



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2026 – 10:40 PM EDT

PDB ID : 4PH9 / pdb_00004ph9
Title : The structure of Ibuprofen bound to cyclooxygenase-2
Authors : Orlando, B.J.; Lucido, M.J.; Malkowski, M.G.
Deposited on : 2014-05-05
Resolution : 1.81 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

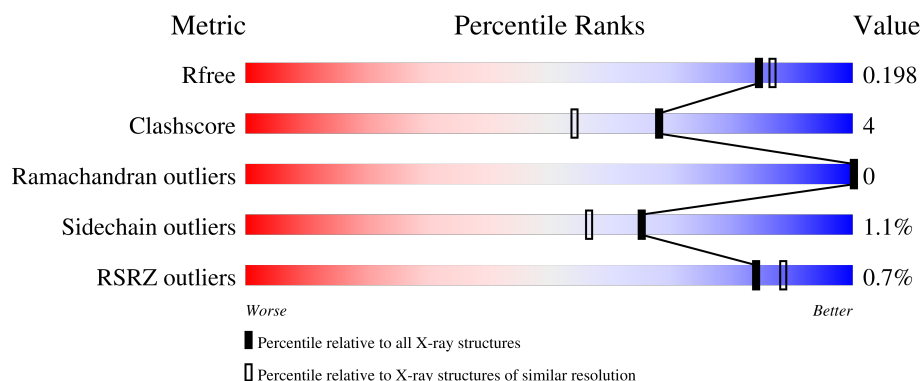
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	551	92% 8%
1	B	551	94% 6%
2	C	2	100%
2	D	2	50% 50%
3	E	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
8	AKR	A	609	-	X	X	-
8	AKR	A	610	-	X	-	-
8	AKR	B	611	-	X	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10527 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	5	0
			4515	2909	759	821	26			
1	B	551	Total	C	N	O	S	0	3	0
			4500	2901	757	816	26			

There are 4 discrepancies between the modelled and reference sequences:

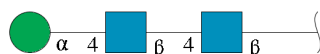
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	HIS	-	expression tag	UNP Q05769
A	34	HIS	-	expression tag	UNP Q05769
B	33	HIS	-	expression tag	UNP Q05769
B	34	HIS	-	expression tag	UNP Q05769

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



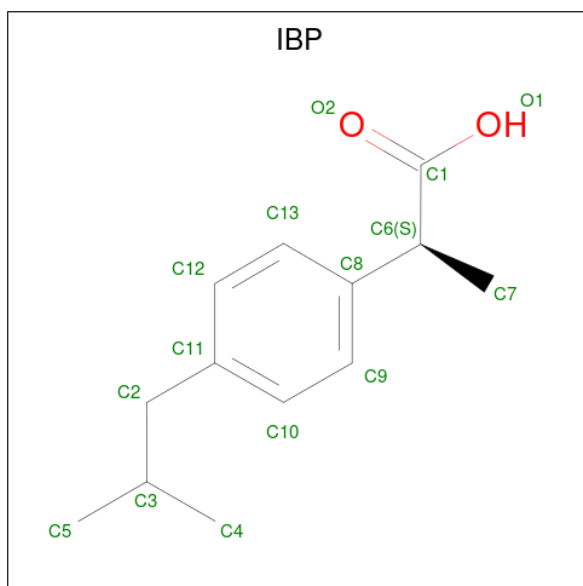
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



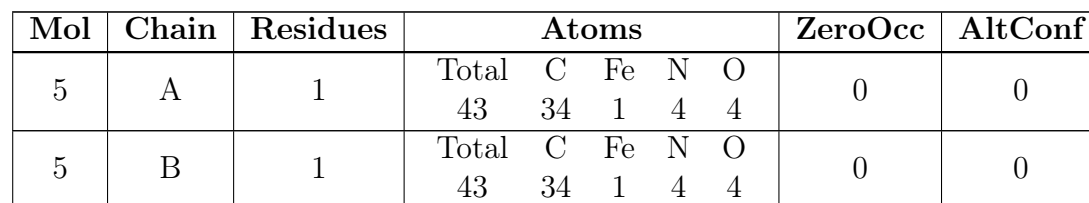
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is IBUPROFEN (CCD ID: IBP) (formula: $C_{13}H_{18}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			15	13	2		
4	B	1	Total	C	O	0	0
			15	13	2		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



- # BOG
-
- The diagram illustrates the chemical structure of Biotin (BOG). It features a fused bicyclic core consisting of a cyclohexane ring and a five-membered imidazolidine ring. The stereocenters are labeled as C1(R), C2(R), C3(S), C4(S), and C5(R). The hydroxyl groups are labeled O1, O2, O3, O4, O5, and O6. The side chain is a branched alkyl chain starting from C1' and extending to C8'.

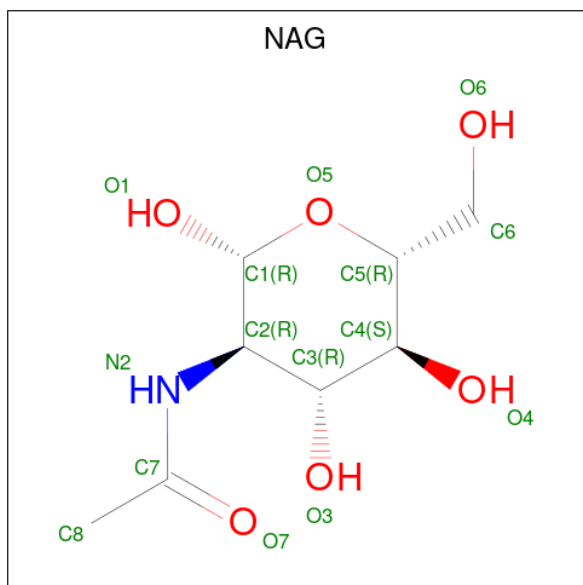
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 20	C 14	O 6	0	0
6	A	1	Total 20	C 14	O 6	0	0



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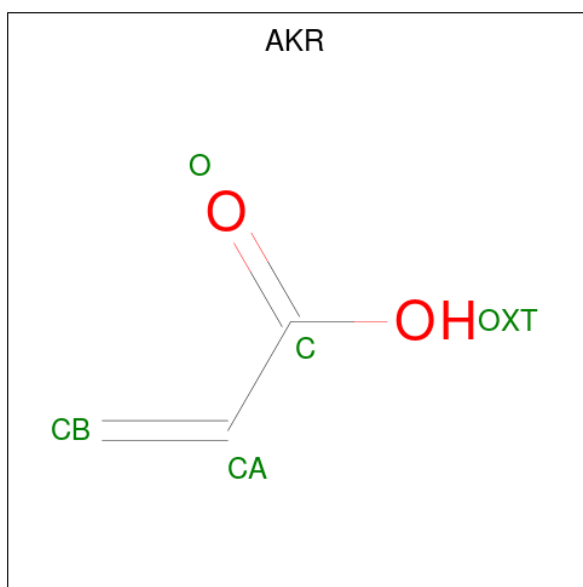
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



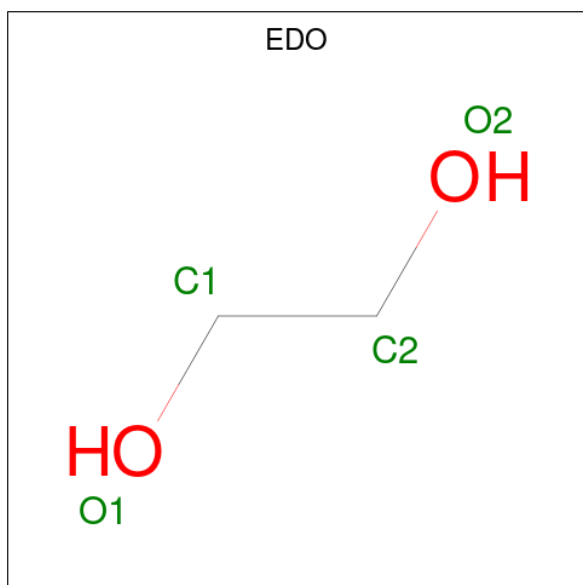
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is ACRYLIC ACID (CCD ID: AKR) (formula: $C_3H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			5	3	2		
8	A	1	Total	C	O	0	0
			5	3	2		
8	B	1	Total	C	O	0	0
			5	3	2		
8	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

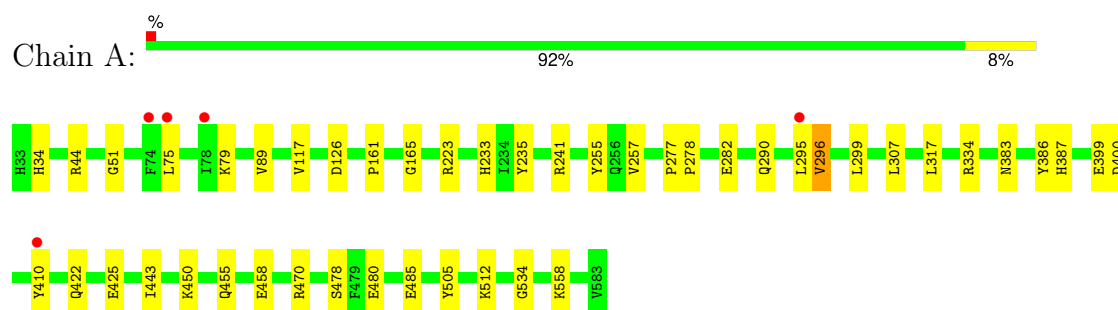
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	545	Total O 545 545	0	0
10	B	582	Total O 582 582	0	0

