



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 07:41 PM BST

PDB ID : 4PH9
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

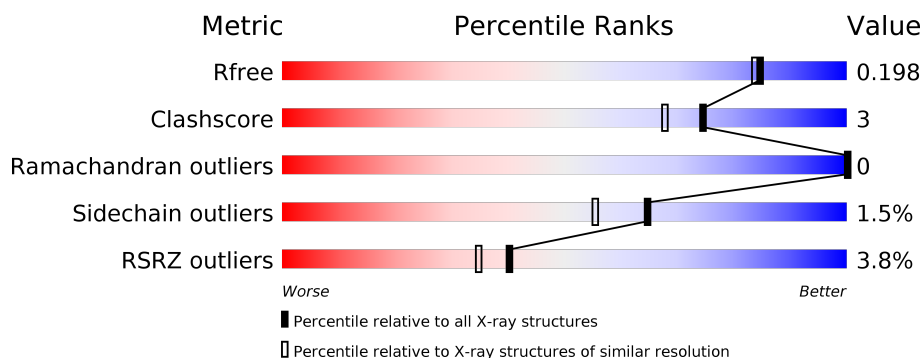
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	551	<div> <div>4%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	B	551	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
3	E	3	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>

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	-
8	AKR	B	611	-	-	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:

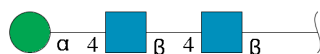
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	HIS	-	expression tag	UNP Q05769
A	34	HIS	-	expression tag	UNP Q05769
B	33	HIS	-	expression tag	UNP Q05769
B	34	HIS	-	expression tag	UNP Q05769

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



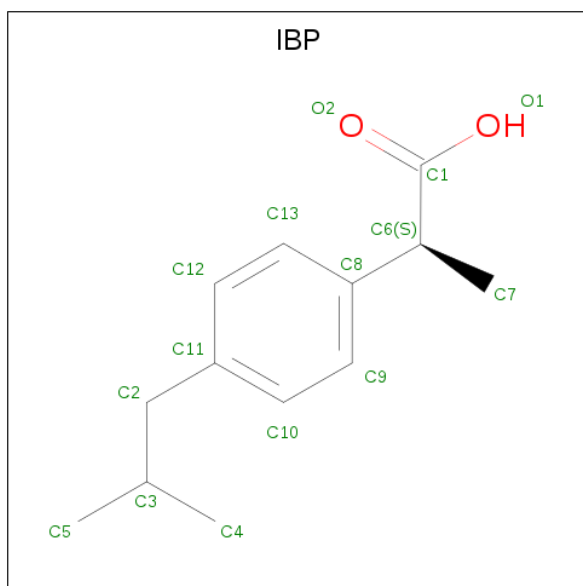
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



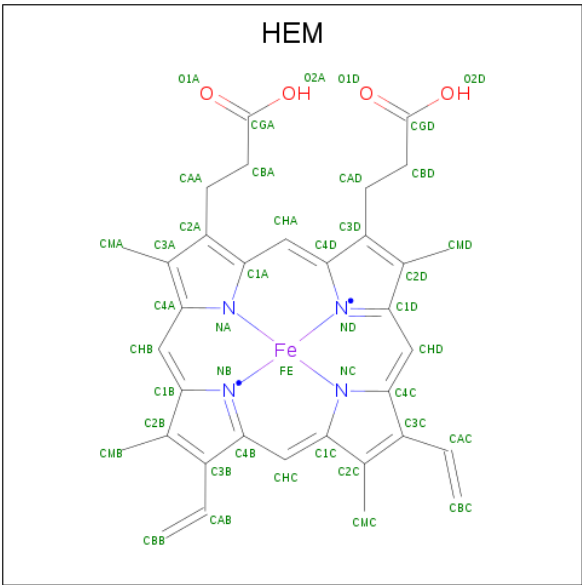
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is IBUPROFEN (three-letter code: IBP) (formula: $C_{13}H_{18}O_2$).



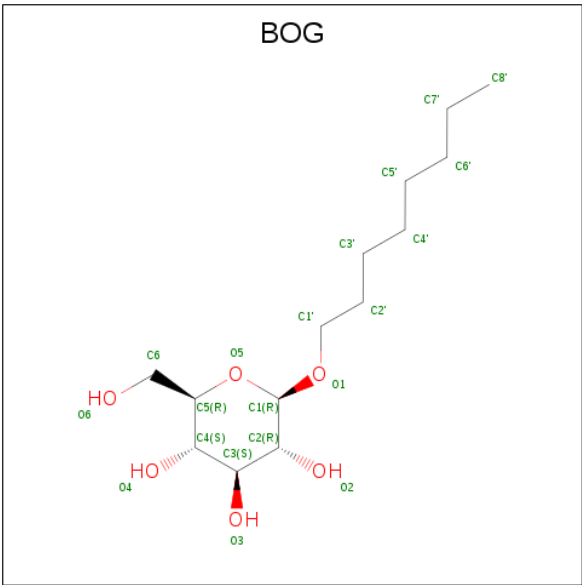
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			15	13	2		
4	B	1	Total	C	O	0	0
			15	13	2		

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



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

- Molecule 6 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



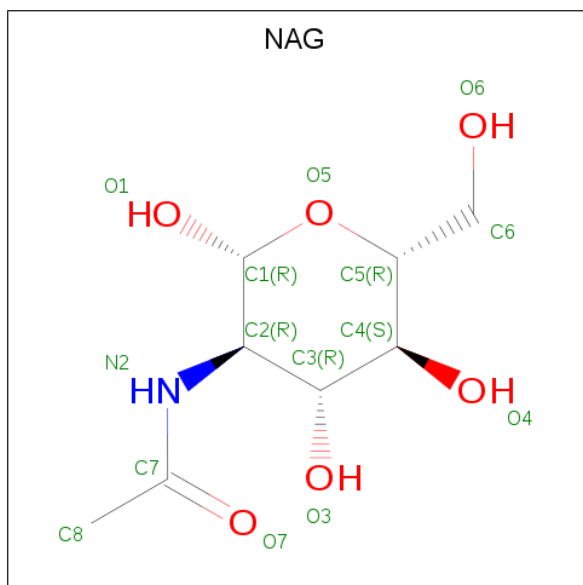
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			20	14	6		
6	A	1	Total	C	O	0	0
			20	14	6		

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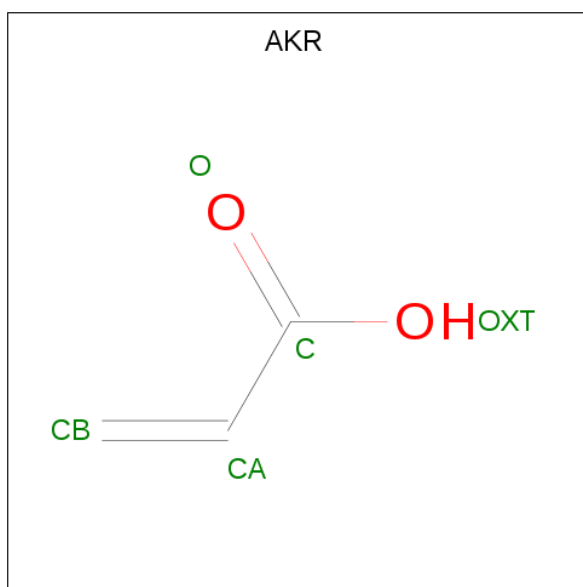
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			20	14	6		

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



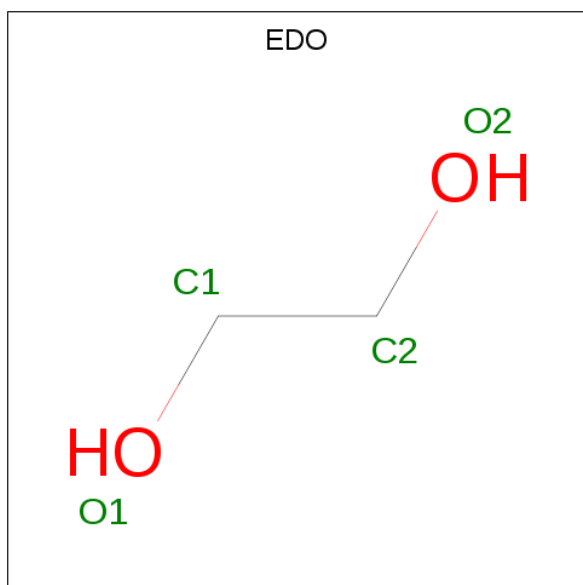
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is ACRYLIC ACID (three-letter code: 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 (three-letter code: 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

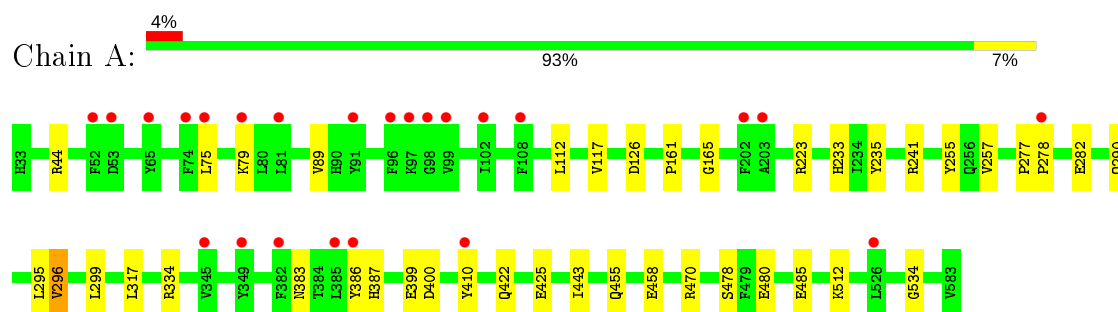
- Molecule 10 is water.

