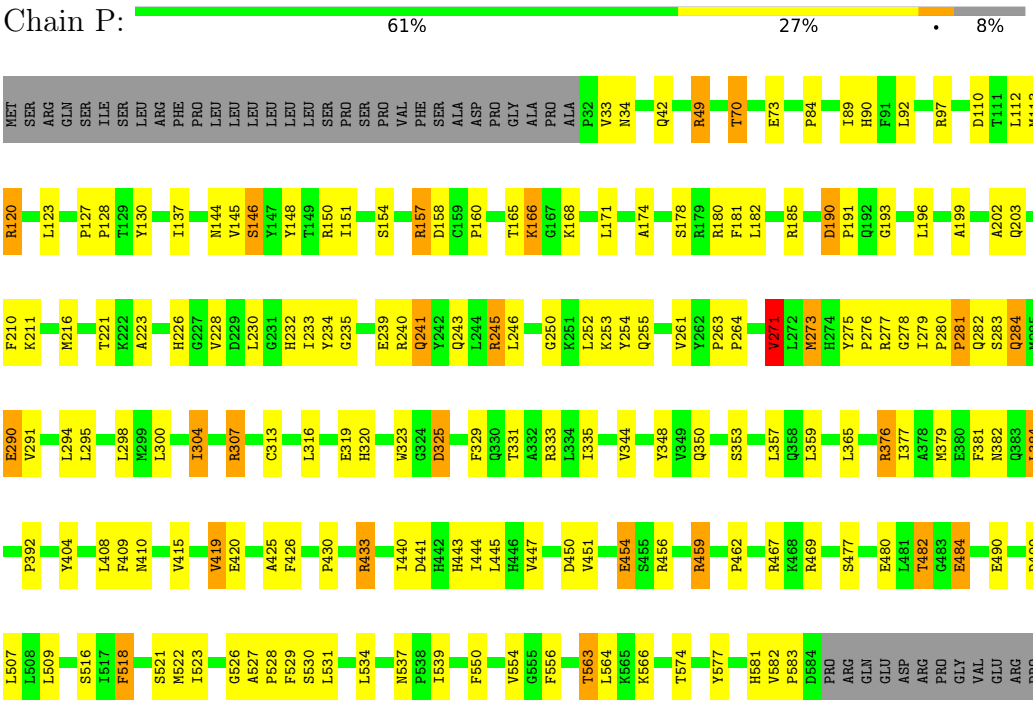
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	52	Total	O	0	0
			52	52		

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. 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. 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.

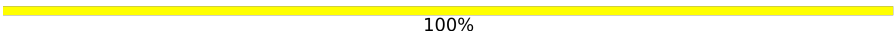
• Molecule 1: Prostaglandin G/H synthase 1

Chain P:



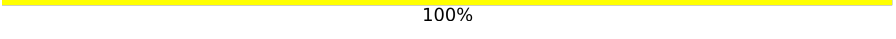
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:



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

Chain C:



• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	181.41Å 181.41Å 103.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.69 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-2.70) 99.6 (29.69-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.74 (at 2.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.292 0.320 , 0.351	Depositor DCC
R_{free} test set	1400 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	62.7	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 28.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	4652	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BOG, HEM, IMS, NAG, BMA

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	P	0.53	0/4547	0.67	0/6189

There are no bond length outliers.

There are no bond angle outliers.

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	P	4408	0	4243	156	0
2	A	28	0	25	0	0
2	C	28	0	25	0	0
3	B	39	0	34	4	0
4	P	24	0	22	0	0
5	P	30	0	25	26	0
6	P	43	0	30	4	0
7	P	52	0	0	6	0
All	All	4652	0	4404	160	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 18.