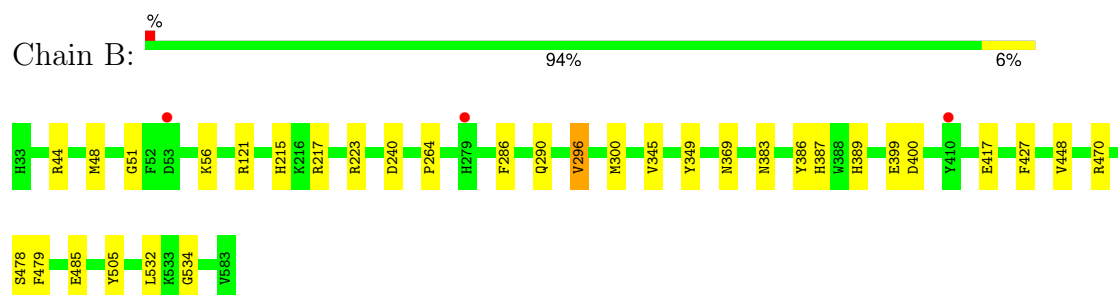
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

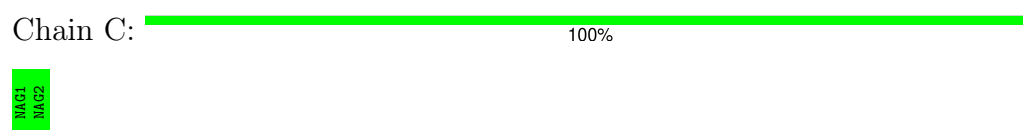
- Molecule 1: Prostaglandin G/H synthase 2



- Molecule 1: Prostaglandin G/H synthase 2



- 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



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

Chain E:  33% 67%

MAG1
MAG2
MAG3

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.94Å 132.23Å 180.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.55 – 1.81 35.55 – 1.81	Depositor EDS
% Data completeness (in resolution range)	98.0 (35.55-1.81) 88.2 (35.55-1.81)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, R_{free}	0.160 , 0.197 0.161 , 0.198	Depositor DCC
R_{free} test set	6431 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.1	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	0.97	EDS
Total number of atoms	10527	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: BOG, HEM, IBP, EDO, AKR, MAN, 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	0.68	0/4644	0.85	5/6295 (0.1%)
1	B	0.67	0/4629	0.84	5/6275 (0.1%)
All	All	0.68	0/9273	0.85	10/12570 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	HIS	CA-C-N	6.80	126.50	119.56
1	A	34	HIS	C-N-CA	6.80	126.50	119.56
1	B	51	GLY	N-CA-C	-6.51	102.04	110.69
1	A	51	GLY	N-CA-C	-6.22	102.04	110.80
1	A	505	TYR	CA-C-N	-5.13	113.75	119.19
1	A	505	TYR	C-N-CA	-5.13	113.75	119.19
1	B	389	HIS	CA-C-N	-5.06	114.40	119.56
1	B	389	HIS	C-N-CA	-5.06	114.40	119.56
1	B	505	TYR	CA-C-N	-5.04	113.85	119.19
1	B	505	TYR	C-N-CA	-5.04	113.85	119.19

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	4515	0	4402	35	0
1	B	4500	0	4393	27	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	E	39	0	34	1	0
4	A	15	0	17	0	0
4	B	15	0	17	0	0
5	A	43	0	30	2	0
5	B	43	0	30	3	0
6	A	40	0	56	3	0
6	B	20	0	28	0	0
7	A	28	0	26	0	0
7	B	14	0	13	0	0
8	A	10	0	6	6	0
8	B	10	0	6	7	0
9	A	24	0	36	4	0
9	B	28	0	42	2	0
10	A	545	0	0	10	1
10	B	582	0	0	4	1
All	All	10527	0	9186	66	1

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 4.

All (66) 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:B:215:HIS:ND1	10:B:1238:HOH:O	2.11	0.84
1:A:126:ASP:OD2	10:A:1087:HOH:O	2.00	0.79
1:B:479:PHE:H	8:B:611:AKR:HA1	1.49	0.78
1:A:295:LEU:HG	1:A:296:VAL:HG12	1.69	0.75
1:A:241:ARG:HH11	8:A:610:AKR:HA1	1.56	0.70
1:B:223:ARG:NH2	10:B:1246:HOH:O	2.14	0.65
1:B:44[B]:ARG:HD3	1:B:470:ARG:HD2	1.78	0.64
1:A:455:GLN:NE2	10:A:1129:HOH:O	2.31	0.63
1:A:480:GLU:HB2	8:A:609:AKR:HB3	1.85	0.58
1:B:264:PRO:HG2	1:B:300[B]:MET:HE1	1.86	0.57
1:A:443:ILE:HD11	6:A:603:BOG:H6'2	1.86	0.56
1:A:223:ARG:NH1	10:A:994:HOH:O	2.39	0.56
1:A:558:LYS:NZ	10:A:703:HOH:O	2.39	0.55
1:A:117:VAL:HG22	6:A:604:BOG:H3'1	1.88	0.55
1:B:479:PHE:N	8:B:611:AKR:HA1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ARG:NH1	3:E:2:NAG:O7	2.40	0.54
1:A:399:GLU:HG2	1:A:422:GLN:OE1	2.08	0.53
1:A:44[B]:ARG:HD3	1:A:470:ARG:HD2	1.91	0.53
1:B:383:ASN:O	1:B:387:HIS:HD2	1.93	0.52
5:A:602:HEM:HBC2	5:A:602:HEM:HHD	1.91	0.51
1:A:480:GLU:H	8:A:609:AKR:CA	2.24	0.51
5:B:602:HEM:HMB1	5:B:602:HEM:HBB2	1.92	0.51
1:B:240:ASP:HB3	8:B:610:AKR:HB3	1.93	0.50
1:A:255:TYR:CZ	9:A:614:EDO:H21	2.46	0.50
1:A:480:GLU:H	8:A:609:AKR:HA1	1.76	0.50
1:B:478:SER:HB2	8:B:611:AKR:HA1	1.93	0.49
1:A:383:ASN:O	1:A:387:HIS:HD2	1.95	0.49
10:A:1163:HOH:O	9:B:615:EDO:H21	2.11	0.49
1:B:479:PHE:H	8:B:611:AKR:CA	2.20	0.49
1:B:286:PHE:HD2	1:B:300[B]:MET:HE2	1.78	0.49
1:A:295:LEU:CG	1:A:296:VAL:HG12	2.42	0.48
1:B:286:PHE:CD2	1:B:300[B]:MET:HE2	2.49	0.48
9:A:613:EDO:H12	1:B:48:MET:HE1	1.94	0.48
1:A:425:GLU:OE1	10:A:975:HOH:O	2.20	0.48
1:A:400:ASP:OD1	1:A:400:ASP:N	2.48	0.47
1:A:534:GLY:HA3	9:A:616:EDO:O2	2.15	0.47
1:A:480:GLU:HG3	8:A:609:AKR:HA1	1.97	0.47
1:A:512:LYS:NZ	10:A:872:HOH:O	2.47	0.47
1:B:448:VAL:HG13	5:B:602:HEM:HBA1	1.97	0.47
1:A:295:LEU:HA	1:A:410:TYR:CE1	2.50	0.46
1:A:161:PRO:HD2	1:A:165:GLY:O	2.15	0.46
1:A:235:TYR:CE2	1:A:334:ARG:HG3	2.51	0.46
1:A:89:VAL:HG11	6:A:604:BOG:H4'2	1.98	0.46
1:A:257:VAL:O	10:A:701:HOH:O	2.20	0.46
1:B:121:ARG:HG3	1:B:532:LEU:HD12	1.97	0.45
1:A:450:LYS:NZ	10:A:1033:HOH:O	2.49	0.45
1:A:75:LEU:O	1:A:79:LYS:HG2	2.16	0.45
1:A:307:LEU:C	1:A:307:LEU:HD23	2.42	0.44
1:B:44[B]:ARG:HD2	10:B:1031:HOH:O	2.18	0.44
1:B:345:VAL:HA	1:B:349:TYR:HB3	2.00	0.44
1:A:296:VAL:HG13	1:A:299:LEU:HD12	2.00	0.43
1:A:296:VAL:HG22	1:A:299:LEU:H	1.82	0.43
1:B:534:GLY:HA3	9:B:616:EDO:O2	2.18	0.43
1:A:458[B]:GLU:OE1	10:A:1229:HOH:O	2.21	0.43
1:A:478:SER:HB2	8:A:609:AKR:CB	2.49	0.43
1:B:478:SER:HB2	8:B:611:AKR:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:SER:CA	8:B:611:AKR:HA1	2.50	0.42
1:B:427:PHE:HD1	1:B:427:PHE:HA	1.71	0.42
1:B:369:ASN:HB3	10:B:1257:HOH:O	2.19	0.42
5:A:602:HEM:HBB2	5:A:602:HEM:HMB2	2.02	0.41
1:B:399:GLU:HB3	1:B:400:ASP:H	1.56	0.41
9:A:613:EDO:H11	1:B:56:LYS:HG2	2.02	0.41
1:A:317:LEU:HD23	1:A:317:LEU:HA	1.89	0.41
1:A:277:PRO:HA	1:A:278:PRO:HD3	1.94	0.40
1:B:286:PHE:HD2	1:B:300[A]:MET:HG2	1.87	0.40
1:B:296:VAL:HG21	5:B:602:HEM:CBB	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:749:HOH:O	10:B:737:HOH:O[7_555]	2.16	0.04

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	554/551 (100%)	541 (98%)	13 (2%)	0	100	100
1	B	552/551 (100%)	539 (98%)	13 (2%)	0	100	100
All	All	1106/1102 (100%)	1080 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	498/493 (101%)	492 (99%)	6 (1%)	63	54
1	B	496/493 (101%)	491 (99%)	5 (1%)	68	60
All	All	994/986 (101%)	983 (99%)	11 (1%)	65	56

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	A	282	GLU
1	A	290	GLN
1	A	296	VAL
1	A	386	TYR
1	A	485	GLU
1	B	290	GLN
1	B	296	VAL
1	B	386	TYR
1	B	417	GLU
1	B	485	GLU