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

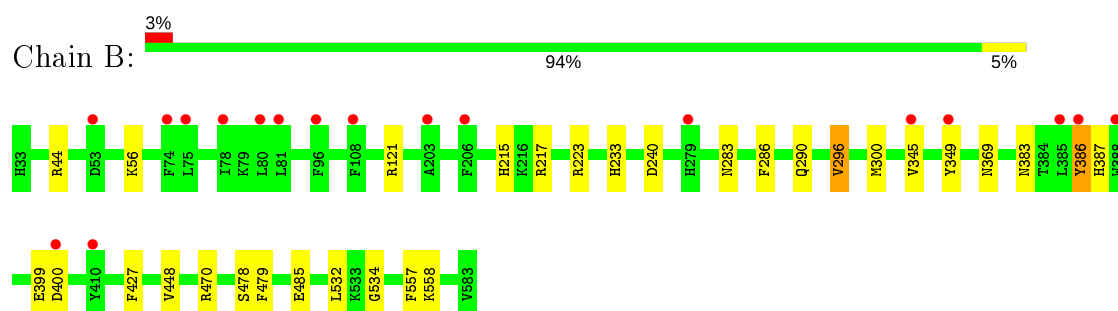
3 Residue-property plots [i](#)

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.

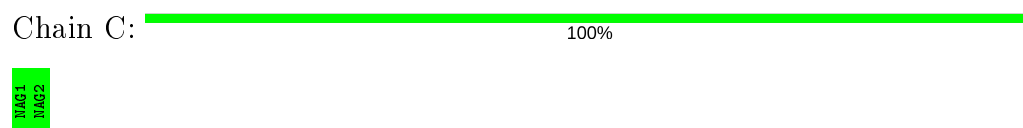
- Molecule 1: Prostaglandin G/H synthase 2



- 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: 


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	120.94 Å 132.23 Å 180.46 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.55 – 1.81 38.56 – 1.81	Depositor EDS
% Data completeness (in resolution range)	98.0 (35.55-1.81) 88.2 (38.56-1.81)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.81 Å)	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 (4.99%)	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)	0.38 , 52.1	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: NAG, AKR, EDO, IBP, HEM, BOG, MAN

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	0.56	0/4644	0.62	0/6295
1	B	0.58	0/4629	0.64	0/6275
All	All	0.57	0/9273	0.63	0/12570

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	A	4515	0	4402	32	0
1	B	4500	0	4393	24	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0
9	B	28	0	42	3	0
10	A	545	0	0	8	1
10	B	582	0	0	4	1
All	All	10527	0	9186	60	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 3.

All (60) 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: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: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
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:HHD	5:A:602:HEM:HBC2	1.91	0.51
1:A:480:GLU:H	8:A:609:AKR:CA	2.24	0.51
5:B:602:HEM:HBB2	5:B:602:HEM:HMB1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:295:LEU:CG	1:A:296:VAL:HG12	2.42	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:75:LEU:O	1:A:79:LYS:HG2	2.16	0.45
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
1:B:478:SER:CA	8:B:611:AKR:HA1	2.50	0.42
1:B:427:PHE:HA	1:B:427:PHE:HD1	1.71	0.42
1:B:369:ASN:HB3	10:B:1257:HOH:O	2.19	0.42
5:A:602:HEM:HMB2	5:A:602:HEM:HBB2	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:B:386:TYR:HH	9:B:618:EDO:C2	2.33	0.41
1:A:317:LEU:HA	1:A:317:LEU:HD23	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

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	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

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%)	491 (99%)	7 (1%)	67	58
1	B	496/493 (101%)	488 (98%)	8 (2%)	62	53
All	All	994/986 (101%)	979 (98%)	15 (2%)	65	55

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
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	233	HIS

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Mol	Chain	Res	Type
1	B	283	ASN
1	B	290	GLN
1	B	296	VAL
1	B	386	TYR
1	B	485	GLU
1	B	557	PHE
1	B	558	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	C	1	1,2	14,14,15	0.26	0	17,19,21	0.66	0
2	NAG	C	2	2	14,14,15	0.53	0	17,19,21	0.43	0
2	NAG	D	1	1,2	14,14,15	0.58	1 (7%)	17,19,21	0.71	1 (5%)
2	NAG	D	2	2	14,14,15	0.24	0	17,19,21	0.37	0
3	NAG	E	1	1,3	14,14,15	0.23	0	17,19,21	0.63	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	1.20	0	15,15,17	1.87	3 (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
2	NAG	C	1	1,2	-	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	1,2	-	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	1,3	-	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)
2	D	1	NAG	O5-C1	-2.02	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	MAN	C1-O5-C5	5.73	119.96	112.19
3	E	3	MAN	O2-C2-C3	-2.72	104.68	110.14
3	E	3	MAN	O5-C1-C2	2.72	114.97	110.77
2	D	1	NAG	C1-O5-C5	2.24	115.23	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

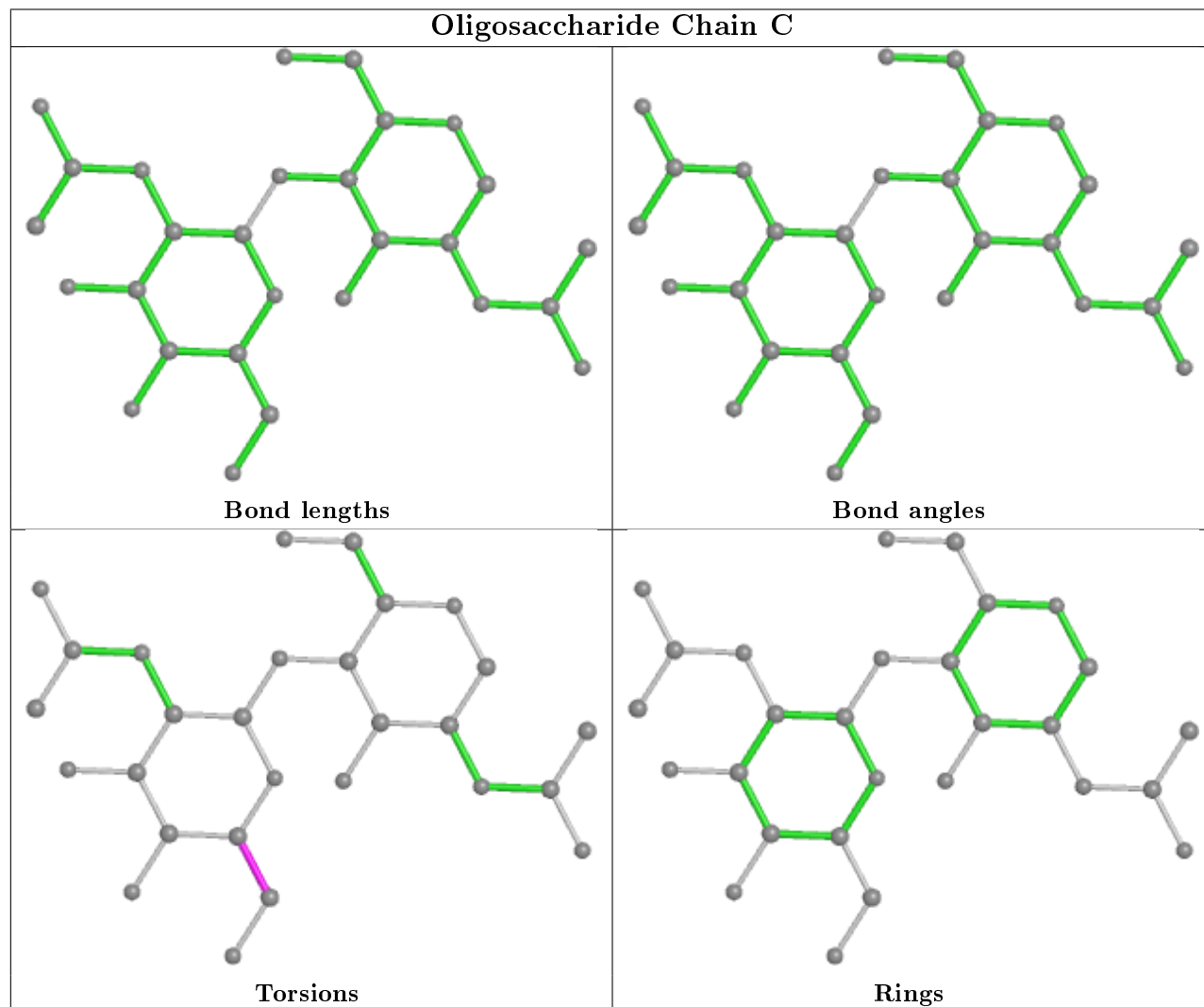
Mol	Chain	Res	Type	Atoms
3	E	3	MAN	O5-C5-C6-O6
3	E	3	MAN	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