All (160) 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:P:151:ILE:HG22	1:P:469:ARG:NH1	1.56	1.19
1:P:280:PRO:HA	1:P:284:GLN:HG3	1.23	1.13
1:P:459:ARG:HH21	1:P:459:ARG:HG2	1.17	1.04
1:P:151:ILE:HG22	1:P:469:ARG:HH12	1.05	1.04
1:P:84:PRO:HG2	1:P:89:ILE:HD11	1.43	0.98
1:P:208:GLN:HE22	1:P:228:VAL:HA	1.29	0.96
1:P:527:ALA:HB3	1:P:528:PRO:HD3	1.48	0.94
1:P:90:HIS:HE1	5:P:700:IMS:H202	1.33	0.93
1:P:151:ILE:CG2	1:P:469:ARG:HH12	1.84	0.90
1:P:563:THR:HG22	1:P:566:LYS:H	1.36	0.90
1:P:527:ALA:HA	5:P:700:IMS:H5	1.52	0.89
1:P:433:ARG:HH11	1:P:433:ARG:HG2	1.39	0.88
1:P:49:ARG:HH11	1:P:49:ARG:HG2	1.39	0.86
1:P:157:ARG:HA	1:P:459:ARG:HH11	1.42	0.85
1:P:388:HIS:HB3	1:P:444:ILE:HD12	1.58	0.84
1:P:353:SER:CB	5:P:700:IMS:H163	2.08	0.82
1:P:527:ALA:HA	5:P:700:IMS:C5	2.09	0.81
1:P:208:GLN:NE2	1:P:228:VAL:HA	1.97	0.78
1:P:516:SER:HB3	5:P:700:IMS:H212	1.63	0.78
1:P:90:HIS:CE1	5:P:700:IMS:H202	2.16	0.78
1:P:344:VAL:O	1:P:348:TYR:HB3	1.84	0.77
1:P:459:ARG:HH21	1:P:459:ARG:CG	1.96	0.74
1:P:280:PRO:CA	1:P:284:GLN:HG3	2.12	0.74
1:P:353:SER:HB2	5:P:700:IMS:H163	1.69	0.74
1:P:387:TRP:HB2	6:P:601:HEM:HAC	1.70	0.73
1:P:353:SER:HB3	5:P:700:IMS:H163	1.71	0.73
1:P:157:ARG:HA	1:P:459:ARG:NH1	2.05	0.71
3:B:2:NAG:H4	3:B:3:BMA:O2	1.90	0.70
1:P:49:ARG:HH11	1:P:49:ARG:CG	2.04	0.70
1:P:90:HIS:HE1	5:P:700:IMS:C20	2.05	0.69
1:P:459:ARG:HG2	1:P:459:ARG:NH2	1.99	0.69
1:P:171:LEU:HB3	1:P:456:ARG:HH21	1.56	0.69
1:P:359:LEU:HD22	5:P:700:IMS:CL	2.31	0.68
1:P:563:THR:HG22	1:P:566:LYS:N	2.08	0.68
1:P:450:ASP:O	1:P:454:GLU:HG2	1.93	0.67
1:P:531:LEU:HD11	5:P:700:IMS:H11	1.76	0.67
1:P:462:PRO:HB3	1:P:499:ASP:O	1.95	0.67
1:P:226:HIS:CE1	1:P:376:ARG:HD2	2.30	0.66
1:P:335:ILE:HD13	1:P:550:PHE:HB3	1.77	0.64
7:P:789:HOH:O	3:B:2:NAG:H3	1.97	0.64
1:P:151:ILE:CG2	1:P:469:ARG:NH1	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:359:LEU:CD1	5:P:700:IMS:H14	2.28	0.64
1:P:433:ARG:HH11	1:P:433:ARG:CG	2.09	0.64
1:P:151:ILE:HG13	1:P:529:PHE:HZ	1.63	0.63
1:P:577:TYR:CE2	1:P:583:PRO:HD3	2.33	0.63
1:P:116:VAL:O	1:P:120:ARG:HB2	1.97	0.62
1:P:353:SER:HA	5:P:700:IMS:N2	2.14	0.62
1:P:34:ASN:HB2	1:P:158:ASP:OD2	2.00	0.61
1:P:320:HIS:HB3	1:P:323:TRP:CD1	2.36	0.60
1:P:150:ARG:NH1	1:P:154:SER:HB3	2.16	0.60
1:P:171:LEU:HB3	1:P:456:ARG:NH2	2.16	0.60
1:P:273:MET:SD	1:P:286:ALA:HA	2.42	0.59
1:P:388:HIS:HB3	1:P:444:ILE:CD1	2.31	0.59
1:P:211:LYS:HB2	1:P:223:ALA:HB2	1.84	0.59
1:P:300:LEU:HD22	1:P:426:PHE:HE2	1.67	0.58
1:P:359:LEU:CD2	5:P:700:IMS:H14	2.34	0.58
1:P:295:LEU:HB2	1:P:298:LEU:HD23	1.86	0.58
1:P:230:LEU:HG	1:P:233:ILE:HD12	1.85	0.57
1:P:281:PRO:O	1:P:284:GLN:HB2	2.05	0.56
1:P:276:PRO:HA	7:P:773:HOH:O	2.04	0.56
1:P:353:SER:O	5:P:700:IMS:H201	2.05	0.56
1:P:433:ARG:HG2	1:P:433:ARG:NH1	2.12	0.56
1:P:477:SER:OG	1:P:480:GLU:HB2	2.05	0.56
1:P:154:SER:HB2	1:P:459:ARG:HB2	1.87	0.56
1:P:261:VAL:HB	1:P:307:ARG:HD2	1.86	0.56
1:P:359:LEU:HD13	5:P:700:IMS:H14	1.85	0.56
1:P:240:ARG:HG3	1:P:271:VAL:HG21	1.88	0.56
1:P:130:TYR:HB2	1:P:150:ARG:HG2	1.87	0.56
1:P:209:PHE:HB2	1:P:377:ILE:HG13	1.87	0.56
1:P:235:GLY:HA2	1:P:288:GLY:O	2.05	0.56
1:P:181:PHE:HZ	1:P:490:GLU:HG3	1.71	0.55
1:P:447:VAL:O	1:P:451:VAL:HG23	2.07	0.55
1:P:157:ARG:NE	1:P:157:ARG:H	2.04	0.55
1:P:290:GLU:CB	7:P:783:HOH:O	2.55	0.55
1:P:526:GLY:HA3	5:P:700:IMS:H62	1.88	0.55
1:P:250:GLY:HA2	1:P:325:ASP:OD1	2.07	0.55
1:P:113:MET:O	1:P:117:LEU:HG	2.08	0.54
1:P:261:VAL:HB	1:P:307:ARG:HH11	1.71	0.54
1:P:42:GLN:HG3	1:P:70:THR:HG23	1.90	0.54
1:P:350:GLN:OE1	1:P:359:LEU:HG	2.08	0.54
1:P:178:SER:HB3	1:P:445:LEU:HD11	1.89	0.54
1:P:300:LEU:HD22	1:P:426:PHE:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:379:MET:O	1:P:382:ASN:HB3	2.08	0.53
1:P:34:ASN:CB	1:P:158:ASP:OD2	2.57	0.53
1:P:241:GLN:O	1:P:245:ARG:HG2	2.09	0.52
1:P:523:ILE:HG12	5:P:700:IMS:H223	1.91	0.52
1:P:295:LEU:HD21	1:P:408:LEU:HD23	1.92	0.52
1:P:359:LEU:HD22	5:P:700:IMS:H14	1.90	0.51
1:P:447:VAL:HG13	6:P:601:HEM:HBA2	1.91	0.51
1:P:527:ALA:HB3	1:P:528:PRO:CD	2.31	0.51
1:P:203:GLN:HA	6:P:601:HEM:HBC2	1.92	0.51
1:P:254:TYR:HA	1:P:264:PRO:HD3	1.93	0.51
1:P:255:GLN:HG2	1:P:263:PRO:O	2.09	0.51
1:P:150:ARG:HH12	1:P:154:SER:HB3	1.74	0.51
1:P:425:ALA:HA	7:P:760:HOH:O	2.11	0.50
1:P:404:TYR:CG	1:P:443:HIS:CD2	3.00	0.50
1:P:459:ARG:CG	1:P:459:ARG:NH2	2.65	0.50
1:P:216:MET:HG2	3:B:2:NAG:H82	1.94	0.49
1:P:286:ALA:O	7:P:786:HOH:O	2.20	0.49
1:P:280:PRO:HA	1:P:284:GLN:CG	2.17	0.49
1:P:307:ARG:HH21	1:P:419:VAL:HG11	1.77	0.49
1:P:207:HIS:HB3	1:P:289:GLN:HE21	1.76	0.49
1:P:307:ARG:NH2	1:P:419:VAL:HG11	2.27	0.49
1:P:90:HIS:CE1	5:P:700:IMS:C20	2.89	0.49
1:P:166:LYS:HG3	1:P:499:ASP:HB2	1.95	0.48
1:P:420:GLU:HG2	1:P:574:THR:HB	1.95	0.48
1:P:381:PHE:HD1	1:P:384:LEU:HD22	1.78	0.48
1:P:335:ILE:CD1	1:P:550:PHE:HB3	2.43	0.48
1:P:353:SER:HA	5:P:700:IMS:C18	2.43	0.47
1:P:49:ARG:HG2	1:P:49:ARG:NH1	2.19	0.47
1:P:278:GLY:C	1:P:280:PRO:HD3	2.35	0.47
1:P:280:PRO:N	1:P:281:PRO:HD3	2.30	0.47
1:P:359:LEU:HB3	5:P:700:IMS:CL	2.52	0.47
5:P:700:IMS:C16	5:P:700:IMS:H15	2.45	0.47
1:P:359:LEU:HD22	5:P:700:IMS:C14	2.45	0.46
1:P:234:TYR:CE2	1:P:333:ARG:HG3	2.50	0.46
1:P:441:ASP:OD2	1:P:443:HIS:CD2	2.68	0.46
1:P:199:ALA:O	1:P:202:ALA:HB3	2.15	0.46
1:P:253:LYS:O	1:P:264:PRO:HD3	2.14	0.46
1:P:84:PRO:CG	1:P:89:ILE:HD11	2.29	0.46
1:P:116:VAL:HG11	5:P:700:IMS:C12	2.46	0.46
1:P:144:ASN:OD1	1:P:146:SER:HB2	2.16	0.46
1:P:49:ARG:CG	1:P:49:ARG:NH1	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:240:ARG:HD2	7:P:755:HOH:O	2.15	0.45
1:P:313:CYS:HA	1:P:316:LEU:HD12	1.98	0.45
1:P:210:PHE:CE1	1:P:382:ASN:HA	2.51	0.45
1:P:518:PHE:CD1	1:P:522:MET:HG2	2.50	0.45
1:P:137:ILE:HD12	1:P:137:ILE:H	1.81	0.44
1:P:359:LEU:HD13	5:P:700:IMS:C14	2.47	0.44
1:P:42:GLN:HG3	1:P:70:THR:CG2	2.47	0.44
1:P:171:LEU:HD13	1:P:456:ARG:HE	1.83	0.43
1:P:482:THR:O	1:P:484:GLU:N	2.51	0.43
1:P:190:ASP:HA	1:P:191:PRO:HD3	1.84	0.43
1:P:127:PRO:HB2	1:P:128:PRO:HD2	2.00	0.43
1:P:182:LEU:HB3	1:P:440:ILE:HD13	2.00	0.42
1:P:331:THR:O	1:P:335:ILE:HG12	2.19	0.42
1:P:384:LEU:HB2	1:P:507:LEU:CD1	2.49	0.42
1:P:504:TYR:HB3	1:P:505:PRO:HD3	2.00	0.42
1:P:582:VAL:HG23	1:P:583:PRO:HD2	2.01	0.42
1:P:467:ARG:NH1	1:P:521:SER:OG	2.47	0.42
1:P:207:HIS:HE1	6:P:601:HEM:C1D	2.38	0.42
1:P:206:THR:HB	1:P:210:PHE:CD2	2.55	0.42
1:P:239:GLU:O	1:P:243:GLN:HG2	2.20	0.42
1:P:245:ARG:HD2	1:P:329:PHE:CE1	2.55	0.42
1:P:193:GLY:O	1:P:581:HIS:HA	2.19	0.42
1:P:148:TYR:CZ	1:P:221:THR:HB	2.55	0.42
1:P:182:LEU:HB3	1:P:440:ILE:CD1	2.50	0.41
1:P:157:ARG:H	1:P:157:ARG:HE	1.67	0.41
1:P:196:LEU:HD11	1:P:392:PRO:HG3	2.02	0.41
1:P:112:LEU:HD12	1:P:357:LEU:HD13	2.02	0.41
1:P:300:LEU:O	1:P:304:ILE:HD12	2.20	0.41
1:P:282:GLN:O	1:P:283:SER:CB	2.68	0.41
1:P:509:LEU:HD23	1:P:509:LEU:HA	1.80	0.41
1:P:537:ASN:OD1	1:P:539:ILE:HG12	2.19	0.41
1:P:151:ILE:HG13	1:P:529:PHE:CZ	2.50	0.41
1:P:240:ARG:HG3	1:P:271:VAL:CG2	2.49	0.41
1:P:226:HIS:ND1	1:P:376:ARG:HD2	2.36	0.41
1:P:320:HIS:HB3	1:P:323:TRP:CG	2.55	0.41
1:P:110:ASP:HB3	1:P:365:LEU:HD21	2.02	0.41
3:B:2:NAG:C4	3:B:3:BMA:O2	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	P	551/600 (92%)	497 (90%)	46 (8%)	8 (2%)	10 26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	281	PRO
1	P	430	PRO
1	P	174	ALA
1	P	294	LEU
1	P	160	PRO
1	P	290	GLU
1	P	410	ASN
1	P	271	VAL

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	P	468/530 (88%)	416 (89%)	52 (11%)	6 14

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	33	VAL
1	P	49	ARG
1	P	70	THR