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	95	HIS
1	A	256	GLN
1	A	319	GLN
1	A	572	ASN
1	B	319	GLN
1	B	561	ASN
1	B	572	ASN

5.3.3 RNA ⓘ

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	C	1	2,1	14,14,15	0.26	0	17,19,21	0.67	0
2	NAG	C	2	2	14,14,15	0.54	0	17,19,21	0.43	0
2	NAG	D	1	2,1	14,14,15	0.56	0	17,19,21	0.72	1 (5%)
2	NAG	D	2	2	14,14,15	0.25	0	17,19,21	0.39	0
3	NAG	E	1	3,1	14,14,15	0.22	0	17,19,21	0.64	0
3	NAG	E	2	3	14,14,15	0.66	0	17,19,21	0.73	0
3	MAN	E	3	3	11,11,12	1.18	1 (9%)	15,15,17	1.80	2 (13%)

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	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	MAN	E	3	3	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	MAN	O5-C5	2.07	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	MAN	C1-O5-C5	5.80	119.96	112.19
3	E	3	MAN	O2-C2-C3	-2.64	104.68	110.15
2	D	1	NAG	C1-O5-C5	2.27	115.23	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

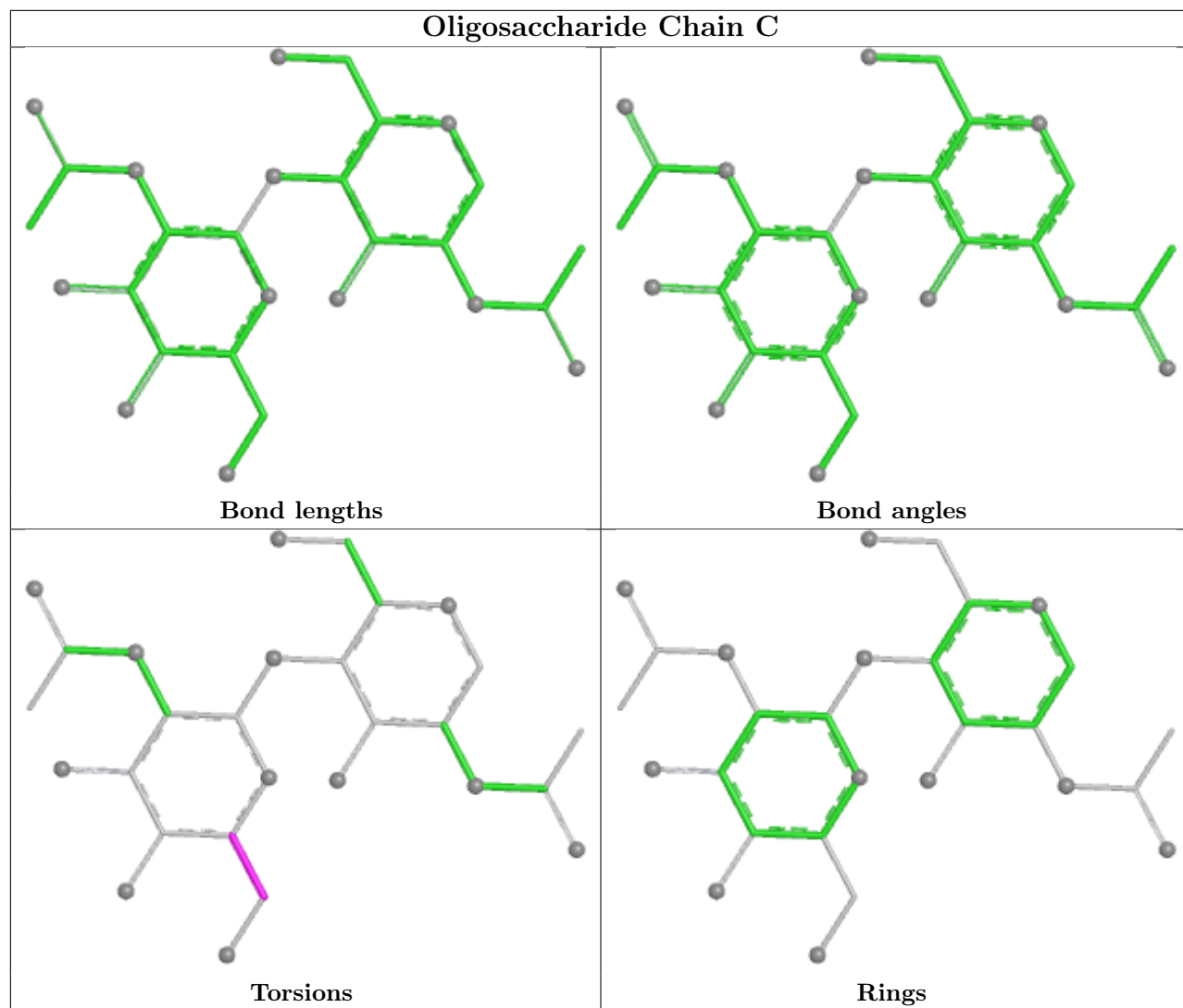
Mol	Chain	Res	Type	Atoms
3	E	3	MAN	O5-C5-C6-O6
3	E	3	MAN	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

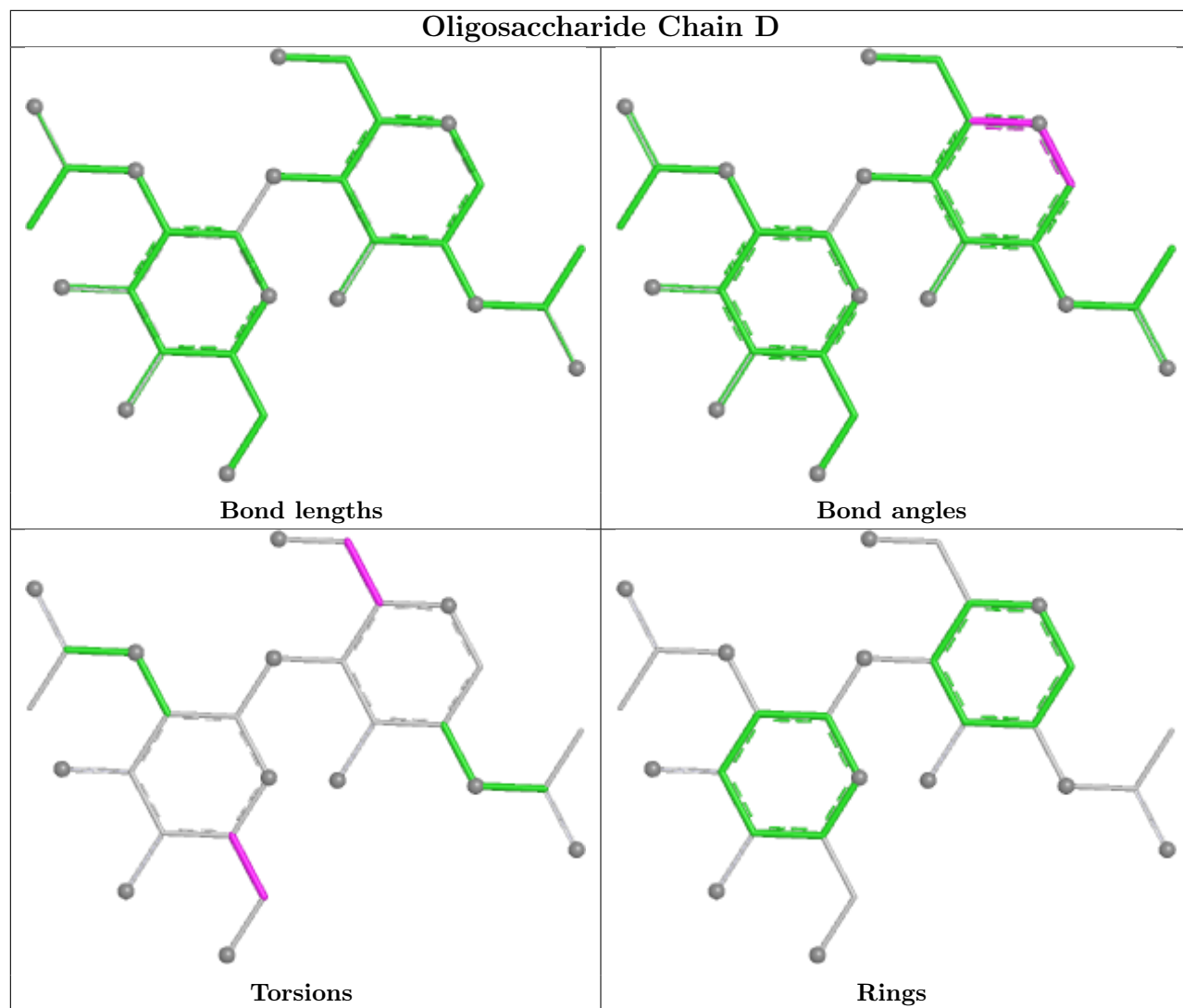
There are no ring outliers.