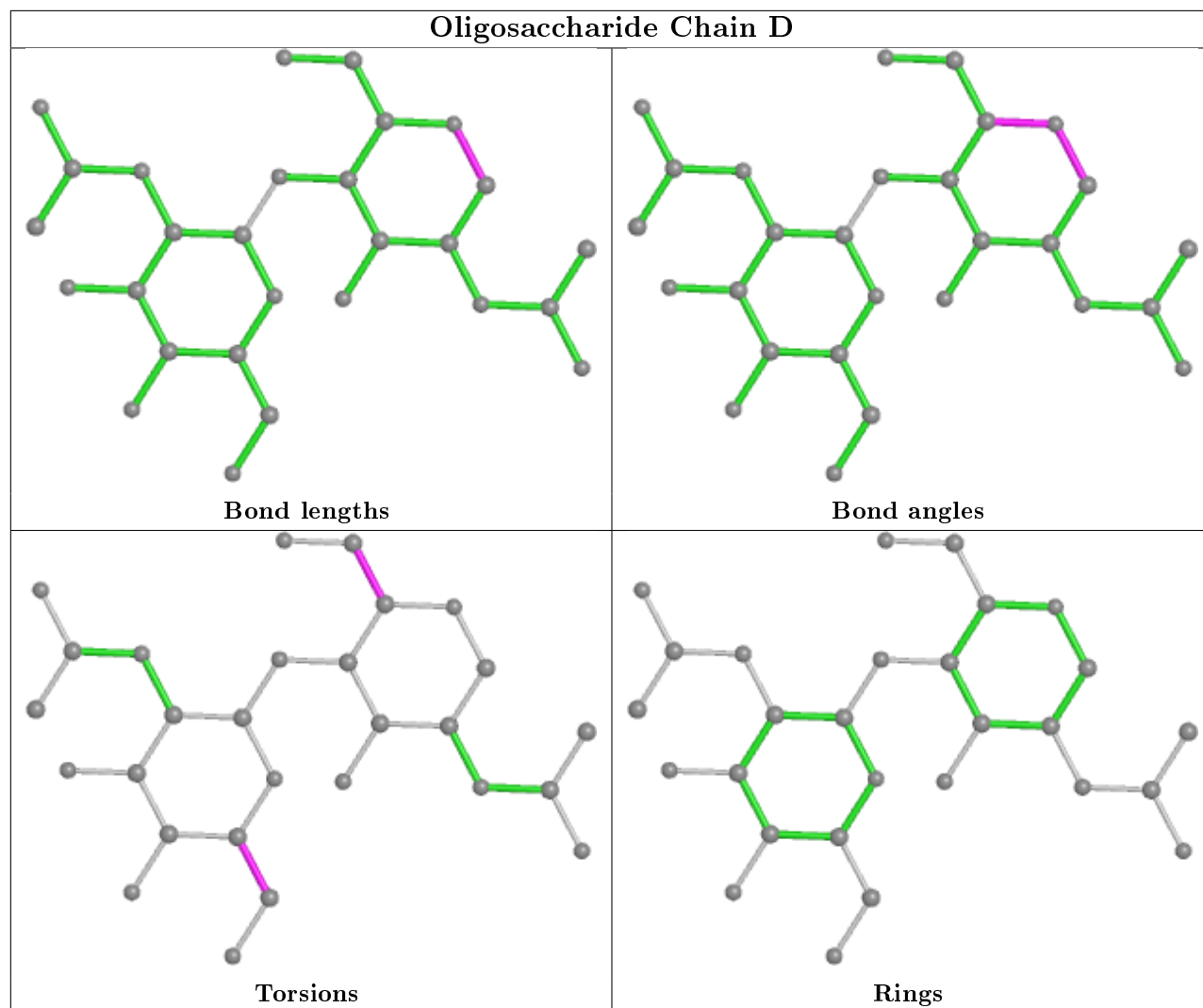
There are no ring outliers.

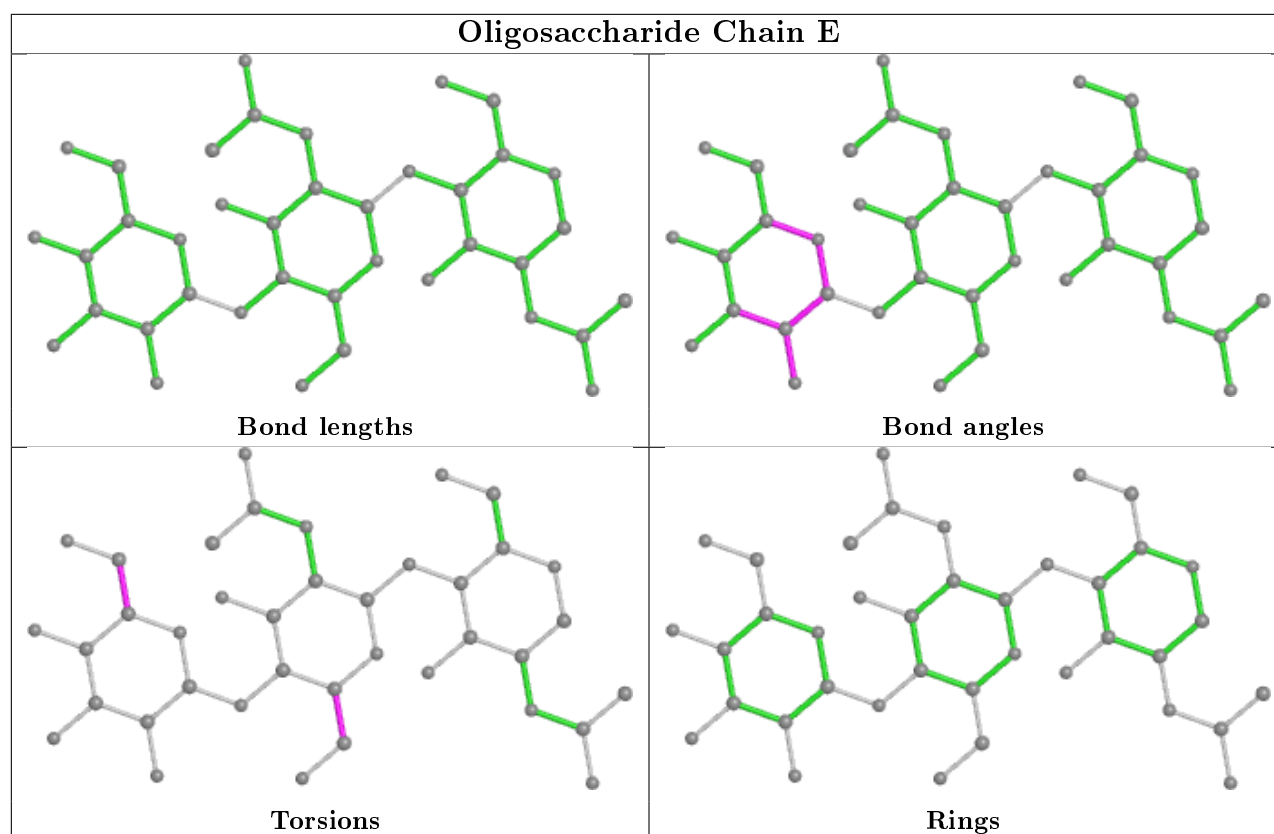
1 monomer is involved in 1 short contact:

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	$\# Z > 2$
9	EDO	A	613	-	3,3,3	0.53	0	2,2,2	0.39	0
8	AKR	A	609	-	1,4,4	0.89	0	0,4,4	0.00	-
8	AKR	B	610	-	1,4,4	0.95	0	0,4,4	0.00	-
9	EDO	B	613	-	3,3,3	0.57	0	2,2,2	0.35	0
9	EDO	B	617	-	3,3,3	0.51	0	2,2,2	0.23	0
7	NAG	A	605	1	14,14,15	0.25	0	17,19,21	1.13	2 (11%)
6	BOG	A	604	-	20,20,20	0.94	1 (5%)	25,25,25	1.06	2 (8%)
7	NAG	A	608	1	14,14,15	0.55	0	17,19,21	0.45	0
9	EDO	B	615	-	3,3,3	0.59	0	2,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	IBP	B	601	-	12,15,15	0.49	0	16,20,20	1.00	1 (6%)
9	EDO	B	614	-	3,3,3	0.65	0	2,2,2	0.51	0
9	EDO	B	618	-	3,3,3	0.36	0	2,2,2	0.89	0
9	EDO	A	612	-	3,3,3	0.43	0	2,2,2	0.46	0
9	EDO	A	616	-	3,3,3	0.55	0	2,2,2	0.30	0
5	HEM	A	602	1,10	27,50,50	2.12	6 (22%)	17,82,82	1.94	6 (35%)
8	AKR	B	611	-	1,4,4	1.04	0	0,4,4	0.00	-
6	BOG	A	603	-	20,20,20	0.90	1 (5%)	25,25,25	1.16	1 (4%)
4	IBP	A	601	-	12,15,15	0.51	0	16,20,20	0.93	1 (6%)
9	EDO	A	611	-	3,3,3	0.80	0	2,2,2	0.51	0
9	EDO	A	614	-	3,3,3	0.54	0	2,2,2	0.37	0
9	EDO	A	615	-	3,3,3	0.62	0	2,2,2	0.60	0
6	BOG	B	603	-	20,20,20	0.93	1 (5%)	25,25,25	1.00	0
5	HEM	B	602	1,10	27,50,50	2.02	6 (22%)	17,82,82	2.06	6 (35%)
9	EDO	B	616	-	3,3,3	0.56	0	2,2,2	0.34	0
7	NAG	B	609	1	14,14,15	0.57	0	17,19,21	0.70	0
8	AKR	A	610	-	1,4,4	1.05	0	0,4,4	0.00	-
9	EDO	B	612	-	3,3,3	0.67	0	2,2,2	0.63	0

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
9	EDO	A	613	-	-	0/1/1/1	-
8	AKR	A	609	-	-	0/0/2/2	-
8	AKR	B	610	-	-	0/0/2/2	-
9	EDO	B	613	-	-	0/1/1/1	-
9	EDO	B	617	-	-	1/1/1/1	-
7	NAG	A	605	1	-	1/6/23/26	0/1/1/1
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	B	615	-	-	0/1/1/1	-
4	IBP	B	601	-	-	1/8/12/12	0/1/1/1
9	EDO	B	614	-	-	0/1/1/1	-
9	EDO	B	618	-	-	1/1/1/1	-
9	EDO	A	612	-	-	0/1/1/1	-
9	EDO	A	616	-	-	0/1/1/1	-
5	HEM	A	602	1,10	-	0/6/54/54	-
8	AKR	B	611	-	-	0/0/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BOG	A	603	-	-	7/11/31/31	0/1/1/1
4	IBP	A	601	-	-	0/8/12/12	0/1/1/1
9	EDO	A	611	-	-	0/1/1/1	-
9	EDO	A	614	-	-	0/1/1/1	-
9	EDO	A	615	-	-	0/1/1/1	-
6	BOG	B	603	-	-	7/11/31/31	0/1/1/1
5	HEM	B	602	1,10	-	0/6/54/54	-
9	EDO	B	616	-	-	1/1/1/1	-
7	NAG	B	609	1	-	0/6/23/26	0/1/1/1
8	AKR	A	610	-	-	0/0/2/2	-
9	EDO	B	612	-	-	0/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	602	HEM	C3D-C2D	4.97	1.52	1.37
5	A	602	HEM	C3D-C2D	4.86	1.52	1.37
5	A	602	HEM	C3C-C2C	-4.81	1.33	1.40
5	B	602	HEM	C3C-C2C	-3.90	1.35	1.40
5	B	602	HEM	C3B-C2B	-3.72	1.35	1.40
5	A	602	HEM	C3B-CAB	3.55	1.55	1.47
5	A	602	HEM	C3C-CAC	3.51	1.55	1.47
5	B	602	HEM	C3B-CAB	3.50	1.55	1.47
5	A	602	HEM	C3B-C2B	-3.40	1.35	1.40
5	B	602	HEM	C3C-CAC	3.37	1.54	1.47
6	B	603	BOG	O5-C1	2.94	1.49	1.41
6	A	604	BOG	O5-C1	2.78	1.48	1.41
6	A	603	BOG	O5-C1	2.70	1.48	1.41
5	A	602	HEM	CAA-C2A	2.29	1.55	1.52
5	B	602	HEM	CAA-C2A	2.04	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	602	HEM	CBD-CAD-C3D	-5.49	102.37	112.48
5	A	602	HEM	CBD-CAD-C3D	-4.99	103.29	112.48
6	A	603	BOG	C1'-O1-C1	4.07	120.59	113.84
5	B	602	HEM	CMB-C2B-C3B	3.08	130.45	124.68
4	B	601	IBP	C12-C13-C8	-2.75	118.43	121.20
7	A	605	NAG	C1-O5-C5	2.72	115.87	112.19
5	A	602	HEM	CMD-C2D-C3D	2.59	129.82	124.94
5	A	602	HEM	CMD-C2D-C1D	-2.58	124.49	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HEM	CMB-C2B-C3B	2.54	129.42	124.68
5	B	602	HEM	CBA-CAA-C2A	-2.35	108.15	112.49
5	A	602	HEM	CBA-CAA-C2A	-2.33	108.18	112.49
6	A	604	BOG	C1'-O1-C1	-2.23	110.15	113.84
5	A	602	HEM	CAD-CBD-CGD	-2.15	109.07	112.67
5	B	602	HEM	C4A-C3A-C2A	2.11	108.46	107.00
7	A	605	NAG	C4-C3-C2	-2.08	107.98	111.02
4	A	601	IBP	C12-C13-C8	-2.05	119.13	121.20
5	B	602	HEM	CMD-C2D-C3D	2.03	128.78	124.94
5	B	602	HEM	C1D-C2D-C3D	-2.03	105.59	107.00
6	A	604	BOG	O5-C1-C2	2.02	114.63	110.35

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	604	BOG	C2-C1-O1-C1'
6	A	604	BOG	O5-C1-O1-C1'
6	B	603	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	604	BOG	C3'-C4'-C5'-C6'
6	A	603	BOG	C4'-C5'-C6'-C7'
6	A	603	BOG	C2'-C3'-C4'-C5'
6	A	603	BOG	C3'-C4'-C5'-C6'
6	A	604	BOG	C2'-C3'-C4'-C5'
6	B	603	BOG	C2'-C1'-O1-C1
6	A	604	BOG	C1'-C2'-C3'-C4'
9	B	617	EDO	O1-C1-C2-O2
9	B	618	EDO	O1-C1-C2-O2
6	A	604	BOG	C4'-C5'-C6'-C7'
6	A	603	BOG	C1'-C2'-C3'-C4'
6	A	603	BOG	C5'-C6'-C7'-C8'
6	A	603	BOG	C2'-C1'-O1-C1
6	B	603	BOG	C4-C5-C6-O6
6	A	604	BOG	O1-C1'-C2'-C3'
9	B	616	EDO	O1-C1-C2-O2
6	B	603	BOG	O1-C1'-C2'-C3'
6	B	603	BOG	O5-C5-C6-O6
7	A	608	NAG	C4-C5-C6-O6
7	A	605	NAG	C3-C2-N2-C7