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Mol	Chain	Res	Type
1	P	73	GLU
1	P	92	LEU
1	P	97	ARG
1	P	120	ARG
1	P	123	LEU
1	P	145	VAL
1	P	146	SER
1	P	157	ARG
1	P	165	THR
1	P	166	LYS
1	P	168	LYS
1	P	180	ARG
1	P	185	ARG
1	P	190	ASP
1	P	232	HIS
1	P	241	GLN
1	P	245	ARG
1	P	246	LEU
1	P	252	LEU
1	P	271	VAL
1	P	273	MET
1	P	275	TYR
1	P	277	ARG
1	P	279	ILE
1	P	284	GLN
1	P	289	GLN
1	P	291	VAL
1	P	304	ILE
1	P	307	ARG
1	P	319	GLU
1	P	325	ASP
1	P	376	ARG
1	P	384	LEU
1	P	385	TYR
1	P	409	PHE
1	P	415	VAL
1	P	419	VAL
1	P	433	ARG
1	P	454	GLU
1	P	459	ARG
1	P	482	THR
1	P	484	GLU

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Mol	Chain	Res	Type
1	P	518	PHE
1	P	530	SER
1	P	534	LEU
1	P	554	VAL
1	P	556	PHE
1	P	563	THR
1	P	564	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	90	HIS
1	P	134	HIS
1	P	203	GLN
1	P	204	HIS
1	P	207	HIS
1	P	208	GLN
1	P	237	ASN
1	P	241	GLN
1	P	243	GLN
1	P	282	GLN
1	P	358	GLN
1	P	386	HIS
1	P	442	HIS
1	P	443	HIS
1	P	461	GLN
1	P	581	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

7 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	A	1	2,1	14,14,15	0.55	0	17,19,21	1.15	1 (5%)
2	NAG	A	2	2	14,14,15	0.70	0	17,19,21	1.95	4 (23%)
3	NAG	B	1	3,1	14,14,15	0.47	0	17,19,21	1.23	3 (17%)
3	NAG	B	2	3	14,14,15	0.73	0	17,19,21	1.29	2 (11%)
3	BMA	B	3	3	11,11,12	0.78	0	15,15,17	2.75	6 (40%)
2	NAG	C	1	2,1	14,14,15	0.69	0	17,19,21	1.42	3 (17%)
2	NAG	C	2	2	14,14,15	0.68	0	17,19,21	1.22	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	A	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	A	2	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	B	2	3	-	5/6/23/26	0/1/1/1
3	BMA	B	3	3	-	1/2/19/22	0/1/1/1
2	NAG	C	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	6/6/23/26	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	3	BMA	C1-C2-C3	6.23	117.32	109.67
3	B	3	BMA	C1-O5-C5	6.16	120.54	112.19
2	A	2	NAG	C4-C3-C2	4.94	118.26	111.02
2	A	1	NAG	O5-C5-C6	3.44	112.60	107.20
2	A	2	NAG	O5-C5-C6	3.42	112.56	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	C3-C4-C5	-3.32	104.31	110.24
3	B	3	BMA	C3-C4-C5	-3.26	104.42	110.24
2	C	2	NAG	C1-O5-C5	3.25	116.60	112.19
3	B	3	BMA	O5-C1-C2	3.12	115.59	110.77
2	A	2	NAG	C3-C4-C5	3.12	115.80	110.24
2	C	1	NAG	O5-C5-C6	3.07	112.01	107.20
2	A	2	NAG	C1-O5-C5	-2.96	108.18	112.19
3	B	2	NAG	C4-C3-C2	2.83	115.17	111.02
3	B	2	NAG	O5-C1-C2	-2.56	107.25	111.29
2	C	1	NAG	O4-C4-C5	2.50	115.51	109.30
3	B	1	NAG	C1-O5-C5	2.47	115.54	112.19
3	B	1	NAG	O4-C4-C3	-2.27	105.10	110.35
2	C	2	NAG	C4-C3-C2	2.22	114.28	111.02
3	B	3	BMA	O4-C4-C5	2.06	114.40	109.30
3	B	1	NAG	O4-C4-C5	2.02	114.32	109.30
3	B	3	BMA	O5-C5-C6	2.02	110.38	107.20

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C3-C2-N2-C7
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	A	1	NAG	C8-C7-N2-C2
2	A	1	NAG	O7-C7-N2-C2
3	B	2	NAG	C8-C7-N2-C2
3	B	2	NAG	O7-C7-N2-C2
2	A	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	A	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
2	C	1	NAG	C4-C5-C6-O6
2	A	1	NAG	O5-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6
3	B	2	NAG	O5-C5-C6-O6
3	B	2	NAG	C1-C2-N2-C7
2	A	1	NAG	C4-C5-C6-O6

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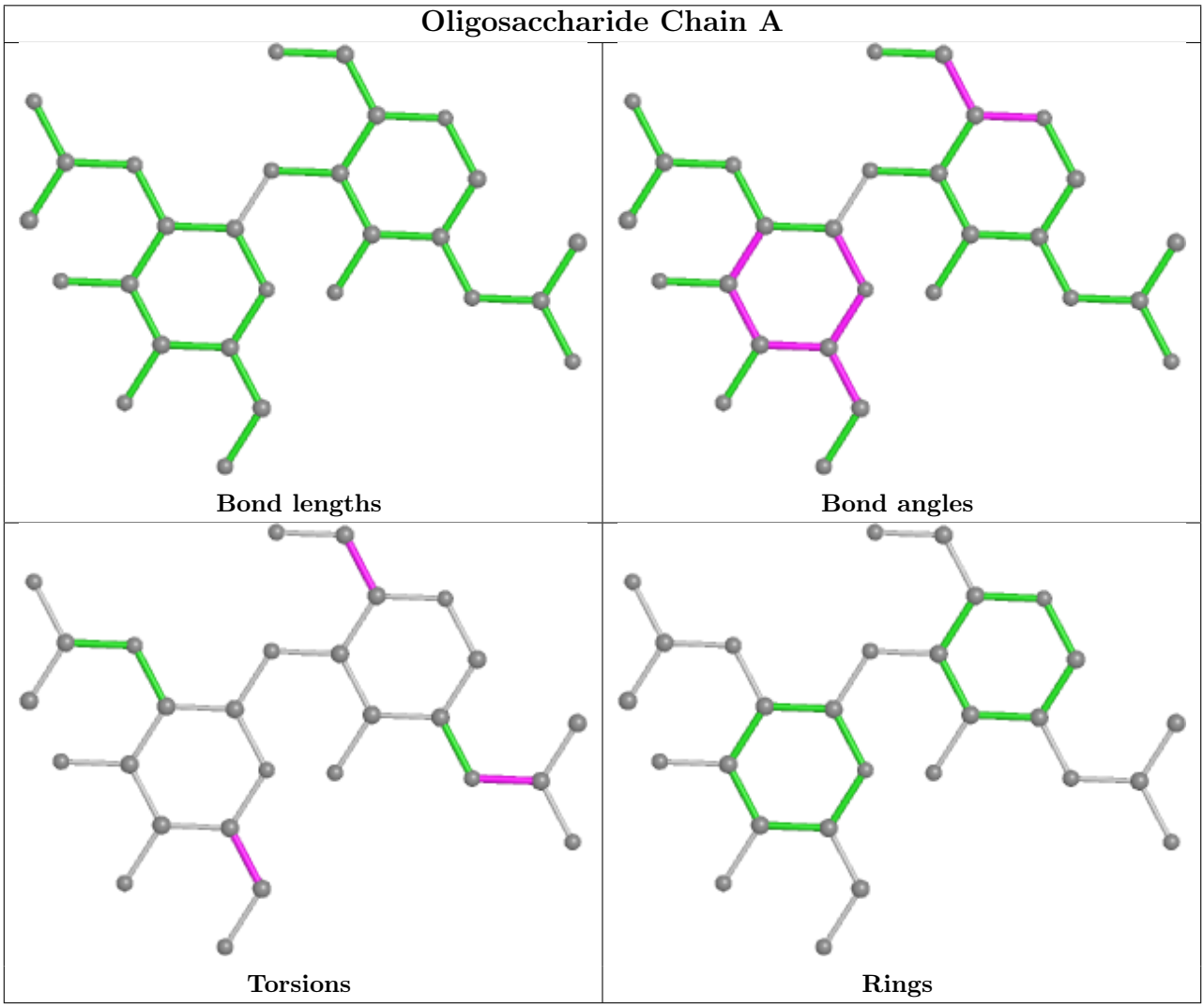
Mol	Chain	Res	Type	Atoms
3	B	3	BMA	O5-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6

There are no ring outliers.