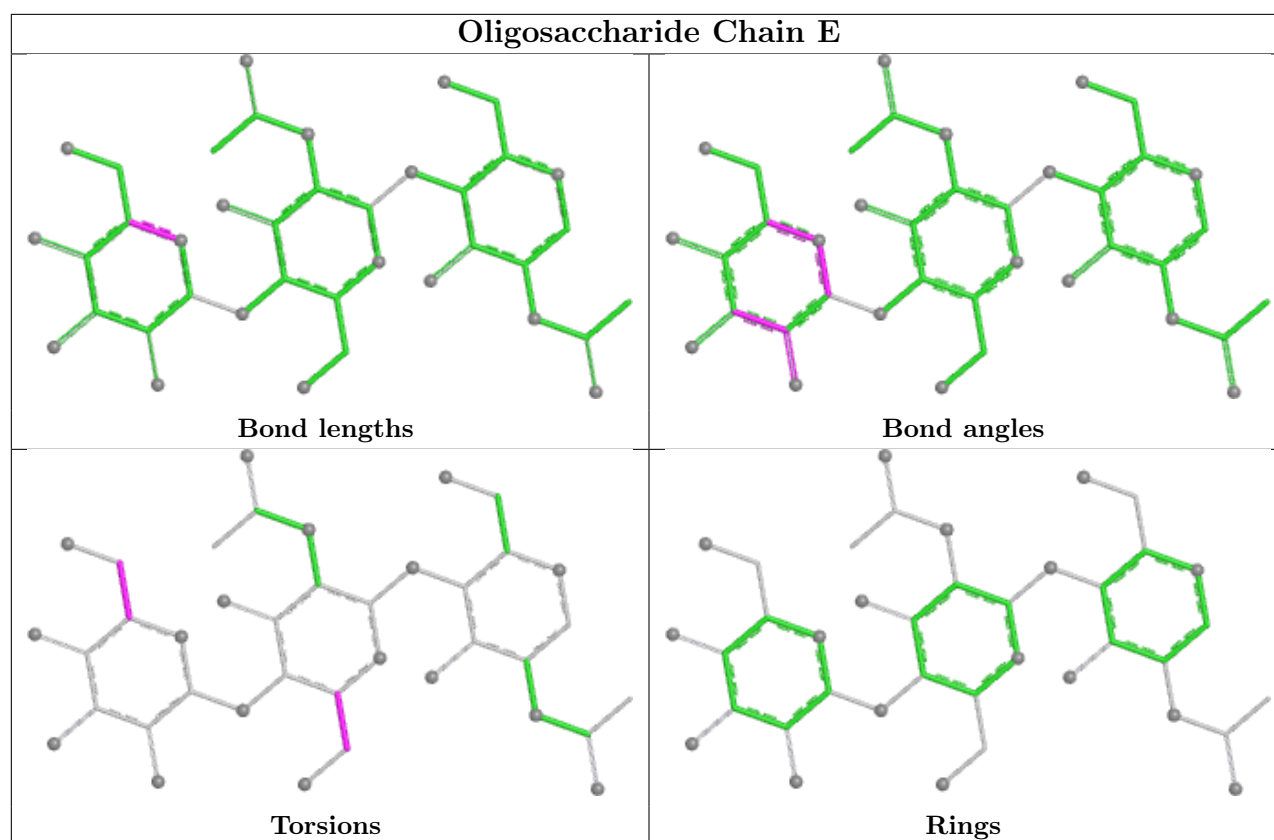
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	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](#)

27 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	$\# Z > 2$
6	BOG	A	603	-	20,20,20	0.89	1 (5%)	25,25,25	1.17	1 (4%)
9	EDO	A	614	-	3,3,3	0.50	0	2,2,2	0.41	0
7	NAG	A	605	1	14,14,15	0.26	0	17,19,21	1.17	3 (17%)
6	BOG	B	603	-	20,20,20	0.92	1 (5%)	25,25,25	0.99	0
5	HEM	B	602	10,1	50,50,50	1.93	9 (18%)	67,82,82	1.54	8 (11%)
9	EDO	B	618	-	3,3,3	0.36	0	2,2,2	0.90	0
9	EDO	A	612	-	3,3,3	0.40	0	2,2,2	0.49	0
8	AKR	B	611	-	4,4,4	1.75	2 (50%)	4,4,4	1.77	2 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	B	613	-	3,3,3	0.54	0	2,2,2	0.39	0
9	EDO	A	615	-	3,3,3	0.59	0	2,2,2	0.63	0
5	HEM	A	602	10,1	50,50,50	1.84	9 (18%)	67,82,82	1.50	10 (14%)
9	EDO	B	612	-	3,3,3	0.64	0	2,2,2	0.62	0
8	AKR	A	610	-	4,4,4	1.46	1 (25%)	4,4,4	1.58	1 (25%)
4	IBP	A	601	-	15,15,15	0.76	1 (6%)	20,20,20	1.08	2 (10%)
8	AKR	A	609	-	4,4,4	1.17	0	4,4,4	1.91	2 (50%)
9	EDO	B	615	-	3,3,3	0.55	0	2,2,2	0.46	0
9	EDO	B	614	-	3,3,3	0.62	0	2,2,2	0.55	0
9	EDO	A	611	-	3,3,3	0.79	0	2,2,2	0.51	0
8	AKR	B	610	-	4,4,4	1.69	1 (25%)	4,4,4	1.08	0
6	BOG	A	604	-	20,20,20	0.93	1 (5%)	25,25,25	1.05	2 (8%)
7	NAG	A	608	1	14,14,15	0.57	0	17,19,21	0.45	0
9	EDO	A	616	-	3,3,3	0.50	0	2,2,2	0.35	0
9	EDO	B	617	-	3,3,3	0.48	0	2,2,2	0.28	0
9	EDO	A	613	-	3,3,3	0.50	0	2,2,2	0.41	0
7	NAG	B	609	1	14,14,15	0.62	1 (7%)	17,19,21	0.71	0
9	EDO	B	616	-	3,3,3	0.52	0	2,2,2	0.38	0
4	IBP	B	601	-	15,15,15	0.63	0	20,20,20	1.06	1 (5%)

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
6	BOG	A	603	-	-	7/11/31/31	0/1/1/1
9	EDO	A	614	-	-	0/1/1/1	-
7	NAG	A	605	1	-	2/6/23/26	0/1/1/1
6	BOG	B	603	-	-	7/11/31/31	0/1/1/1
5	HEM	B	602	10,1	-	2/14/54/54	-
9	EDO	B	618	-	-	1/1/1/1	-
9	EDO	A	612	-	-	0/1/1/1	-
8	AKR	B	611	-	-	1/2/2/2	-
9	EDO	B	613	-	-	0/1/1/1	-
9	EDO	A	615	-	-	0/1/1/1	-
5	HEM	A	602	10,1	-	3/14/54/54	-
9	EDO	B	612	-	-	0/1/1/1	-
8	AKR	A	610	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IBP	A	601	-	-	1/12/12/12	0/1/1/1
8	AKR	A	609	-	-	2/2/2/2	-
9	EDO	B	615	-	-	0/1/1/1	-
9	EDO	B	614	-	-	0/1/1/1	-
9	EDO	A	611	-	-	0/1/1/1	-
8	AKR	B	610	-	-	2/2/2/2	-
6	BOG	A	604	-	-	7/11/31/31	0/1/1/1
7	NAG	A	608	1	-	1/6/23/26	0/1/1/1
9	EDO	A	616	-	-	0/1/1/1	-
9	EDO	B	617	-	-	1/1/1/1	-
9	EDO	A	613	-	-	1/1/1/1	-
7	NAG	B	609	1	-	0/6/23/26	0/1/1/1
9	EDO	B	616	-	-	1/1/1/1	-
4	IBP	B	601	-	-	0/12/12/12	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	602	HEM	C3D-C2D	7.25	1.52	1.36
5	A	602	HEM	C3D-C2D	7.10	1.52	1.36
5	B	602	HEM	FE-NB	5.48	2.11	1.94
5	A	602	HEM	FE-ND	5.08	2.10	1.94
5	B	602	HEM	FE-NA	4.13	2.08	1.95
5	B	602	HEM	FE-ND	4.12	2.07	1.94
5	A	602	HEM	FE-NB	3.89	2.06	1.94
5	A	602	HEM	CAB-C3B	2.92	1.55	1.47
6	B	603	BOG	O5-C1	2.91	1.49	1.41
5	B	602	HEM	CAB-C3B	2.87	1.55	1.47
5	A	602	HEM	CAC-C3C	2.85	1.55	1.47
6	A	604	BOG	O5-C1	2.76	1.48	1.41
5	B	602	HEM	CAC-C3C	2.75	1.54	1.47
6	A	603	BOG	O5-C1	2.68	1.48	1.41
5	B	602	HEM	CMB-C2B	2.60	1.56	1.50
5	B	602	HEM	FE-NC	2.54	2.03	1.95
5	A	602	HEM	CMB-C2B	2.41	1.55	1.50
8	B	611	AKR	CA-C	2.25	1.52	1.46
5	A	602	HEM	FE-NC	2.19	2.02	1.95
7	B	609	NAG	C1-C2	2.14	1.55	1.52
5	A	602	HEM	CMA-C3A	2.13	1.55	1.50
4	A	601	IBP	O2-C1	2.12	1.28	1.22
5	A	602	HEM	FE-NA	2.10	2.02	1.95
8	B	611	AKR	OXT-C	-2.09	1.25	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	610	AKR	CA-C	2.06	1.52	1.46
5	B	602	HEM	C2A-C3A	-2.04	1.33	1.38
8	B	610	AKR	CA-C	2.03	1.52	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	602	HEM	C4D-ND-C1D	6.43	112.83	105.21
5	A	602	HEM	C4D-ND-C1D	5.49	111.71	105.21
6	A	603	BOG	C1'-O1-C1	4.04	120.59	113.68
5	B	602	HEM	CBD-CAD-C3D	-3.68	102.37	112.53
5	A	602	HEM	C1B-NB-C4B	3.36	109.18	105.21
5	A	602	HEM	CBD-CAD-C3D	-3.34	103.29	112.53
5	A	602	HEM	CHD-C1D-ND	3.21	127.88	124.42
5	B	602	HEM	C1B-NB-C4B	3.11	108.89	105.21
5	B	602	HEM	CHD-C1D-ND	3.02	127.68	124.42
8	A	609	AKR	CB-CA-C	-3.01	116.37	121.50
5	B	602	HEM	CHC-C1C-NC	2.86	127.57	124.45
4	B	601	IBP	C12-C13-C8	-2.76	118.43	121.18
7	A	605	NAG	C1-O5-C5	2.75	115.87	112.19
5	A	602	HEM	CHC-C4B-NB	2.58	127.20	124.42
8	A	610	AKR	OXT-C-CA	2.50	121.00	114.19
5	B	602	HEM	CHA-C4D-ND	2.46	127.41	124.37
5	A	602	HEM	CAC-C3C-C4C	2.43	130.62	124.82
5	B	602	HEM	C3B-C4B-NB	-2.37	107.77	109.47
8	B	611	AKR	OXT-C-CA	2.29	120.44	114.19
4	A	601	IBP	O1-C1-O2	-2.29	118.89	124.08
5	A	602	HEM	CHA-C4D-ND	2.25	127.14	124.37
8	B	611	AKR	OXT-C-O	-2.24	118.14	122.70
5	B	602	HEM	C3D-C4D-ND	-2.20	107.76	110.17
5	A	602	HEM	C3C-C2C-C1C	2.20	109.12	107.05
7	A	605	NAG	C1-C2-N2	2.16	113.84	110.43
5	A	602	HEM	C3B-C4B-NB	-2.09	107.97	109.47
7	A	605	NAG	C4-C3-C2	-2.08	107.98	111.02
6	A	604	BOG	O5-C1-C2	2.07	114.63	110.37
6	A	604	BOG	C1'-O1-C1	-2.07	110.15	113.68
4	A	601	IBP	C12-C13-C8	-2.06	119.13	121.18
5	A	602	HEM	O1D-CGD-CBD	-2.05	116.58	123.09
8	A	609	AKR	OXT-C-CA	2.01	119.66	114.19

There are no chirality outliers.