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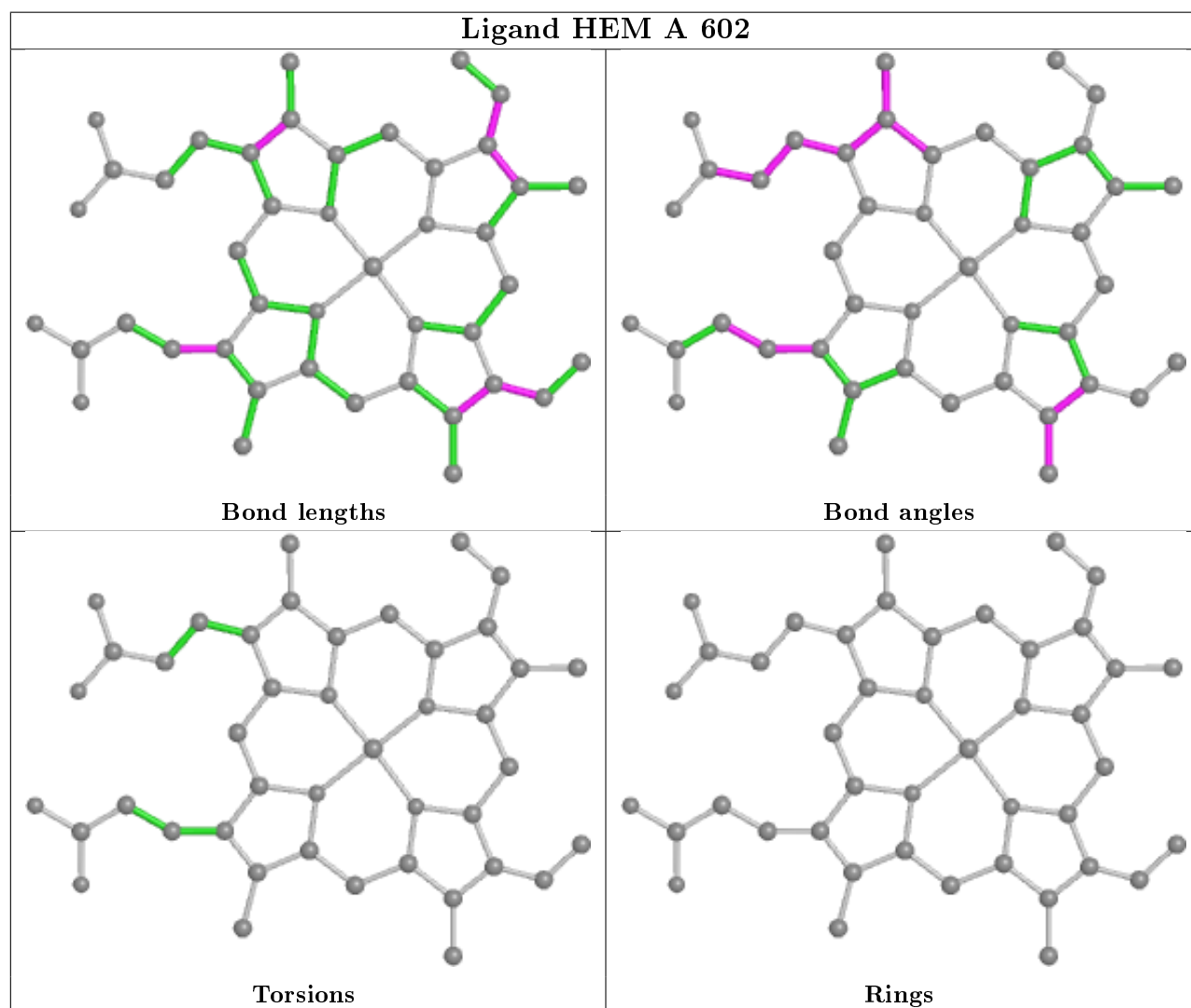
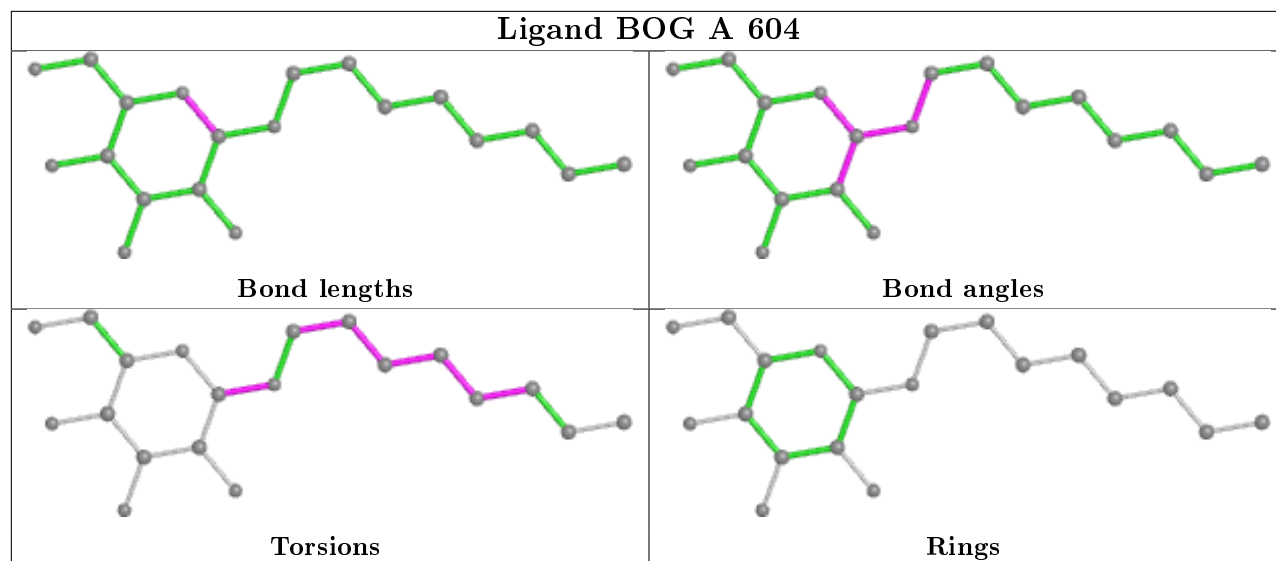
Mol	Chain	Res	Type	Atoms
4	B	601	IBP	C7-C6-C8-C9

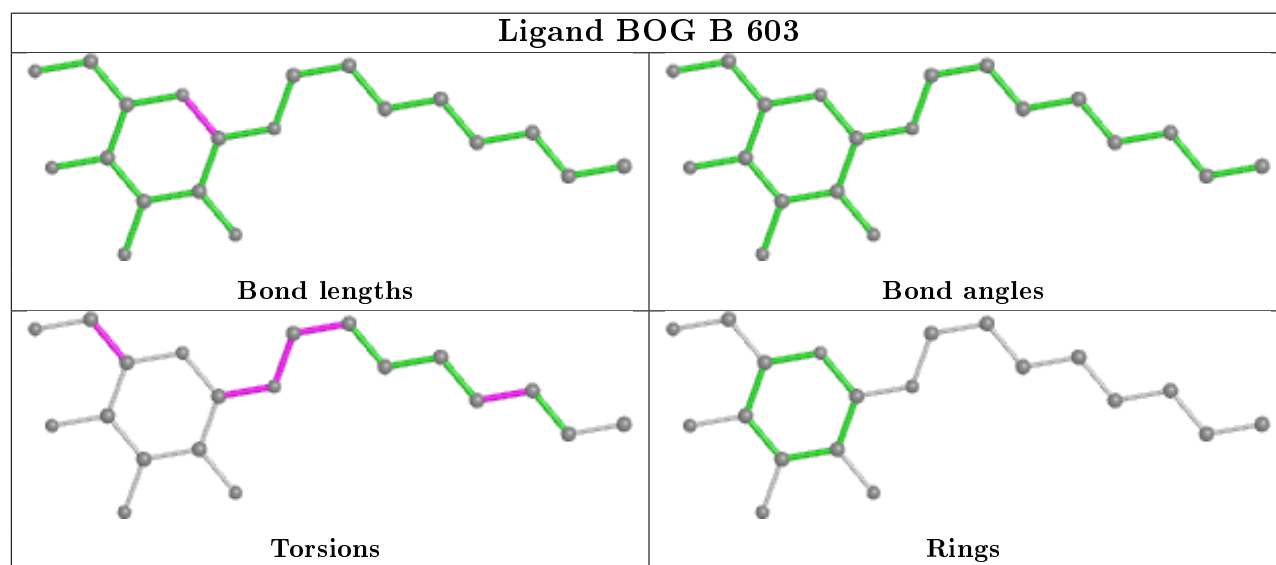
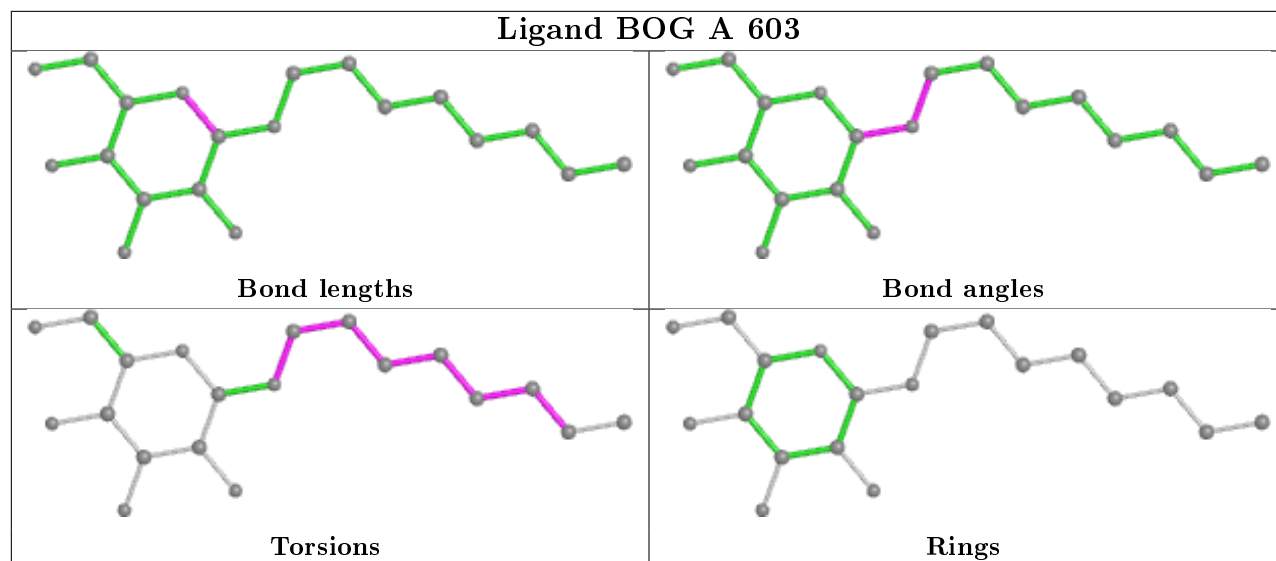
There are no ring outliers.