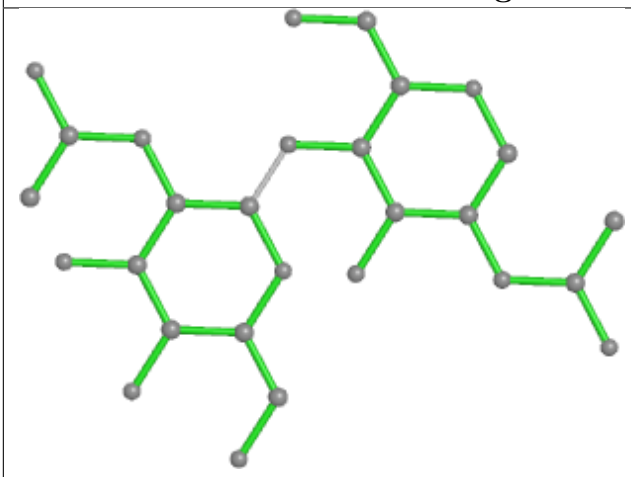
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3	BMA	2	0
3	B	2	NAG	4	0

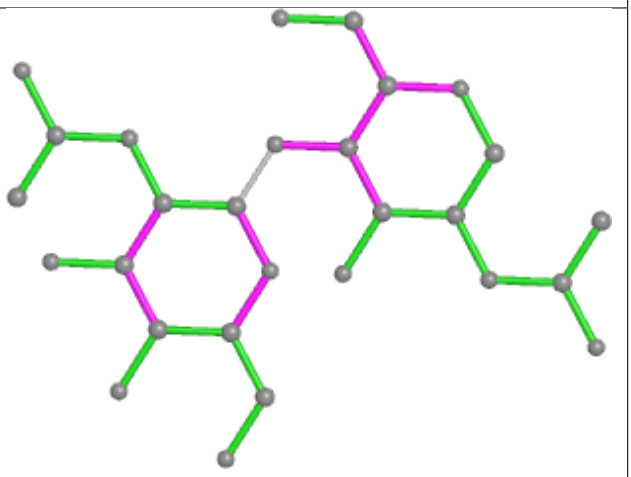
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



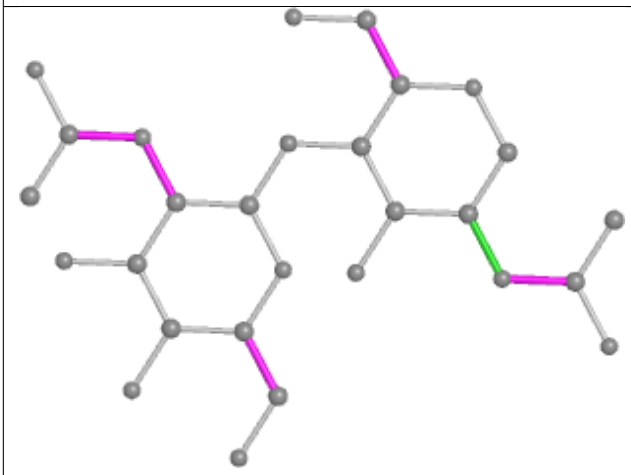
Oligosaccharide Chain C



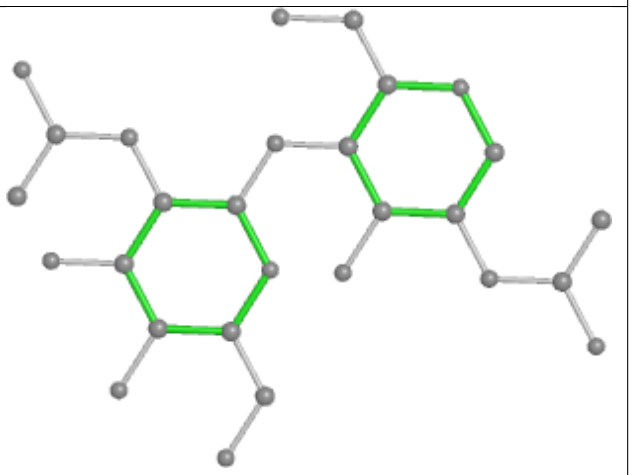
Bond lengths



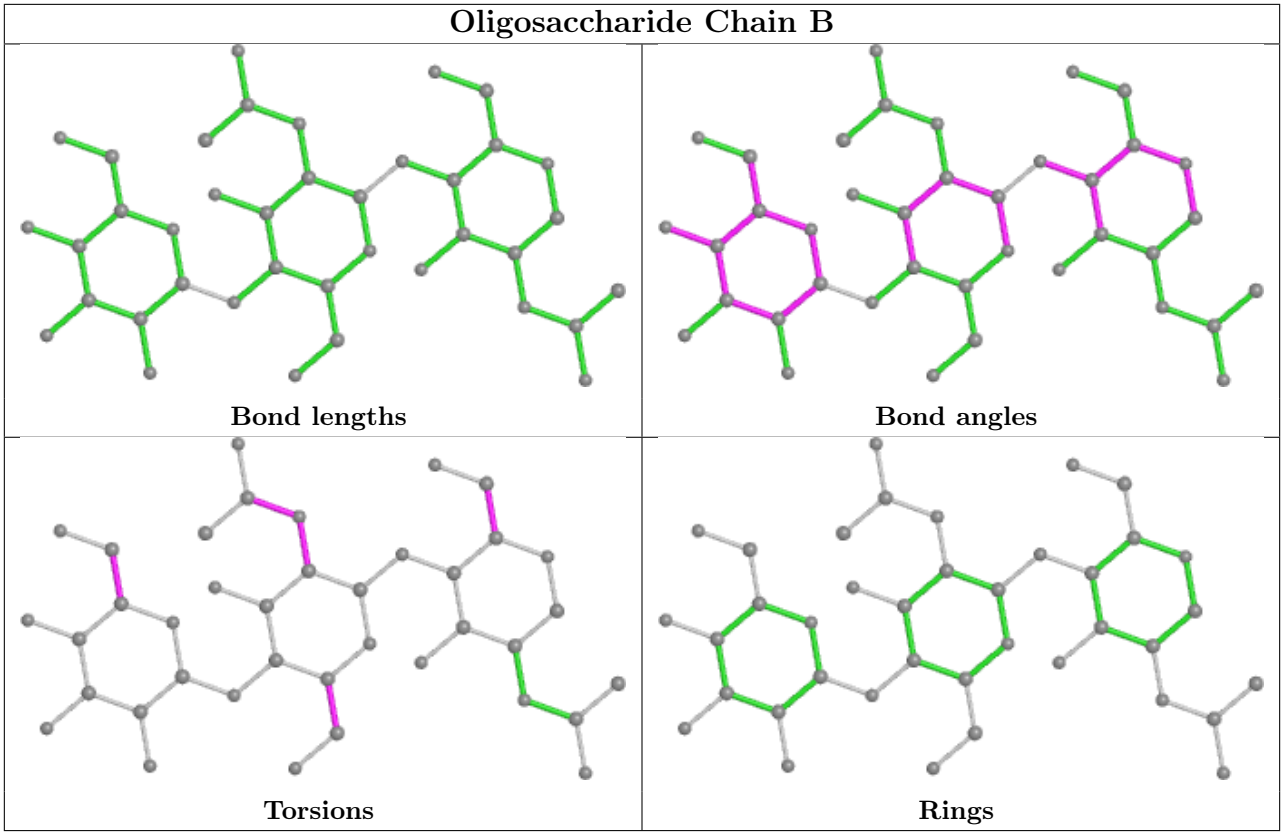
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

4 ligands 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	$\#\|Z\| > 2$
4	BOG	P	750	-	12,12,20	0.54	0	17,17,25	0.70	1 (5%)
5	IMS	P	700	-	29,32,32	2.27	2 (6%)	35,45,45	2.64	14 (40%)
4	BOG	P	751	-	12,12,20	0.46	0	17,17,25	1.02	2 (11%)
6	HEM	P	601	1	41,50,50	1.97	5 (12%)	45,82,82	1.71	9 (20%)

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	BOG	P	750	-	-	0/2/22/31	0/1/1/1
5	IMS	P	700	-	-	8/18/22/22	0/3/3/3
4	BOG	P	751	-	-	0/2/22/31	0/1/1/1
6	HEM	P	601	1	-	0/12/54/54	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	700	IMS	C13-CL	-10.91	1.50	1.74
6	P	601	HEM	C3D-C2D	8.09	1.53	1.36
6	P	601	HEM	C3C-C2C	-4.02	1.34	1.40
5	P	700	IMS	C-N	-3.97	1.33	1.39
6	P	601	HEM	C3C-CAC	3.75	1.55	1.47
6	P	601	HEM	FE-ND	3.57	2.14	1.96
6	P	601	HEM	CAB-C3B	2.88	1.55	1.47