All (41) torsion outliers are listed below:

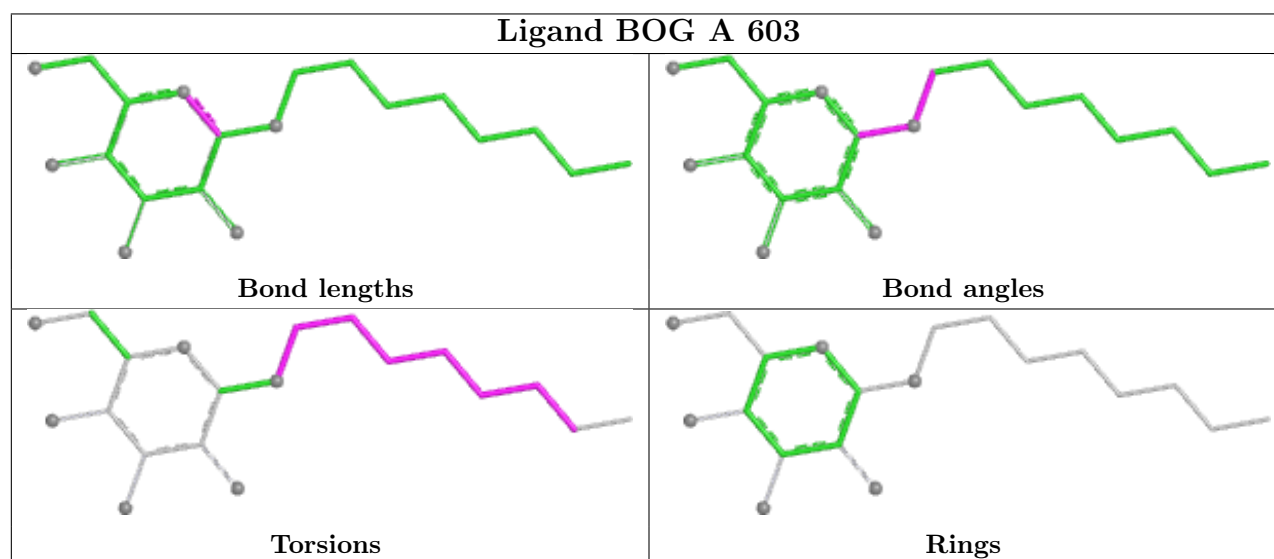
Mol	Chain	Res	Type	Atoms
6	B	603	BOG	C2-C1-O1-C1'
8	A	609	AKR	O-C-CA-CB
8	A	609	AKR	OXT-C-CA-CB
8	A	610	AKR	O-C-CA-CB
8	B	610	AKR	OXT-C-CA-CB
8	B	611	AKR	O-C-CA-CB
6	A	604	BOG	O5-C1-O1-C1'
6	A	604	BOG	C2-C1-O1-C1'
6	B	603	BOG	C4'-C5'-C6'-C7'
6	B	603	BOG	O5-C1-O1-C1'
6	A	603	BOG	O1-C1'-C2'-C3'
6	A	603	BOG	C4'-C5'-C6'-C7'
6	A	604	BOG	C3'-C4'-C5'-C6'
6	A	603	BOG	C2'-C3'-C4'-C5'
6	A	604	BOG	C1'-C2'-C3'-C4'
6	A	604	BOG	C2'-C3'-C4'-C5'
9	B	618	EDO	O1-C1-C2-O2
6	A	603	BOG	C3'-C4'-C5'-C6'
6	A	603	BOG	C1'-C2'-C3'-C4'
6	A	604	BOG	C4'-C5'-C6'-C7'
9	B	617	EDO	O1-C1-C2-O2
6	A	603	BOG	C2'-C1'-O1-C1
6	B	603	BOG	C2'-C1'-O1-C1
6	B	603	BOG	C4-C5-C6-O6
6	A	604	BOG	O1-C1'-C2'-C3'
6	A	603	BOG	C5'-C6'-C7'-C8'
7	A	605	NAG	C1-C2-N2-C7
8	A	610	AKR	OXT-C-CA-CB
5	A	602	HEM	C4C-C3C-CAC-CBC
8	B	610	AKR	O-C-CA-CB
5	A	602	HEM	CAA-CBA-CGA-O2A
5	A	602	HEM	CAA-CBA-CGA-O1A
6	B	603	BOG	O1-C1'-C2'-C3'
9	B	616	EDO	O1-C1-C2-O2
7	A	605	NAG	C3-C2-N2-C7
6	B	603	BOG	O5-C5-C6-O6
5	B	602	HEM	CAA-CBA-CGA-O2A
7	A	608	NAG	C4-C5-C6-O6
5	B	602	HEM	CAA-CBA-CGA-O1A
4	A	601	IBP	O1-C1-C6-C7
9	A	613	EDO	O1-C1-C2-O2

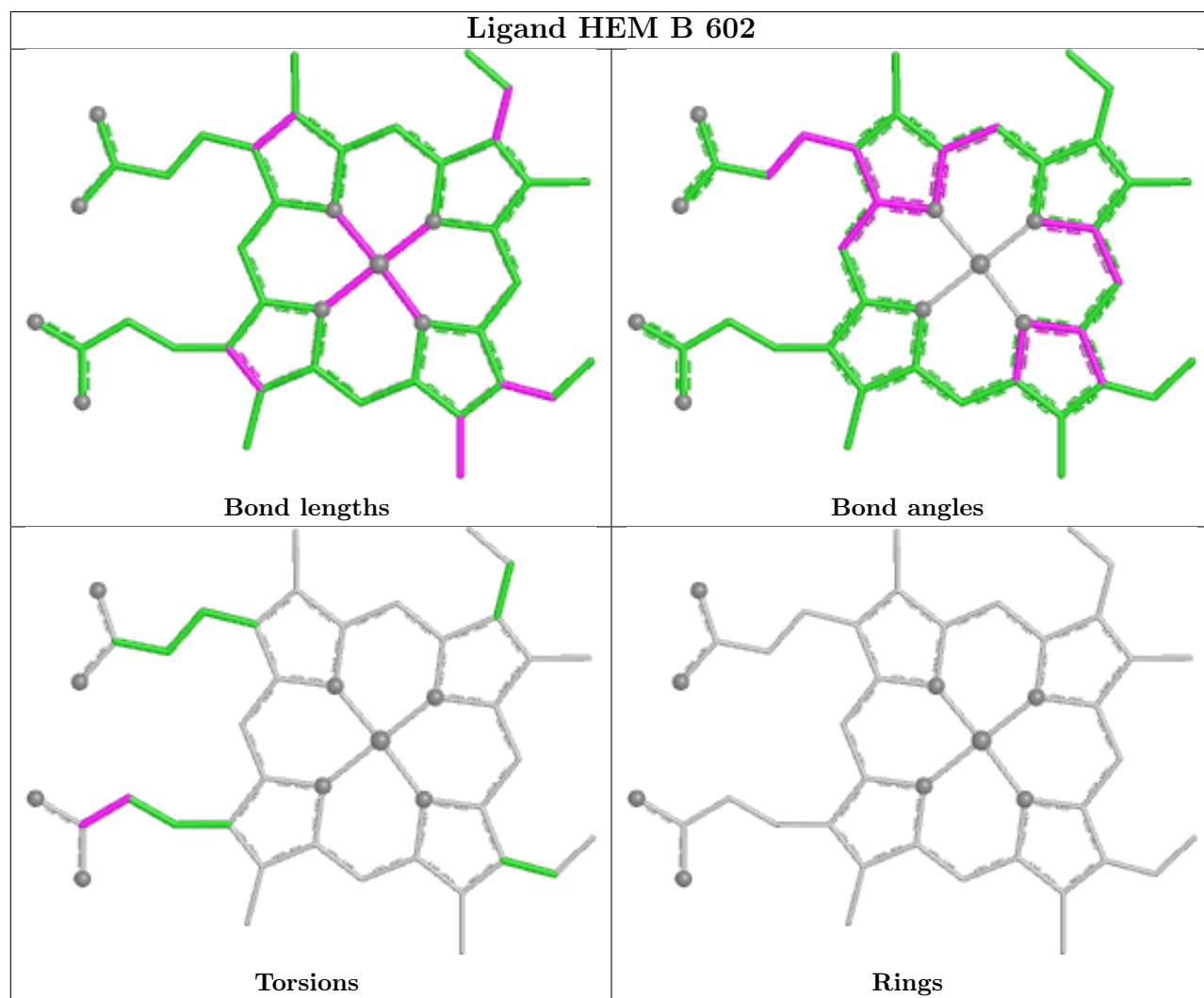
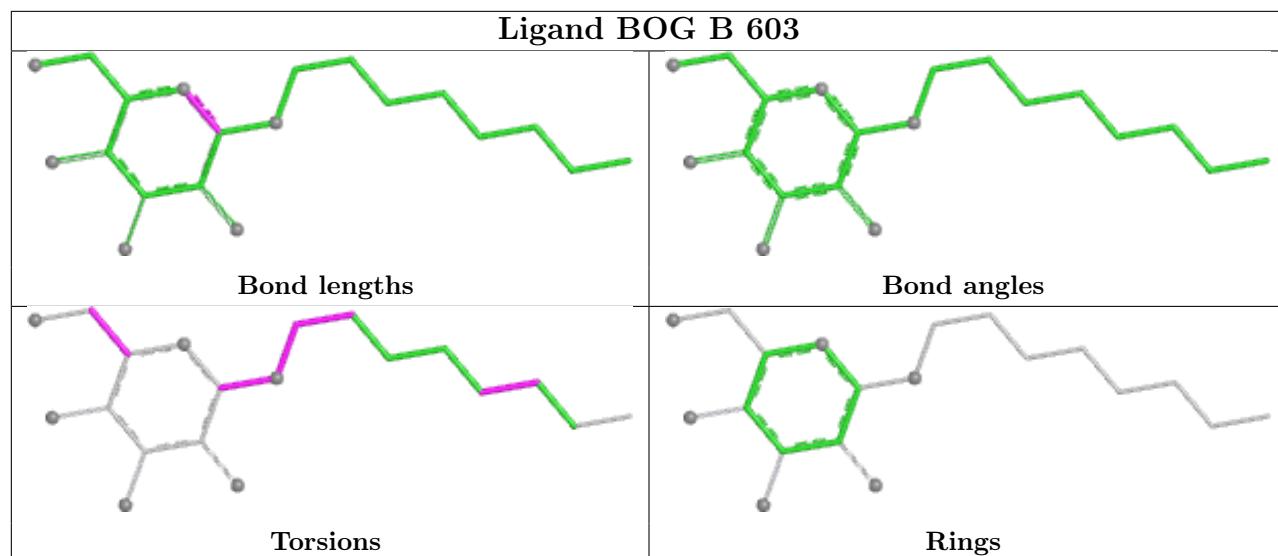
There are no ring outliers.