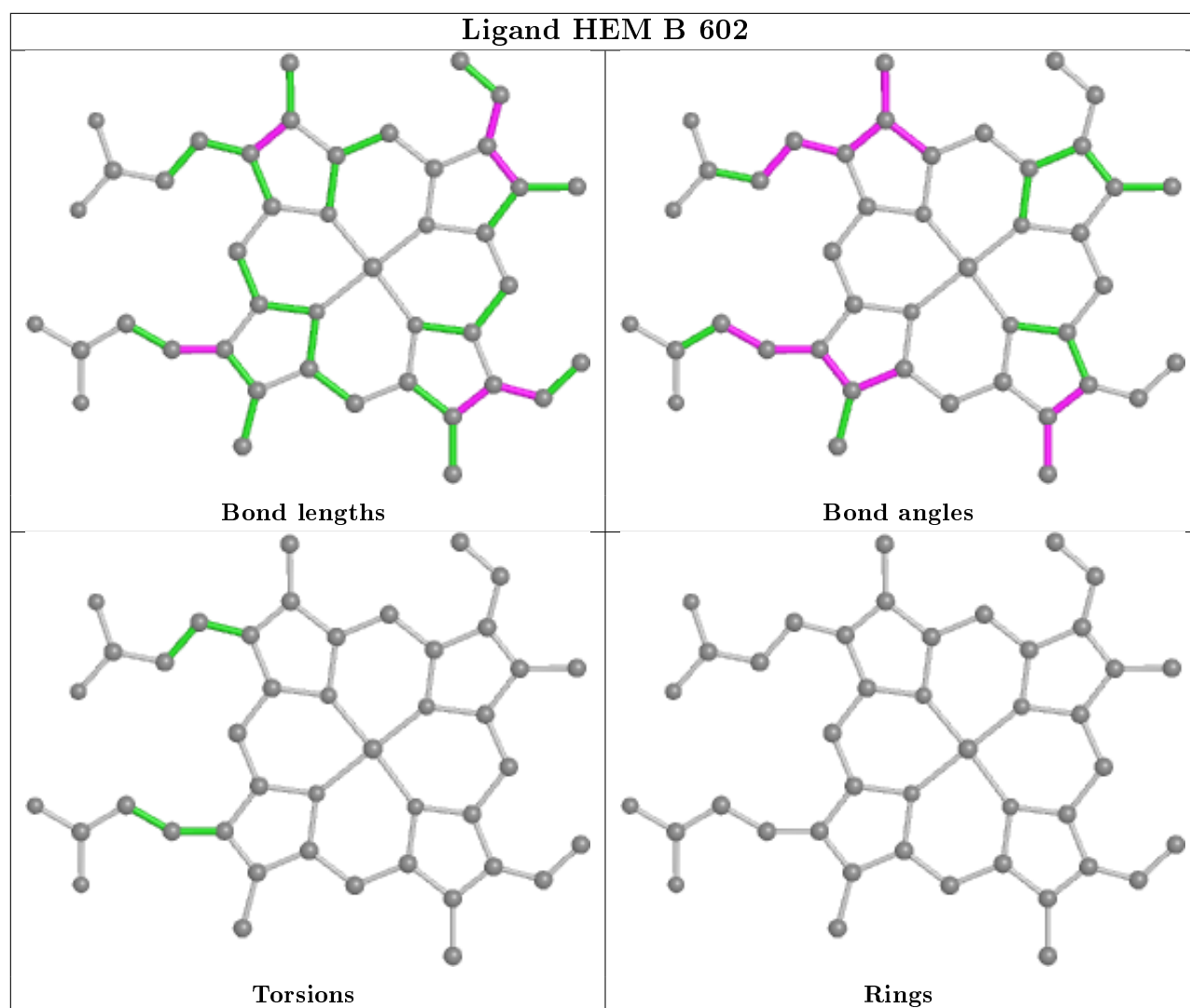
14 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	613	EDO	1	0
8	A	609	AKR	5	0
8	B	610	AKR	1	0
6	A	604	BOG	2	0
9	B	615	EDO	1	0
9	B	618	EDO	1	0
9	A	616	EDO	1	0
5	A	602	HEM	2	0
8	B	611	AKR	6	0
6	A	603	BOG	1	0
9	A	614	EDO	1	0
5	B	602	HEM	3	0
9	B	616	EDO	1	0
8	A	610	AKR	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	551/551 (100%)	-0.16	24 (4%) 34 28	16, 28, 48, 67	0
1	B	551/551 (100%)	-0.25	18 (3%) 46 40	16, 26, 41, 70	0
All	All	1102/1102 (100%)	-0.21	42 (3%) 40 35	16, 27, 45, 70	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	PHE	4.9
1	B	75	LEU	4.0
1	A	96	PHE	3.6
1	A	108	PHE	3.5
1	A	81	LEU	3.5
1	A	75	LEU	3.3
1	A	91	TYR	3.2
1	B	81	LEU	3.1
1	B	74	PHE	3.1
1	B	108	PHE	2.9
1	A	410	TYR	2.8
1	A	526	LEU	2.8
1	B	78	ILE	2.7
1	A	53	ASP	2.7
1	B	349	TYR	2.6
1	B	279	HIS	2.5
1	B	96	PHE	2.4
1	B	388	TRP	2.4
1	B	386	TYR	2.4
1	B	206	PHE	2.4
1	B	410	TYR	2.4
1	B	80	LEU	2.3
1	A	98	GLY	2.3
1	B	345	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	203	ALA	2.3
1	A	386	TYR	2.3
1	A	382	PHE	2.3
1	B	400	ASP	2.3
1	A	99	VAL	2.3
1	A	203	ALA	2.3
1	A	52	PHE	2.2
1	B	385	LEU	2.2
1	A	79	LYS	2.2
1	A	345	VAL	2.2
1	B	53	ASP	2.2
1	A	385	LEU	2.1
1	A	349	TYR	2.1
1	A	278	PRO	2.1
1	A	65	TYR	2.1
1	A	202	PHE	2.1
1	A	102	ILE	2.1
1	A	97	LYS	2.1

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

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

6.3 Carbohydrates ⓘ

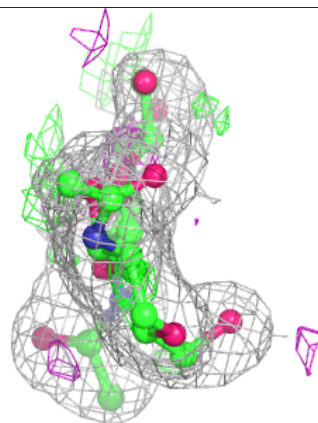
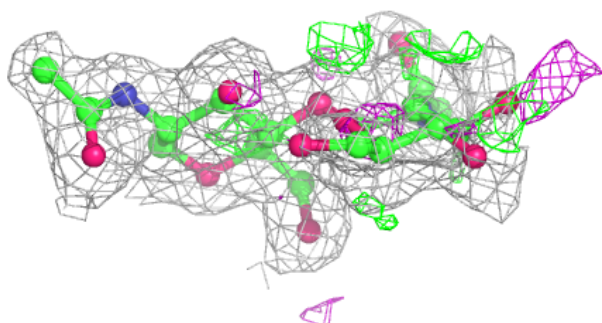
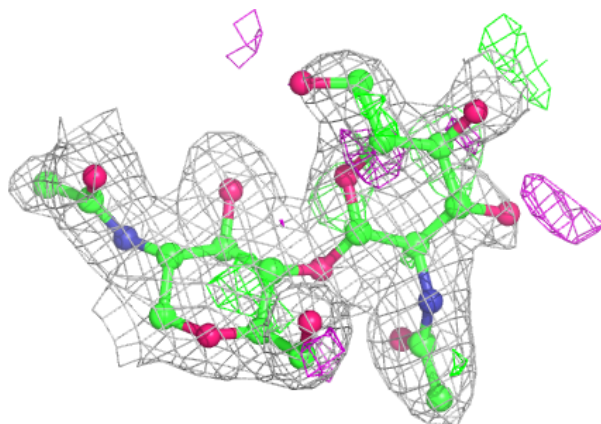
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	E	3	11/12	0.64	0.31	64,68,73,78	0
2	NAG	D	2	14/15	0.70	0.34	68,72,77,82	0
2	NAG	C	2	14/15	0.81	0.25	37,47,55,58	0
2	NAG	D	1	14/15	0.87	0.16	41,49,60,67	0
3	NAG	E	2	14/15	0.88	0.12	37,41,52,61	0
2	NAG	C	1	14/15	0.96	0.07	25,29,35,39	0
3	NAG	E	1	14/15	0.97	0.06	24,31,34,40	0