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	700	IMS	C19-N2-C18	8.80	135.89	122.92
6	P	601	HEM	C4D-ND-C1D	5.45	110.70	105.07
5	P	700	IMS	C10-C9-N	4.76	123.51	117.95
5	P	700	IMS	C17-C18-N2	-4.43	108.74	115.88
6	P	601	HEM	C4C-CHD-C1D	4.27	128.19	122.56
5	P	700	IMS	C21-C19-N2	-4.16	105.28	110.32
5	P	700	IMS	C16-C8-N	3.69	127.02	122.37
5	P	700	IMS	C17-C7-C8	3.50	129.49	126.41
5	P	700	IMS	O1-C9-C10	-3.46	113.50	120.23
5	P	700	IMS	O2-C18-N2	3.10	128.18	122.95
5	P	700	IMS	C6-O-C3	2.93	123.88	117.51
6	P	601	HEM	C1B-NB-C4B	2.87	108.04	105.07
6	P	601	HEM	CHB-C1B-NB	2.75	127.78	124.38
5	P	700	IMS	C11-C10-C15	2.73	122.47	118.59
6	P	601	HEM	C3B-C2B-C1B	2.61	108.42	106.49
6	P	601	HEM	O2D-CGD-CBD	2.53	122.15	114.03
5	P	700	IMS	C7-C17-C18	2.48	121.44	113.94
6	P	601	HEM	CHD-C1D-ND	2.36	127.00	124.43
5	P	700	IMS	C2-C1-C7	-2.36	130.10	134.17
6	P	601	HEM	O1D-CGD-CBD	-2.30	115.69	123.08
4	P	750	BOG	O5-C5-C6	2.28	112.11	106.44
6	P	601	HEM	CMA-C3A-C4A	-2.23	125.03	128.46
5	P	700	IMS	C11-C10-C9	-2.19	115.53	120.26
5	P	700	IMS	C12-C11-C10	-2.17	118.26	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	751	BOG	C1-O5-C5	2.08	117.59	113.66
4	P	751	BOG	C4-C3-C2	-2.05	107.24	110.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	P	700	IMS	C2-C3-O-C6
5	P	700	IMS	C4-C3-O-C6
5	P	700	IMS	C21-C19-C20-O3
5	P	700	IMS	C20-C19-N2-C18
5	P	700	IMS	N2-C19-C20-O3
5	P	700	IMS	C15-C10-C9-N
5	P	700	IMS	C11-C10-C9-N
5	P	700	IMS	C20-C19-C21-C22

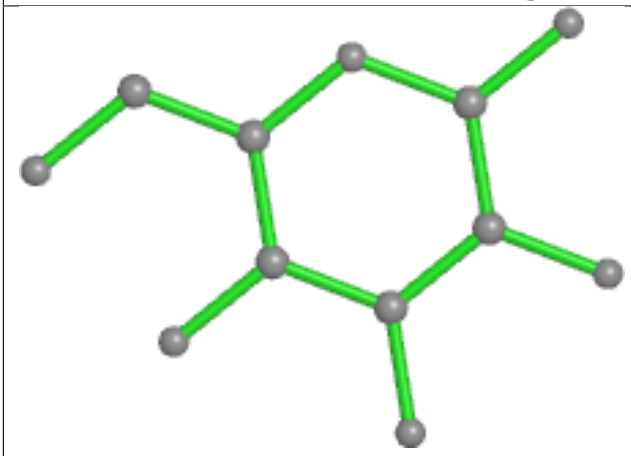
There are no ring outliers.

2 monomers are involved in 30 short contacts:

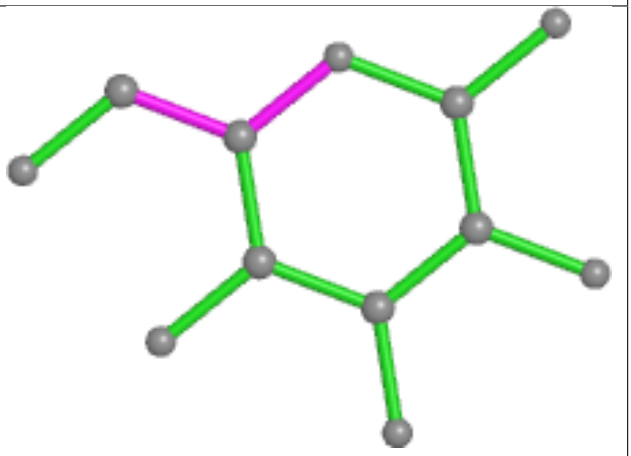
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	700	IMS	26	0
6	P	601	HEM	4	0

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 then 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.