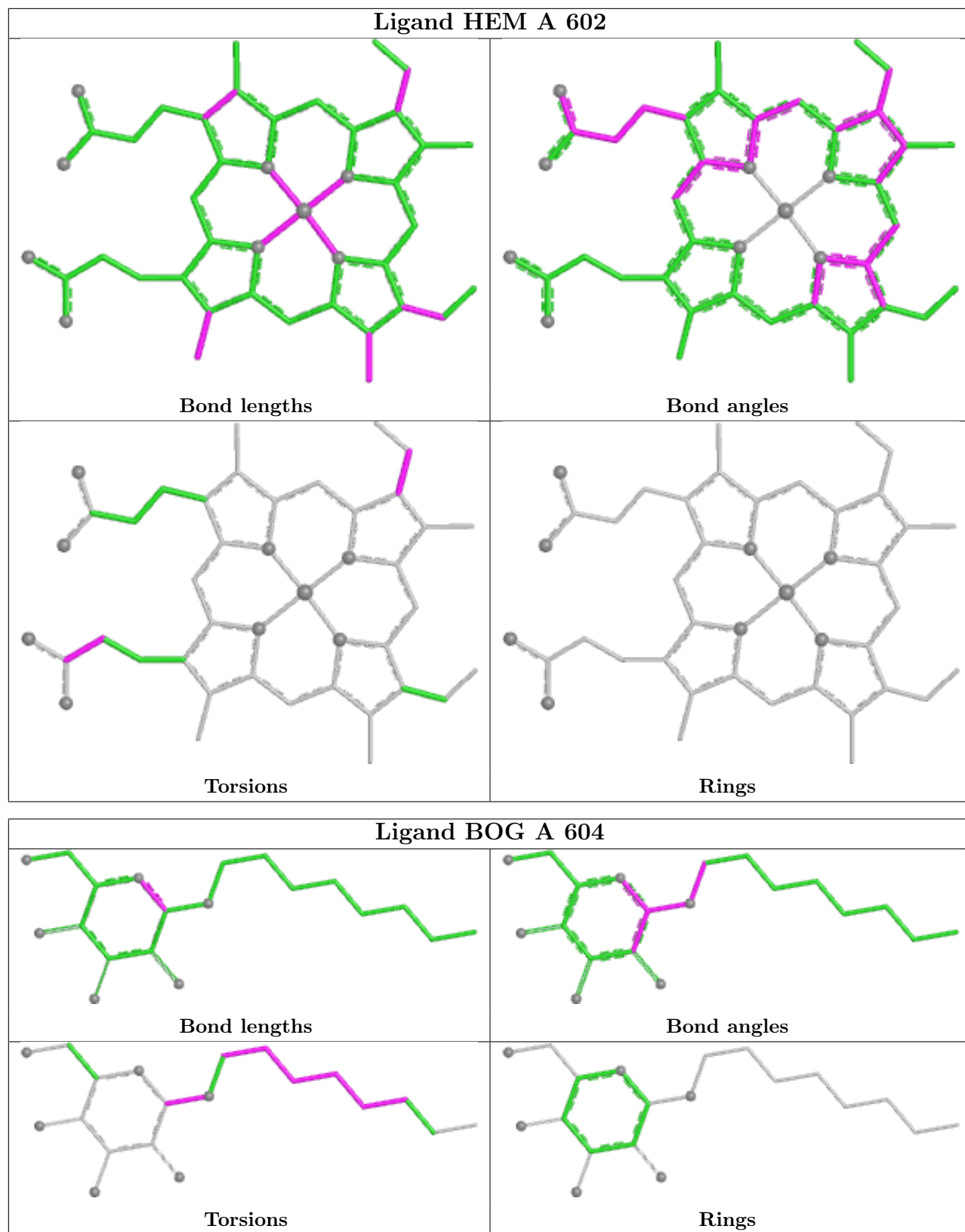
13 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	BOG	1	0
9	A	614	EDO	1	0
5	B	602	HEM	3	0
8	B	611	AKR	6	0
5	A	602	HEM	2	0
8	A	610	AKR	1	0
8	A	609	AKR	5	0
9	B	615	EDO	1	0
8	B	610	AKR	1	0
6	A	604	BOG	2	0
9	A	616	EDO	1	0
9	A	613	EDO	2	0
9	B	616	EDO	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 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 [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	551/551 (100%)	-0.32	5 (0%) 81 85	11, 28, 48, 67	5 (0%)
1	B	551/551 (100%)	-0.41	3 (0%) 87 90	10, 26, 41, 70	3 (0%)
All	All	1102/1102 (100%)	-0.37	8 (0%) 84 88	10, 27, 45, 70	8 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	410	TYR	3.5
1	B	410	TYR	2.9
1	B	279	HIS	2.6
1	B	53	ASP	2.3
1	A	74	PHE	2.3
1	A	78	ILE	2.1
1	A	75	LEU	2.1
1	A	295	LEU	2.1

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

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

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.

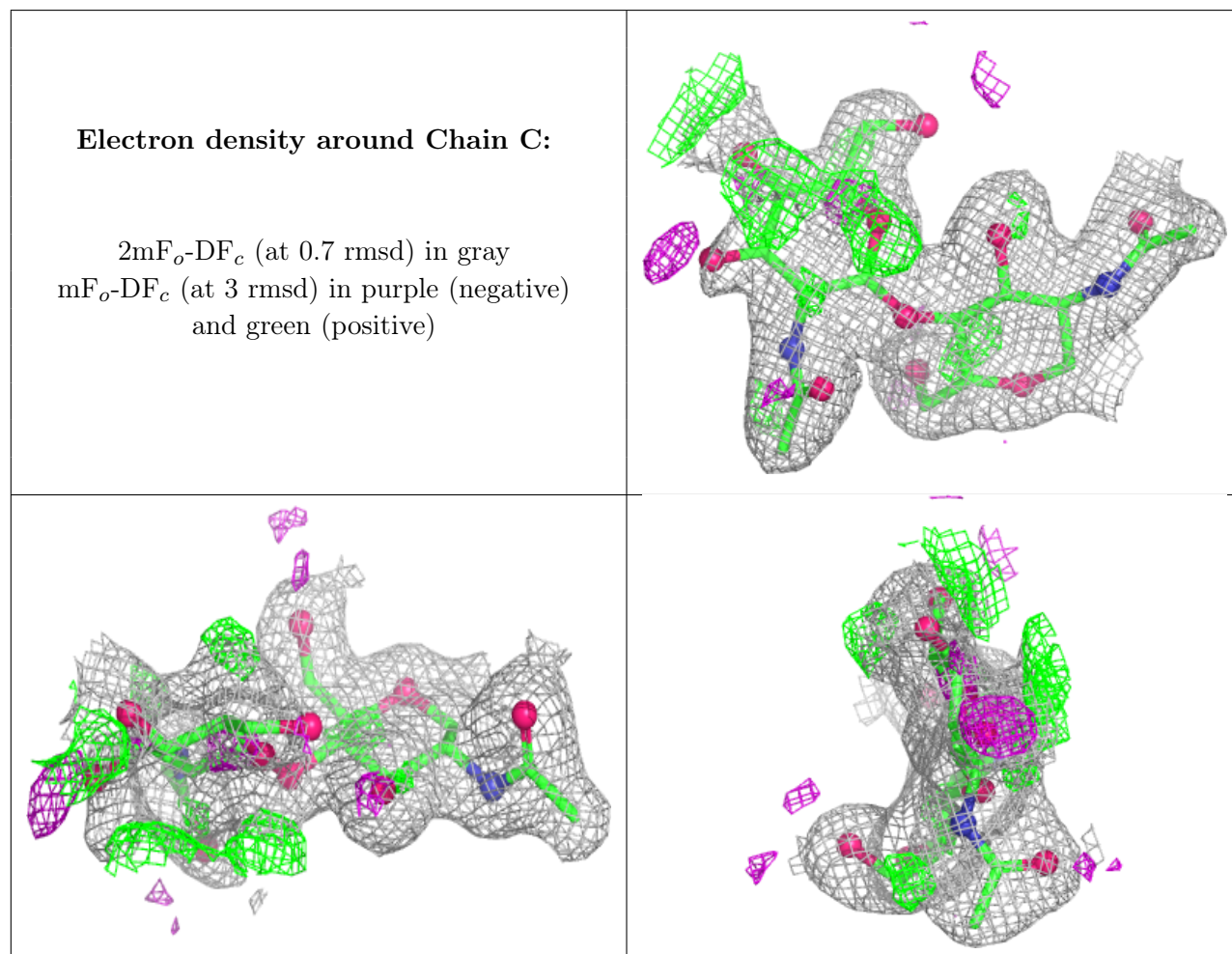
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	E	3	11/12	0.47	0.17	64,68,73,78	0