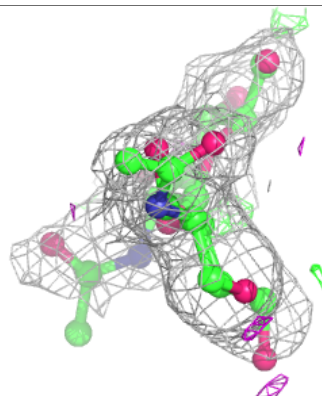
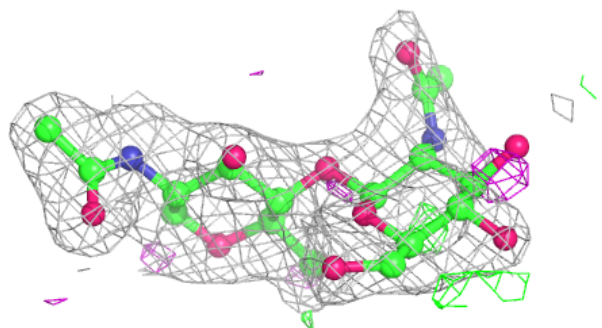
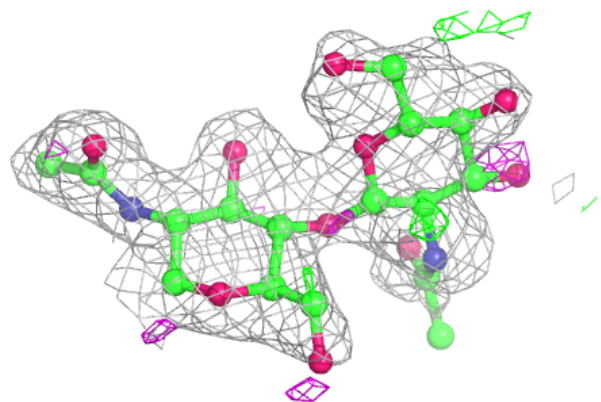
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

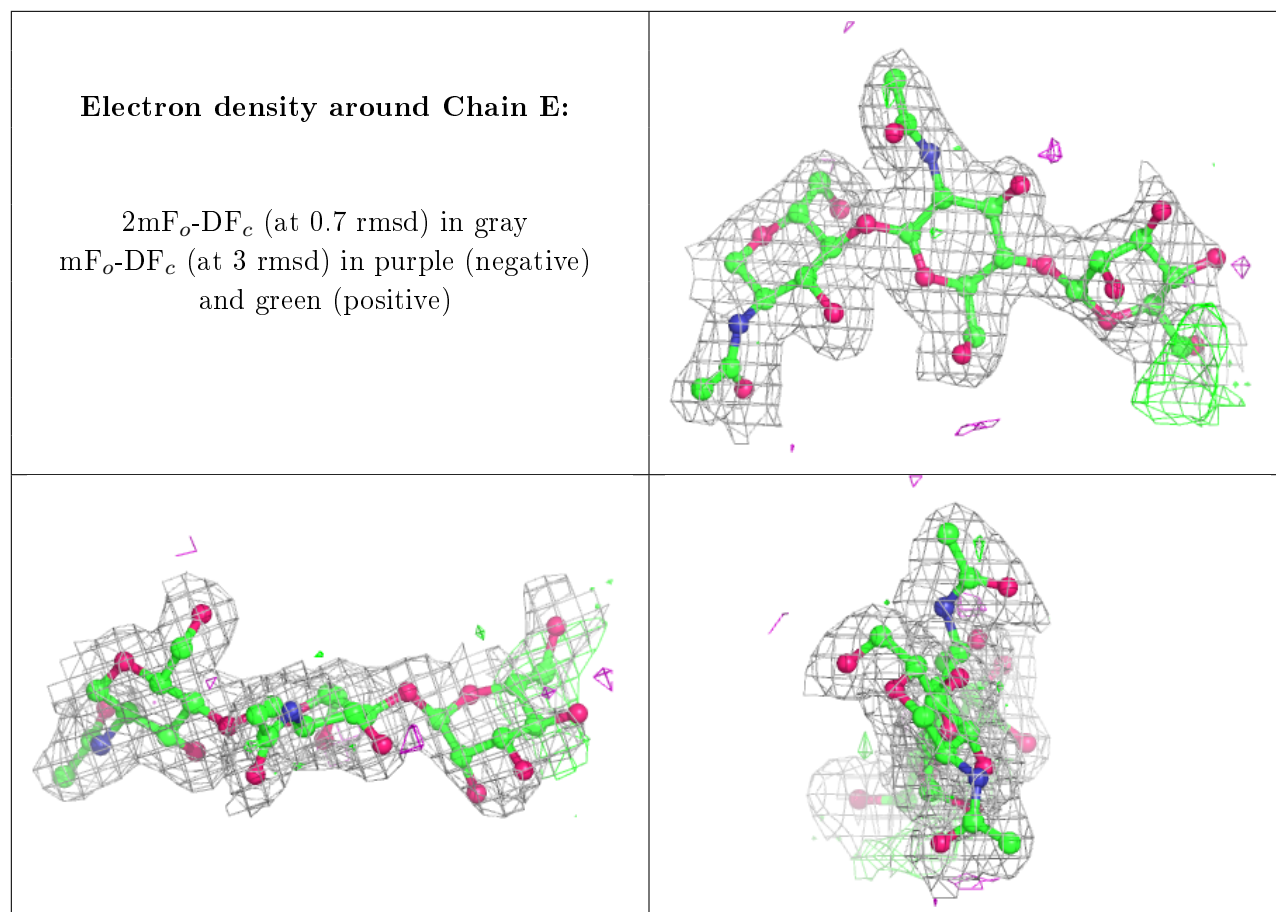
Electron density around Chain C:

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

**Electron density around Chain 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.

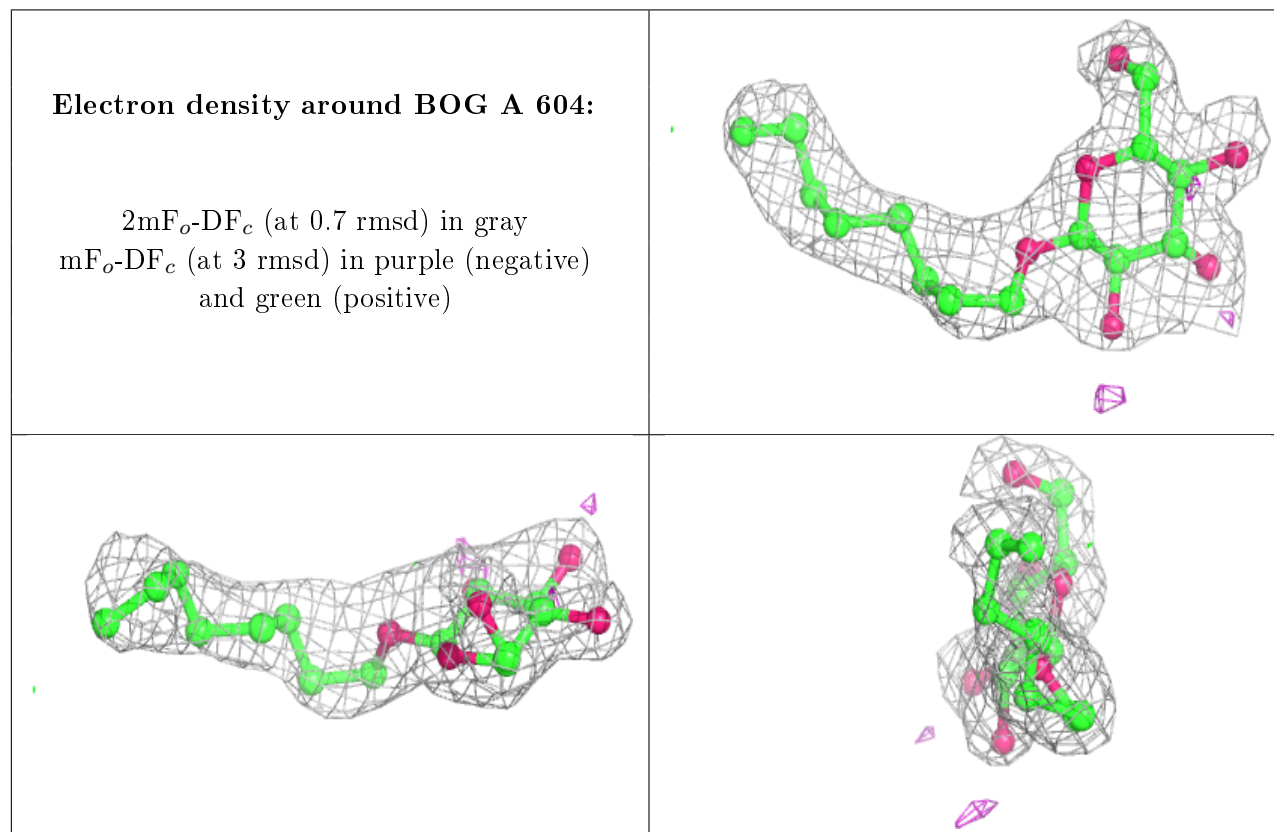
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	EDO	A	613	4/4	0.76	0.31	38,38,41,43	0
9	EDO	B	617	4/4	0.83	0.31	37,41,44,44	0
9	EDO	B	615	4/4	0.83	0.32	34,37,39,54	0
9	EDO	B	612	4/4	0.84	0.16	24,27,30,35	0
9	EDO	A	611	4/4	0.87	0.18	28,31,31,37	0
8	AKR	A	609	5/5	0.87	0.30	28,41,46,47	0
6	BOG	A	604	20/20	0.88	0.15	42,48,52,53	0
6	BOG	B	603	20/20	0.88	0.14	41,44,47,49	0
7	NAG	A	605	14/15	0.88	0.29	48,54,61,64	0
7	NAG	A	608	14/15	0.89	0.28	44,51,58,59	0
8	AKR	B	610	5/5	0.90	0.21	36,38,39,45	0
7	NAG	B	609	14/15	0.91	0.24	34,39,46,46	0