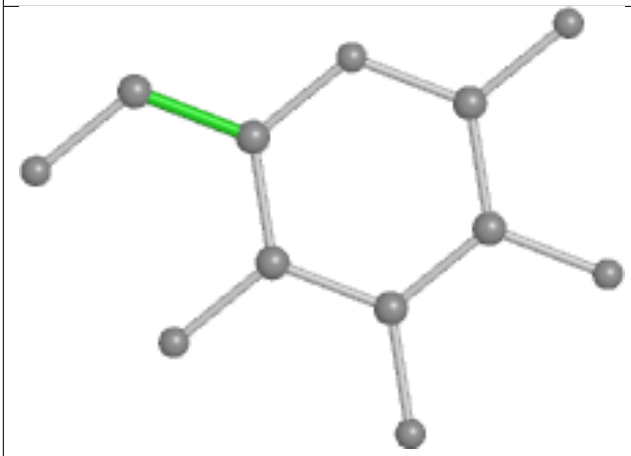
Ligand BOG P 750



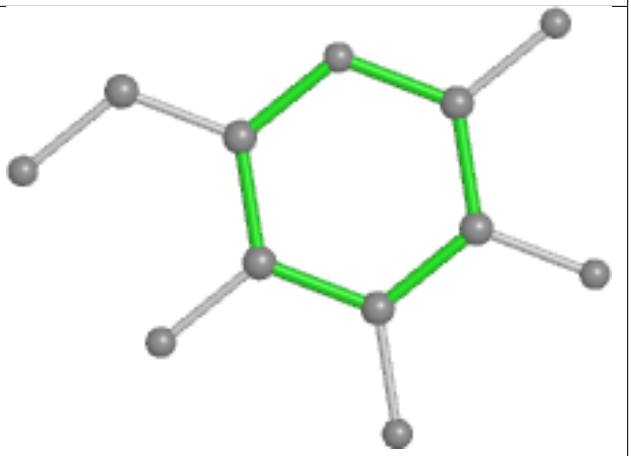
Bond lengths



Bond angles

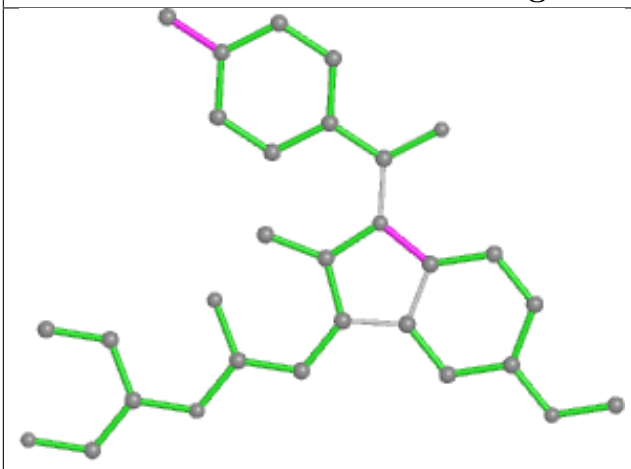


Torsions

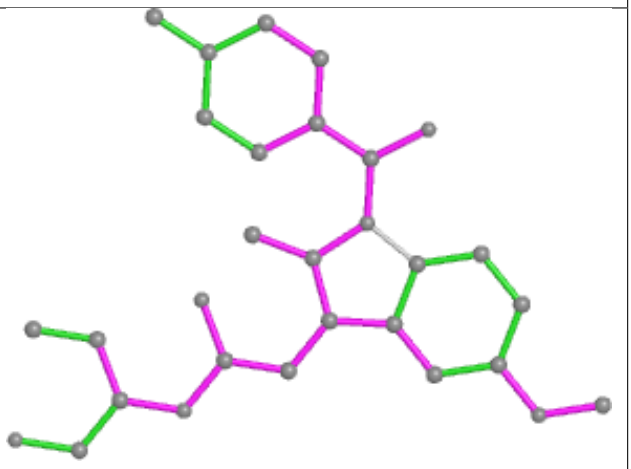


Rings

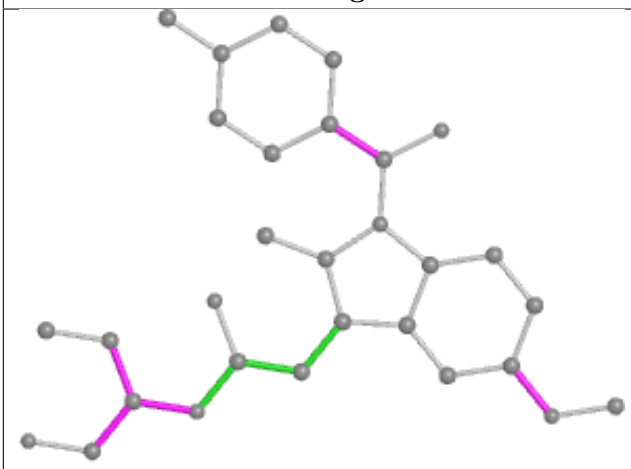
Ligand IMS P 700



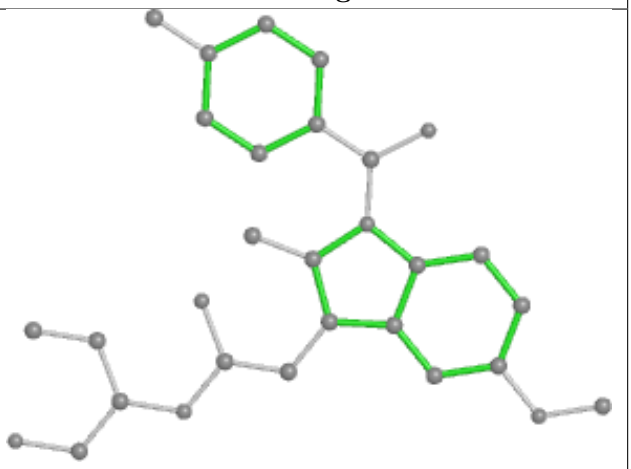
Bond lengths



Bond angles

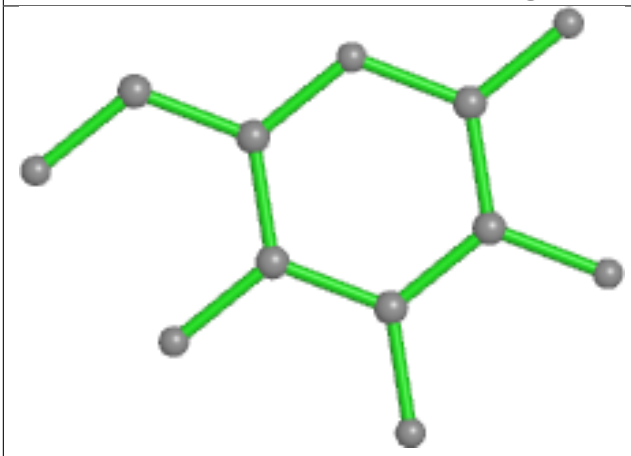


Torsions

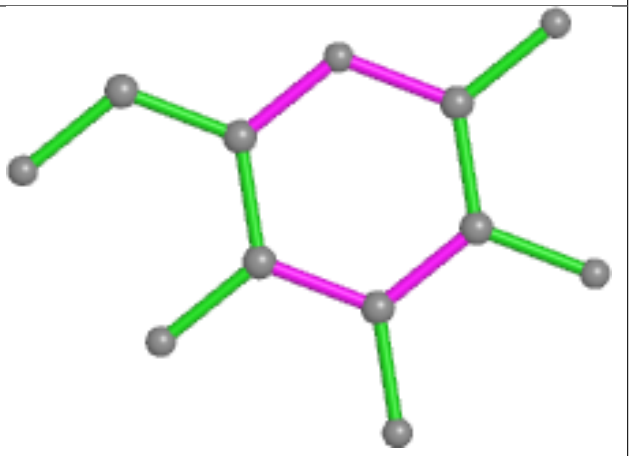


Rings

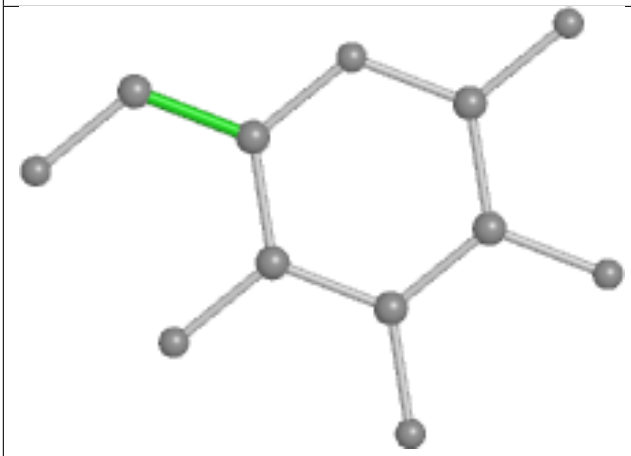
Ligand BOG P 751



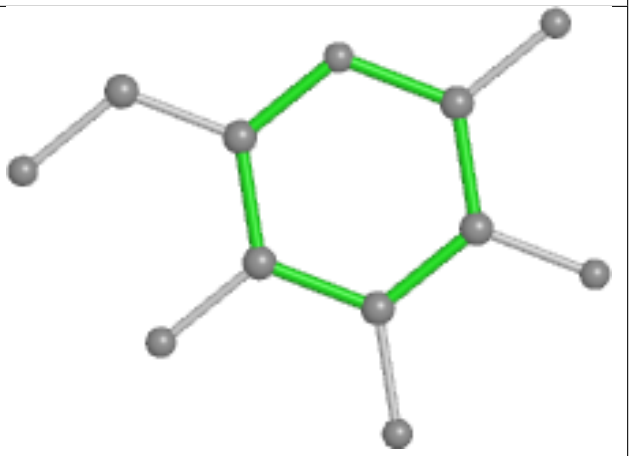
Bond lengths



Bond angles

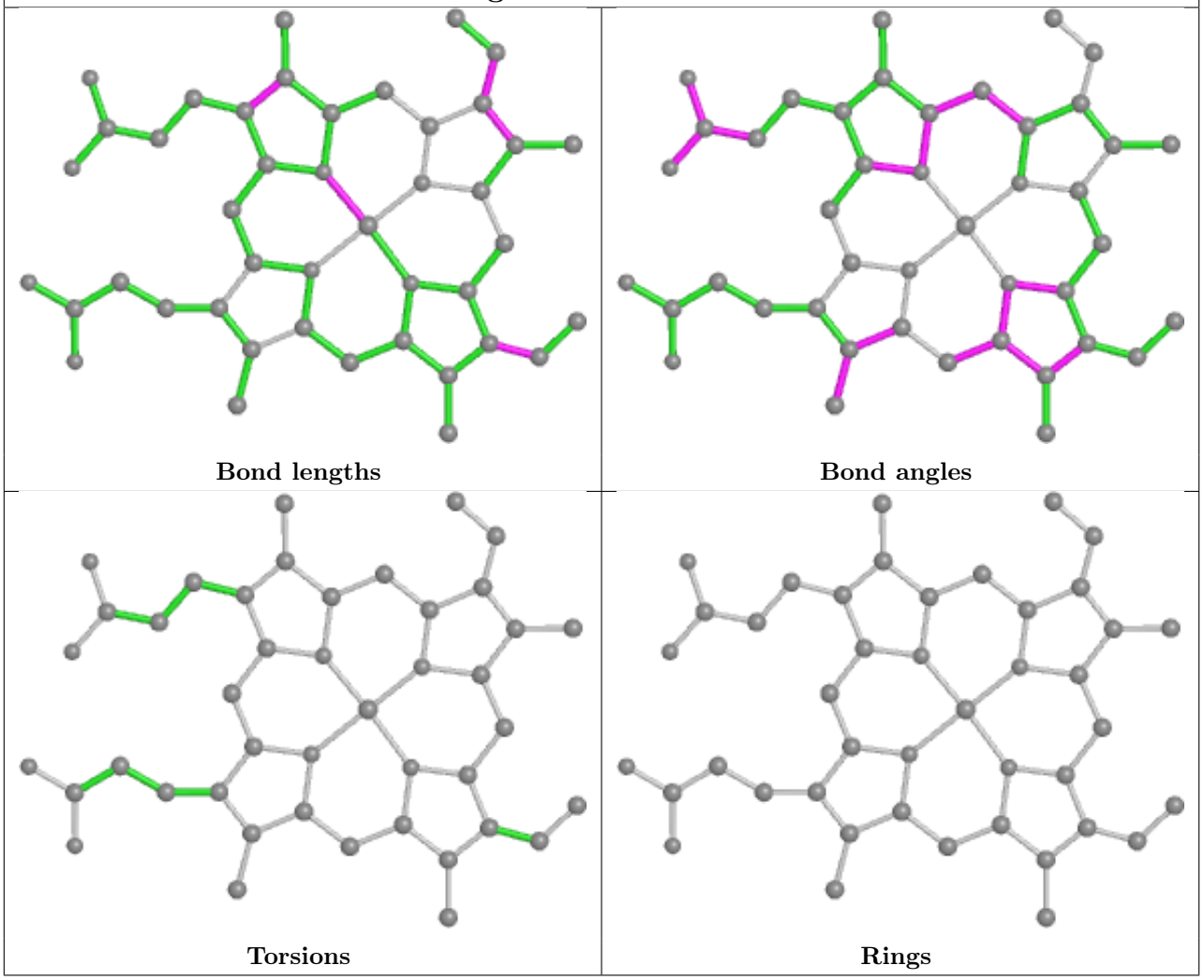


Torsions



Rings

Ligand HEM P 601



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

Unable to reproduce the depositors R factor - this section is therefore empty.