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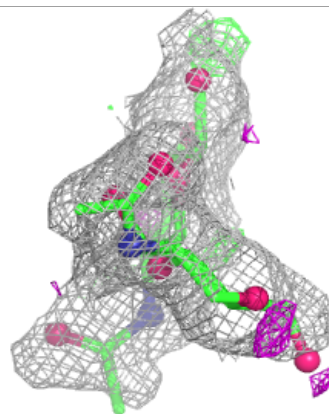
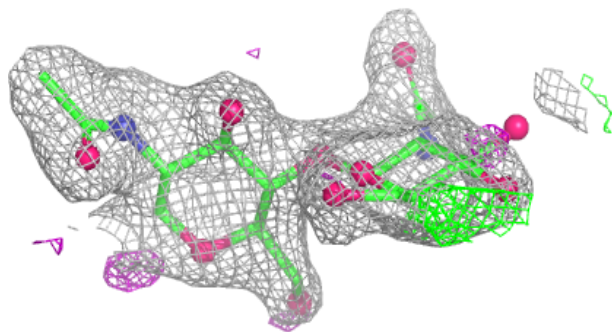
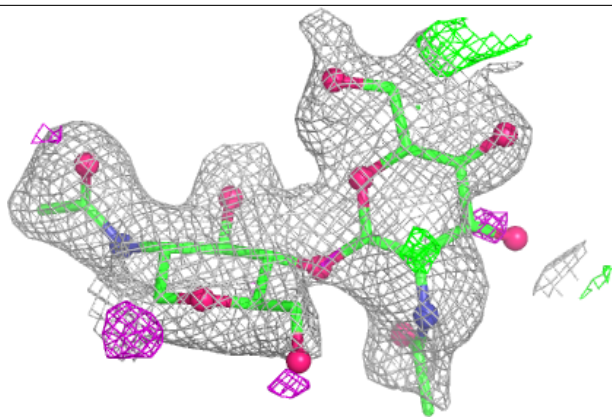
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	2	14/15	0.59	0.14	68,72,77,82	0
2	NAG	C	2	14/15	0.76	0.15	37,47,55,58	0
3	NAG	E	2	14/15	0.86	0.11	37,41,52,61	0
2	NAG	D	1	14/15	0.86	0.11	41,49,60,67	0
2	NAG	C	1	14/15	0.95	0.08	25,29,35,39	0
3	NAG	E	1	14/15	0.96	0.06	24,31,34,40	0

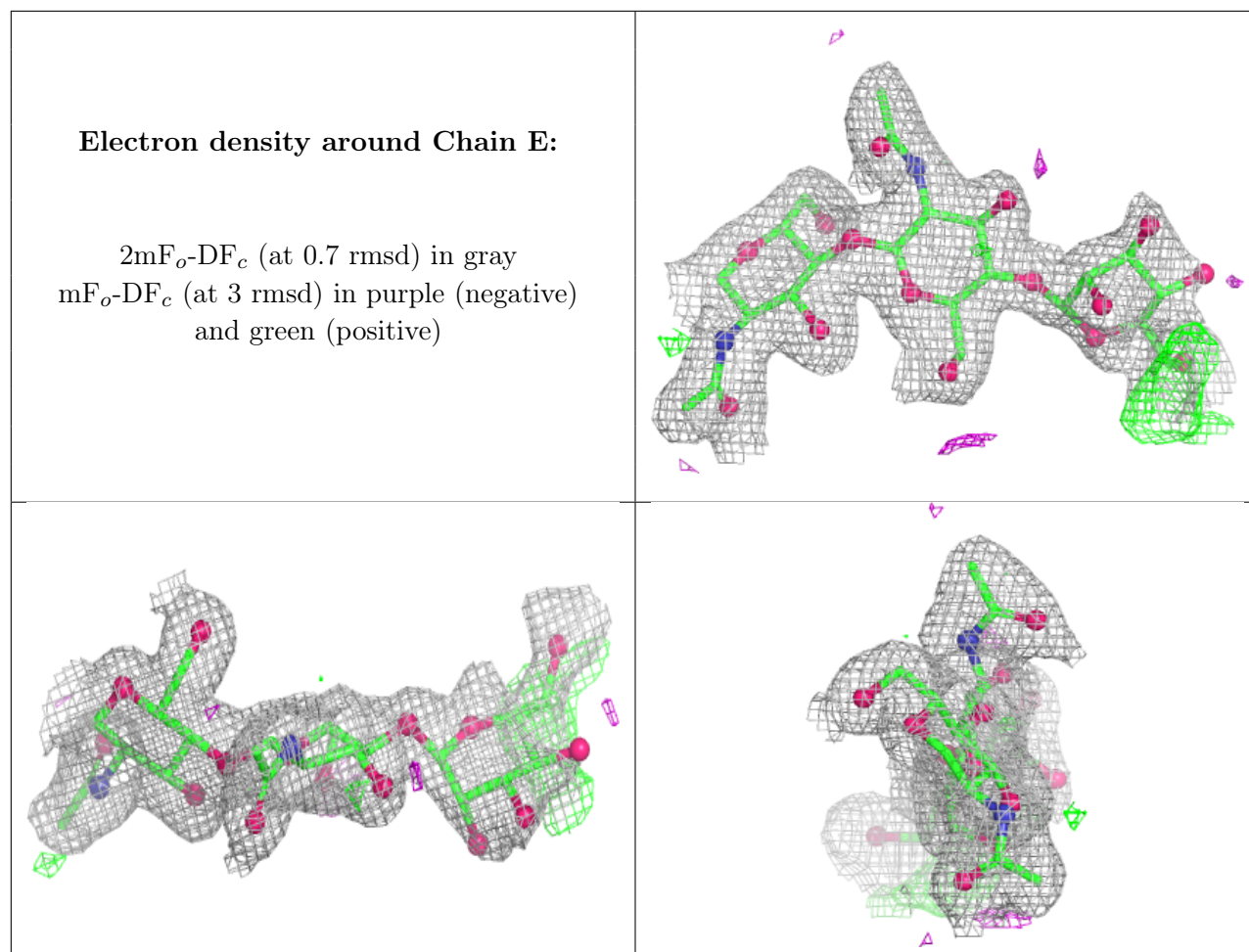
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

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





6.4 Ligands ⓘ

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
7	NAG	A	605	14/15	0.71	0.15	48,54,61,64	0
8	AKR	A	609	5/5	0.81	0.14	28,41,46,47	0
9	EDO	B	615	4/4	0.81	0.23	34,37,39,54	0
7	NAG	A	608	14/15	0.83	0.11	44,51,58,59	0
9	EDO	B	612	4/4	0.85	0.17	24,27,30,35	0
9	EDO	B	617	4/4	0.85	0.16	37,41,44,44	0
6	BOG	A	604	20/20	0.86	0.12	42,48,52,53	0
8	AKR	B	610	5/5	0.86	0.15	36,38,39,45	0
8	AKR	B	611	5/5	0.86	0.14	30,31,42,44	0
9	EDO	A	611	4/4	0.87	0.16	28,31,31,37	0
7	NAG	B	609	14/15	0.87	0.09	34,39,46,46	0

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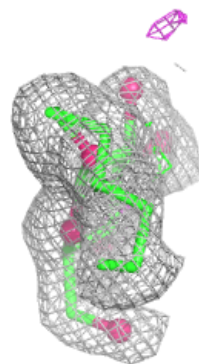
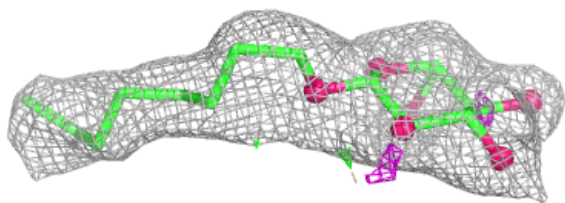
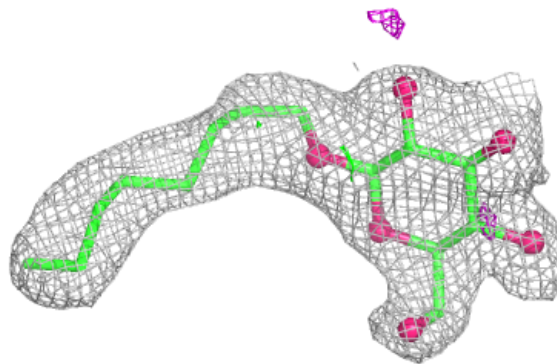
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	AKR	A	610	5/5	0.88	0.13	32,35,43,43	0
6	BOG	B	603	20/20	0.89	0.10	41,44,47,49	0
9	EDO	A	613	4/4	0.89	0.20	38,38,41,43	0
9	EDO	A	615	4/4	0.89	0.12	30,32,35,41	0
9	EDO	B	614	4/4	0.91	0.17	30,35,36,41	0
9	EDO	B	618	4/4	0.91	0.15	27,29,31,33	0
4	IBP	B	601	15/15	0.93	0.07	22,24,29,29	0
9	EDO	A	616	4/4	0.94	0.11	26,28,29,32	0
4	IBP	A	601	15/15	0.94	0.07	24,28,31,33	0
6	BOG	A	603	20/20	0.95	0.08	27,32,38,40	0
9	EDO	B	616	4/4	0.95	0.11	23,28,28,31	0
9	EDO	B	613	4/4	0.96	0.08	22,26,28,29	0
9	EDO	A	612	4/4	0.96	0.08	25,28,30,32	0
9	EDO	A	614	4/4	0.97	0.08	26,27,31,32	0
5	HEM	B	602	43/43	0.98	0.06	18,23,35,56	0
5	HEM	A	602	43/43	0.98	0.06	20,24,34,54	0