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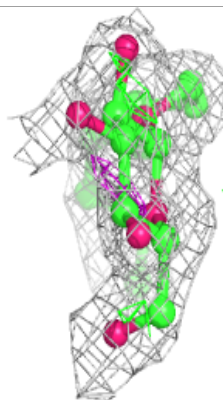
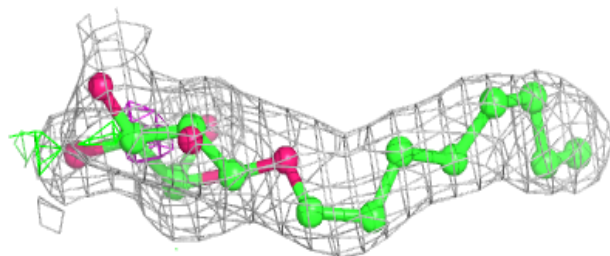
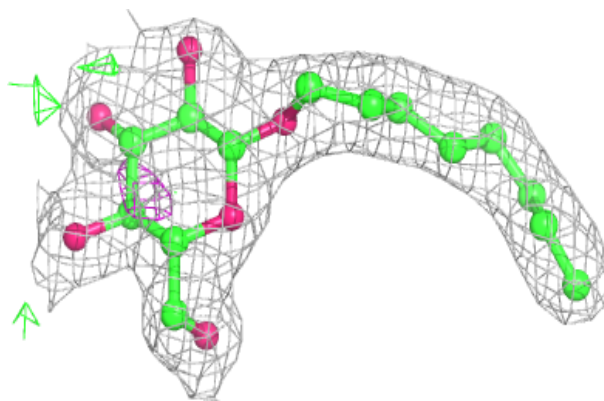
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	EDO	B	618	4/4	0.92	0.14	27,29,31,33	0
8	AKR	A	610	5/5	0.92	0.17	32,35,43,43	0
4	IBP	A	601	15/15	0.92	0.19	24,28,31,33	0
4	IBP	B	601	15/15	0.93	0.21	22,24,29,29	0
9	EDO	A	615	4/4	0.93	0.17	30,32,35,41	0
9	EDO	B	614	4/4	0.93	0.23	30,35,36,41	0
9	EDO	B	616	4/4	0.94	0.11	23,28,28,31	0
9	EDO	A	616	4/4	0.95	0.12	26,28,29,32	0
8	AKR	B	611	5/5	0.95	0.22	30,31,42,44	0
6	BOG	A	603	20/20	0.96	0.09	27,32,38,40	0
9	EDO	A	612	4/4	0.97	0.11	25,28,30,32	0
9	EDO	A	614	4/4	0.97	0.09	26,27,31,32	0
9	EDO	B	613	4/4	0.97	0.08	22,26,28,29	0
5	HEM	A	602	43/43	0.97	0.11	20,24,34,54	0
5	HEM	B	602	43/43	0.98	0.11	18,23,35,56	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.

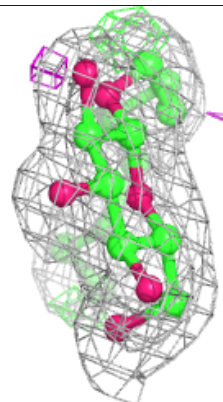
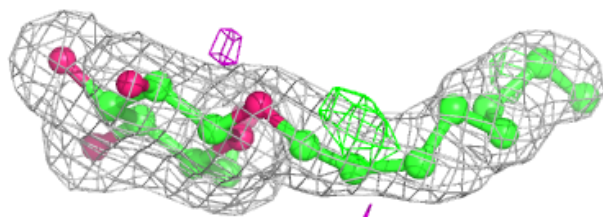
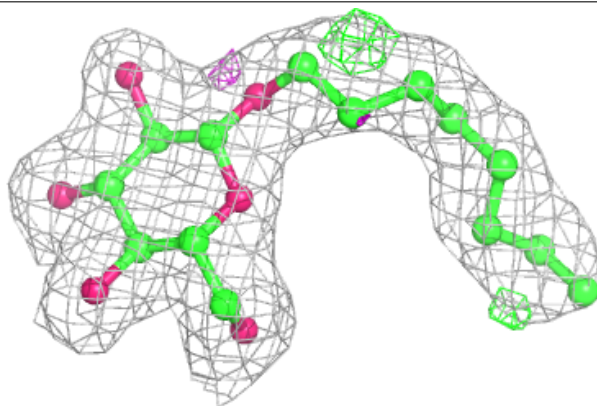


Electron density around BOG B 603:

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

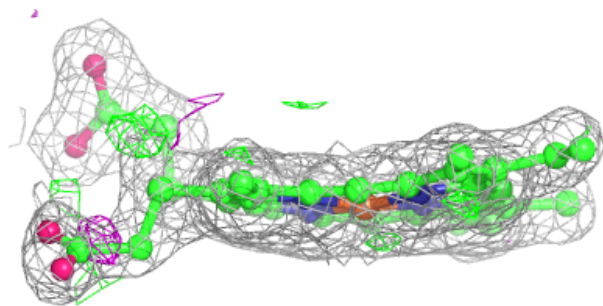
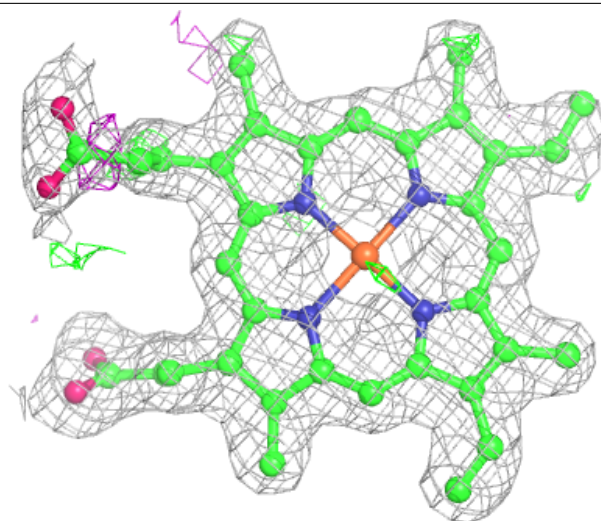
**Electron density around BOG A 603:**

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



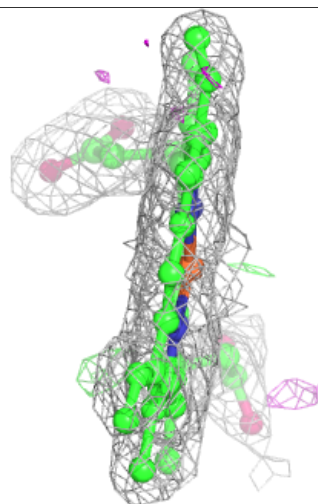
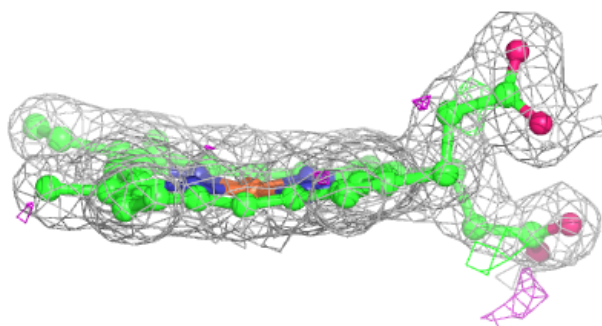
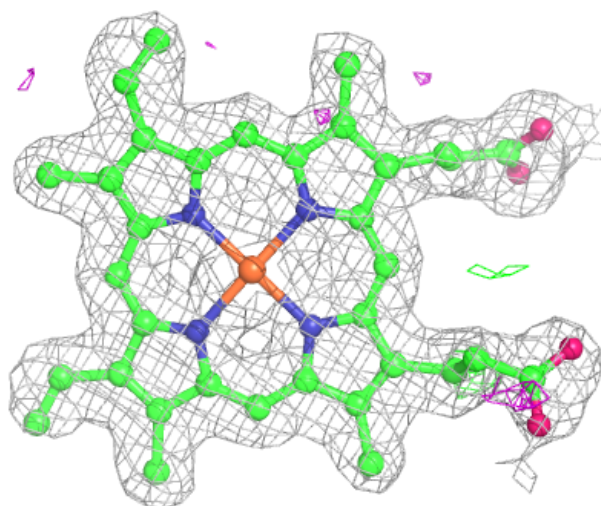
Electron density around HEM A 602:

$2mF_o-DF_c$ (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.