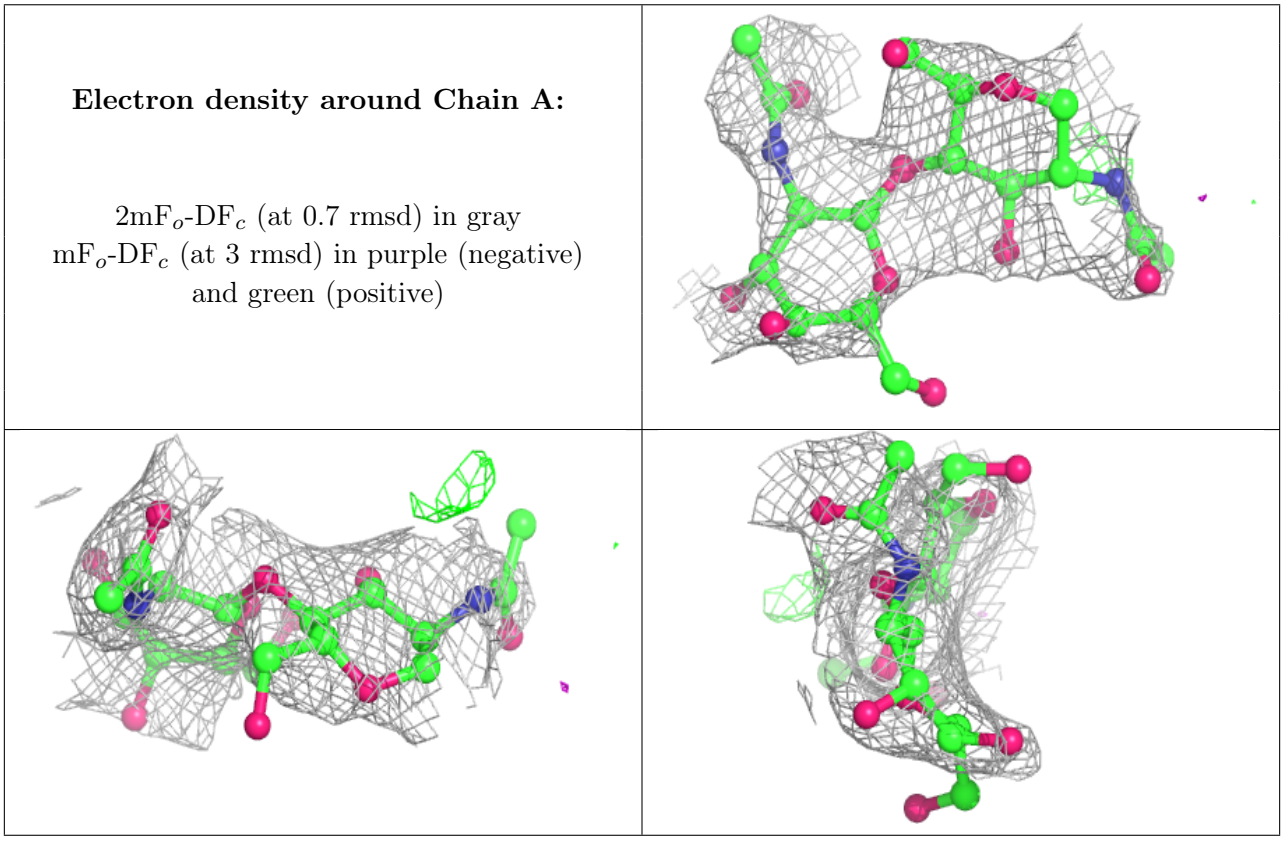
6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

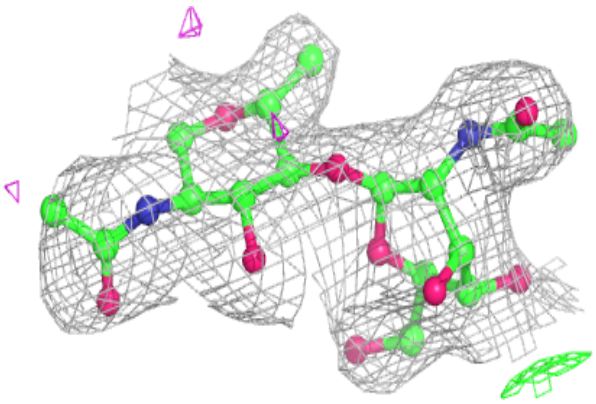
Unable to reproduce the depositors R factor - this section is therefore empty.

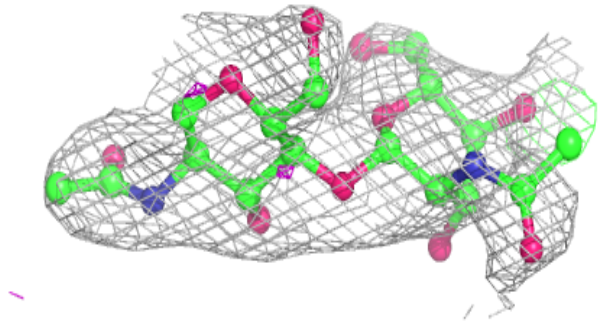
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

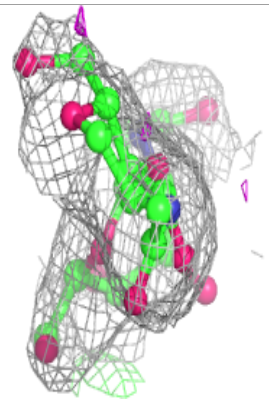


Electron density around Chain C:

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

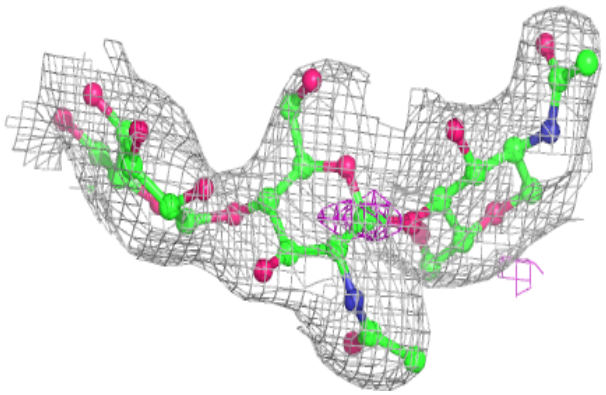


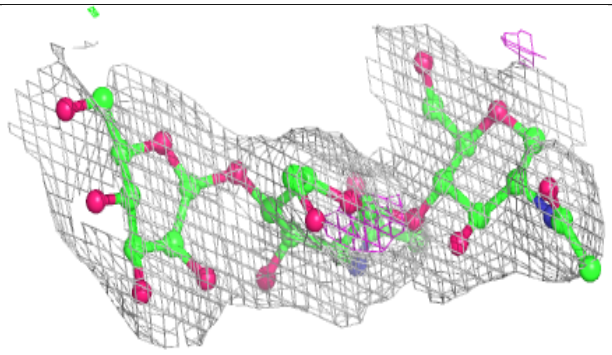


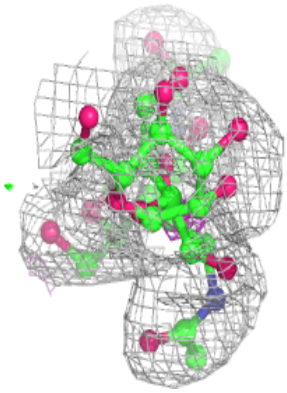


Electron density around Chain B:

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







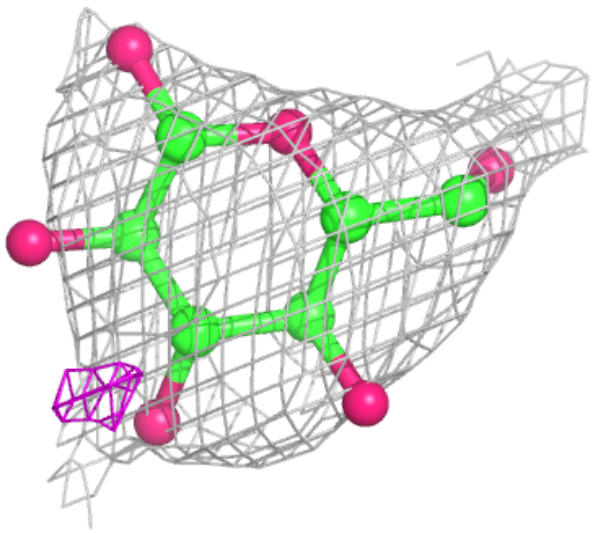
6.4 Ligands (i)

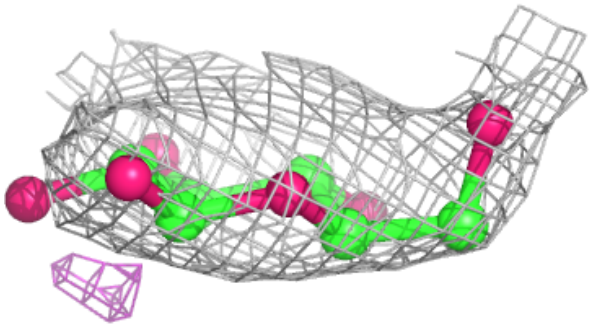
Unable to reproduce the depositors R factor - this section is therefore empty.