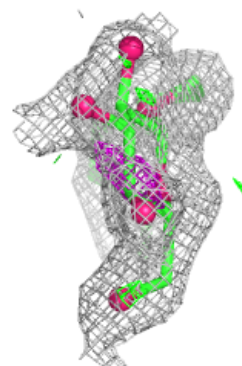
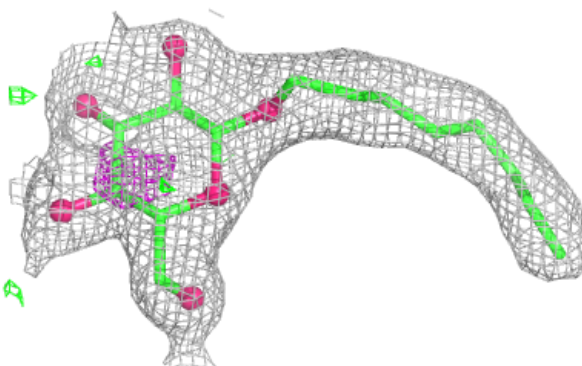
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG A 604:

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

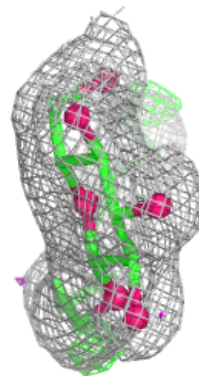
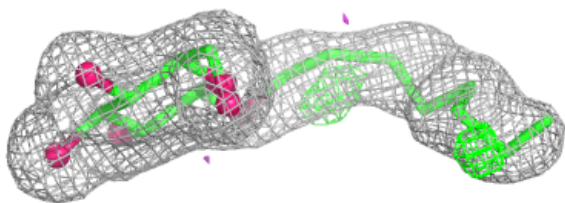
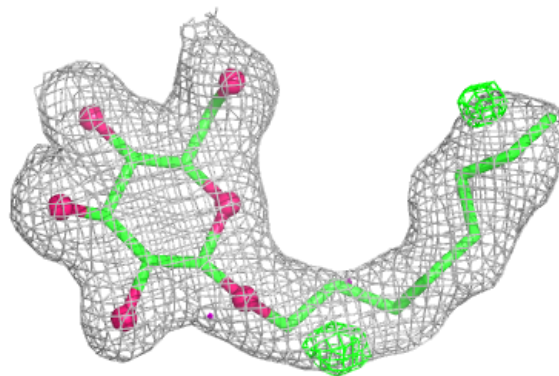
**Electron density around BOG B 603:**

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



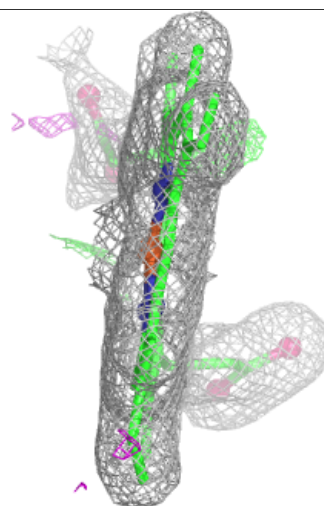
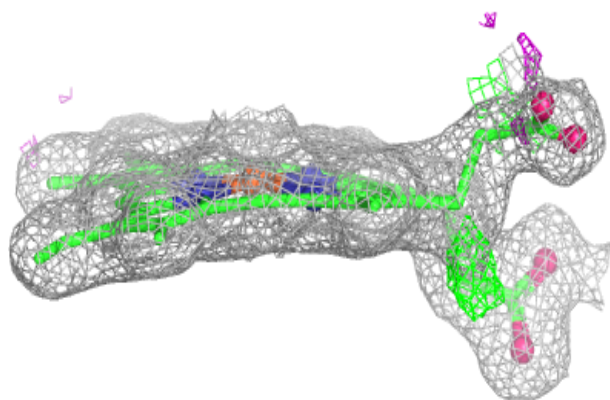
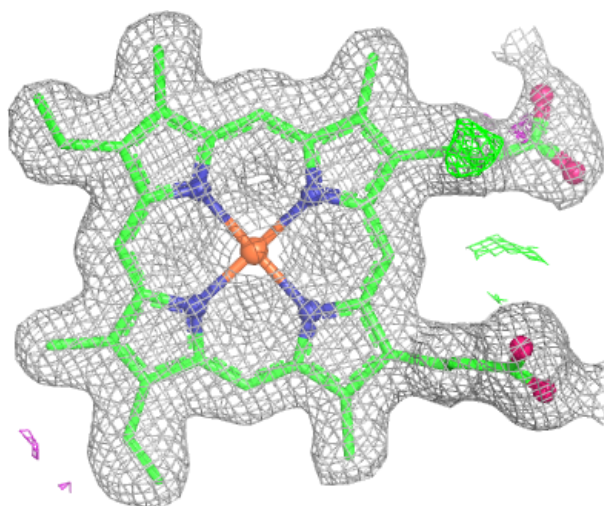
Electron density around BOG A 603:

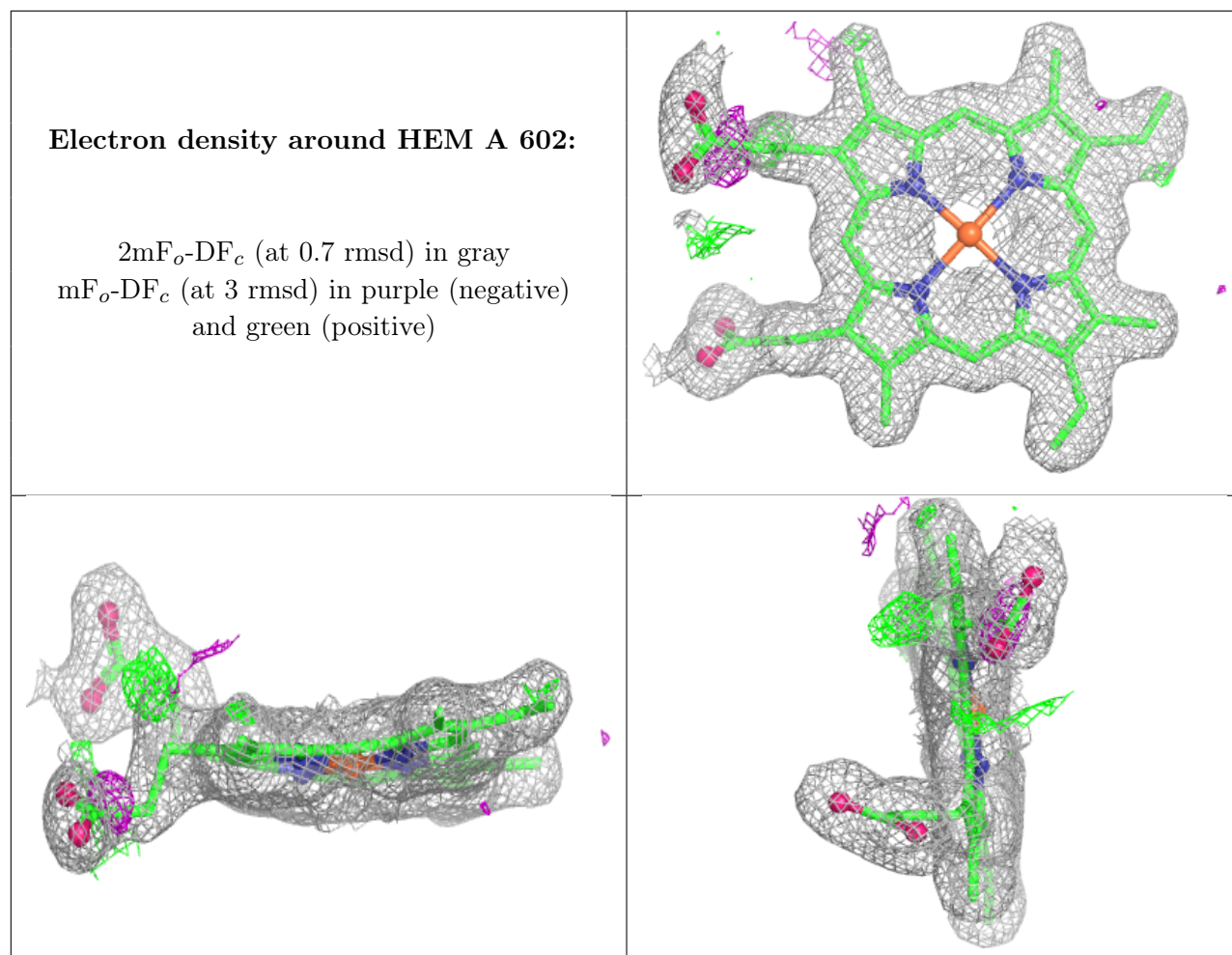
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 602:

$2mF_o-DF_c$ (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.