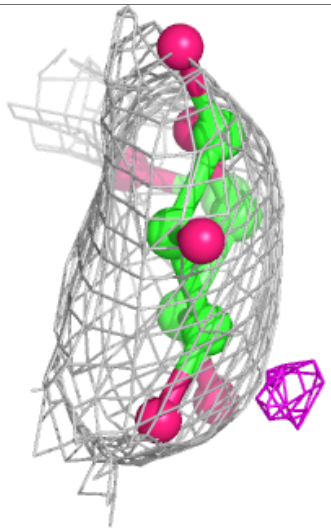
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG P 750:

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

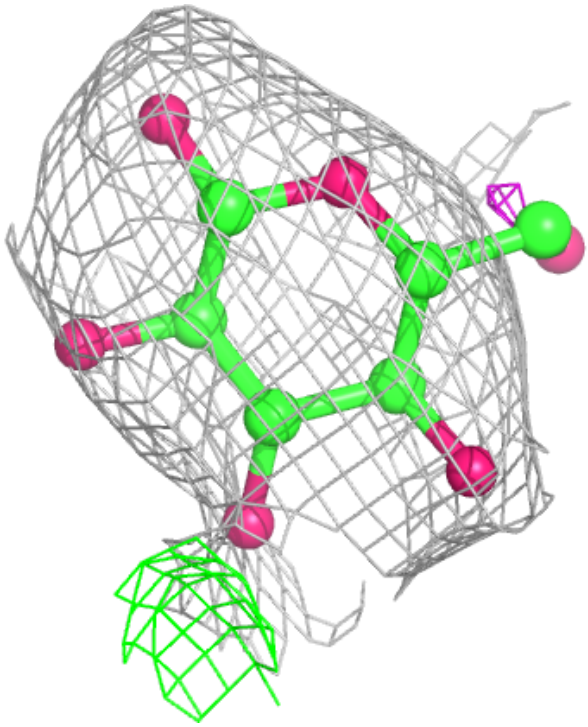


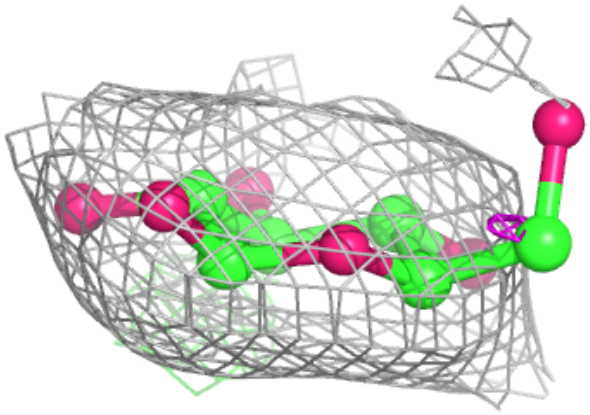


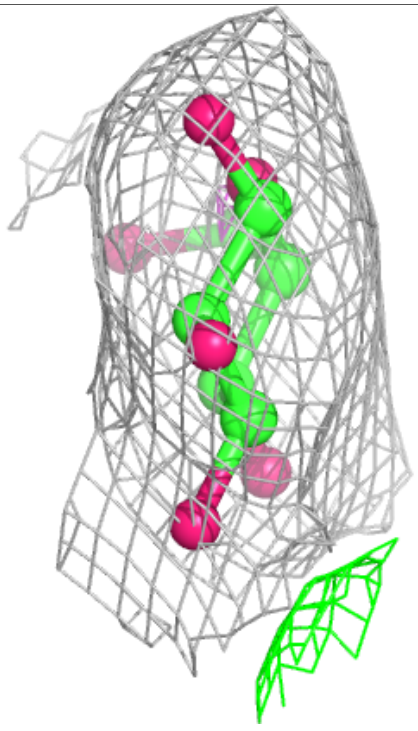


Electron density around BOG P 751:

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

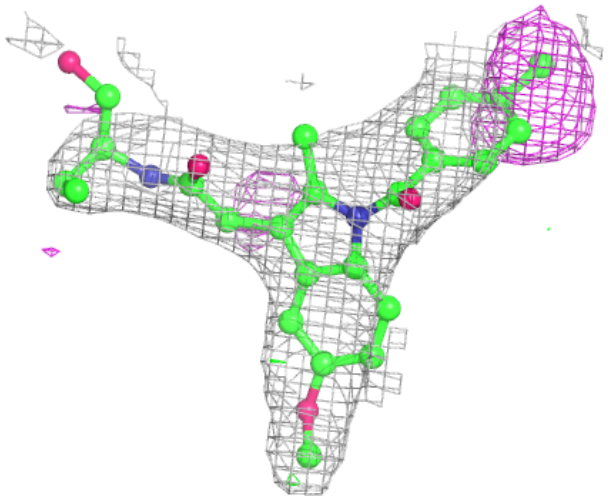


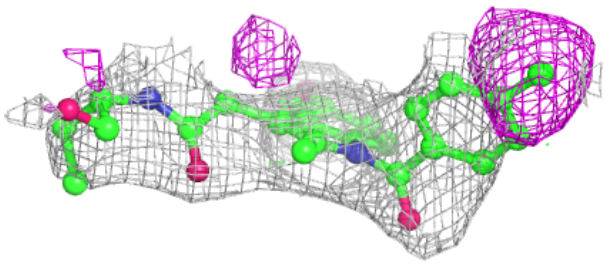


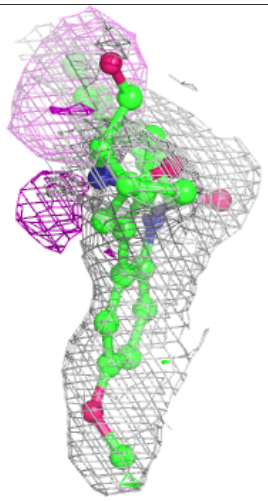


Electron density around IMS P 700:

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

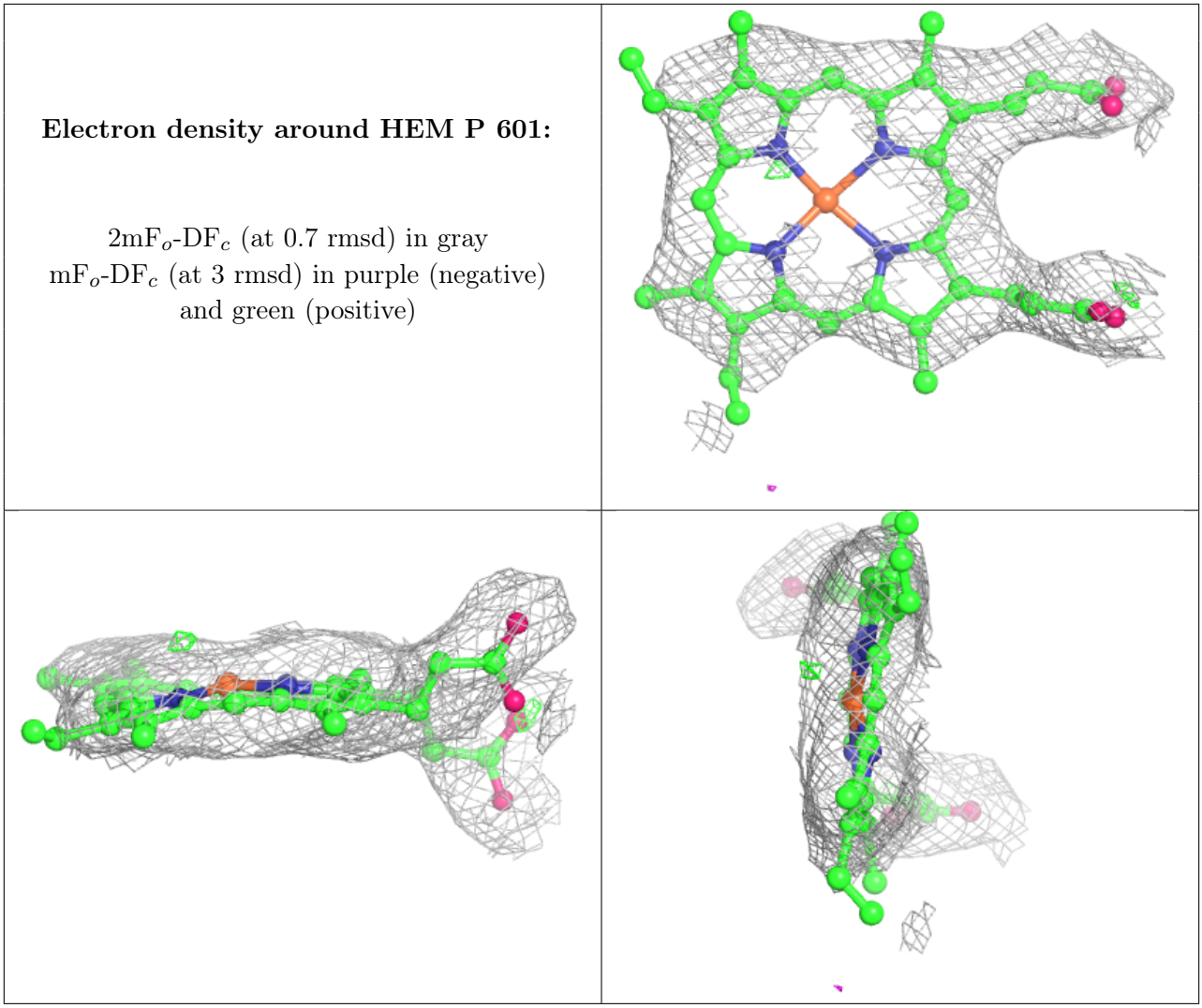






Electron density around HEM P 601:

$2mF_o$-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 (i)

Unable to reproduce the depositors R factor - this section is therefore empty.