



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2023 – 02:16 PM EDT

PDB ID : 4OTJ  
Title : The complex of murine cyclooxygenase-2 with a conjugate of indomefathin and podophyllotoxin, N-{(succinylpodophyllotoxiny)but-4-yl}-2-{1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl}acetamide  
Authors : Xu, S.; Uddin, M.J.; Banerjee, S.; Marnett, L.J.  
Deposited on : 2014-02-13  
Resolution : 2.11 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](mailto: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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

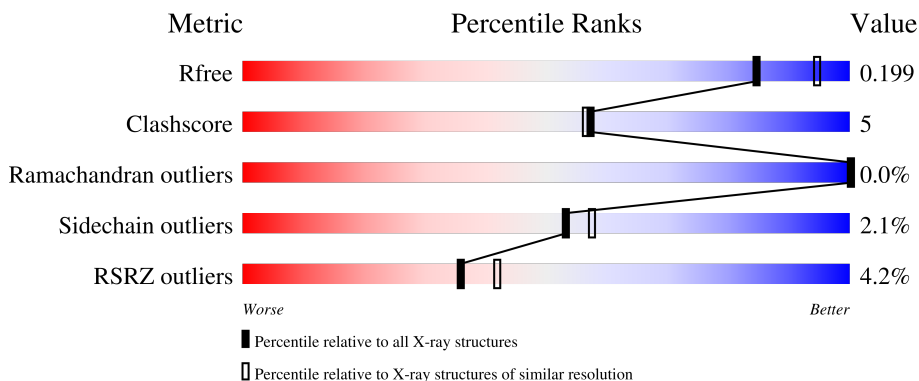
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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.



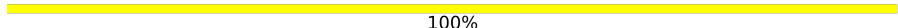


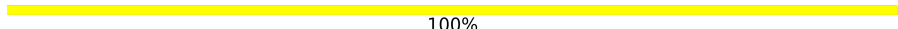
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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  $\geq 3$ , 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	587	 4% 87% 7% • 6%
1	B	587	 4% 85% 8% • 6%
1	C	587	 5% 86% 7% • 6%
1	D	587	 3% 86% 8% • 6%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	E	2	 100%
2	F	2	 50% 50%
2	G	2	 50% 50%
2	H	2	 100%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 20131 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
			Total	C	N	O	S			
1	A	552	4482	2890	753	814	25	0	1	0
1	B	551	4465	2880	748	812	25	0	0	0
1	C	552	4482	2890	753	814	25	0	1	0
1	D	551	4471	2884	748	814	25	0	1	0

- 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
			Total	C	N	O			
2	E	2	28	16	2	10	0	0	0
2	F	2	28	16	2	10	0	0	0
2	G	2	28	16	2	10	0	0	0
2	H	2	28	16	2	10	0	0	0

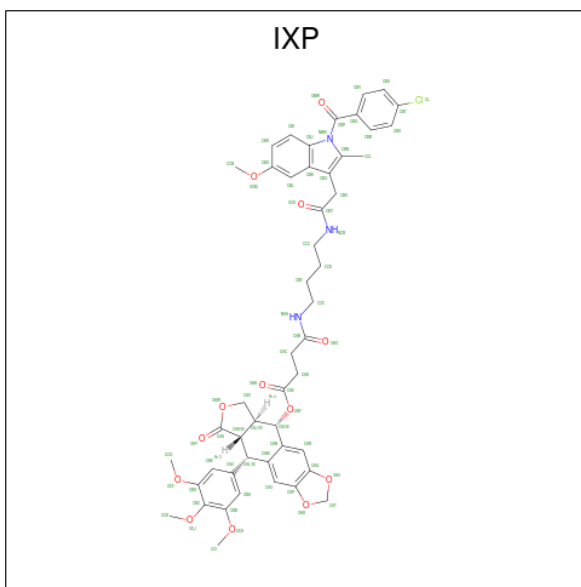
- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

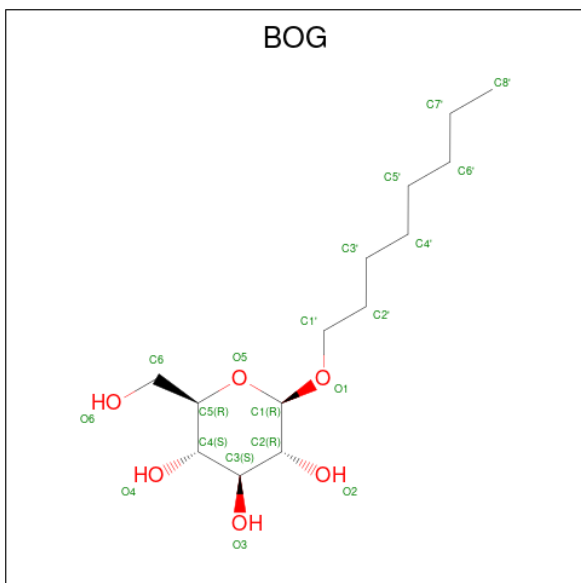
- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
5	A	1	Total 66	C 49	Cl 1	N 3	O 13	34	0
5	B	1	Total 66	C 49	Cl 1	N 3	O 13	36	0
5	C	1	Total 66	C 49	Cl 1	N 3	O 13	41	0
5	D	1	Total 66	C 49	Cl 1	N 3	O 13	34	0

- Molecule 6 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



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

- Molecule 7 is water.

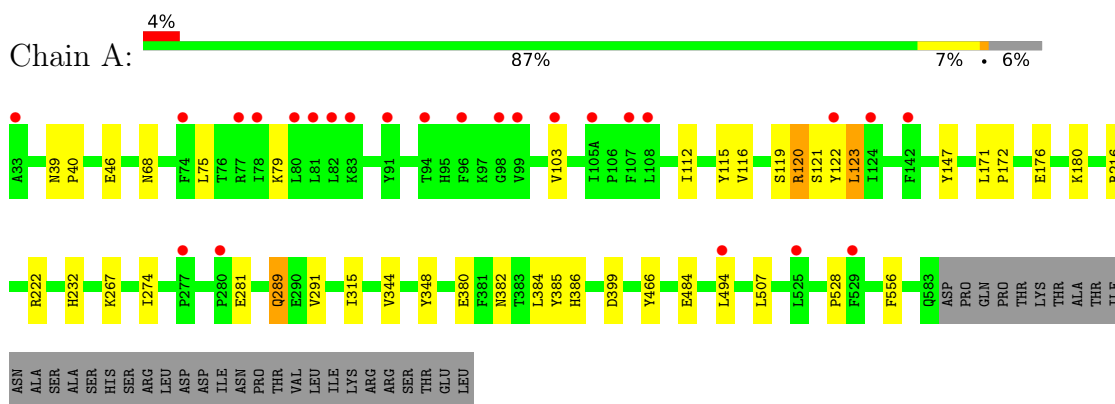
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	340	Total	O	0	0
			340	340		
7	B	336	Total	O	0	0
			336	336		
7	C	406	Total	O	0	0
			406	406		
7	D	449	Total	O	0	0
			449	449		



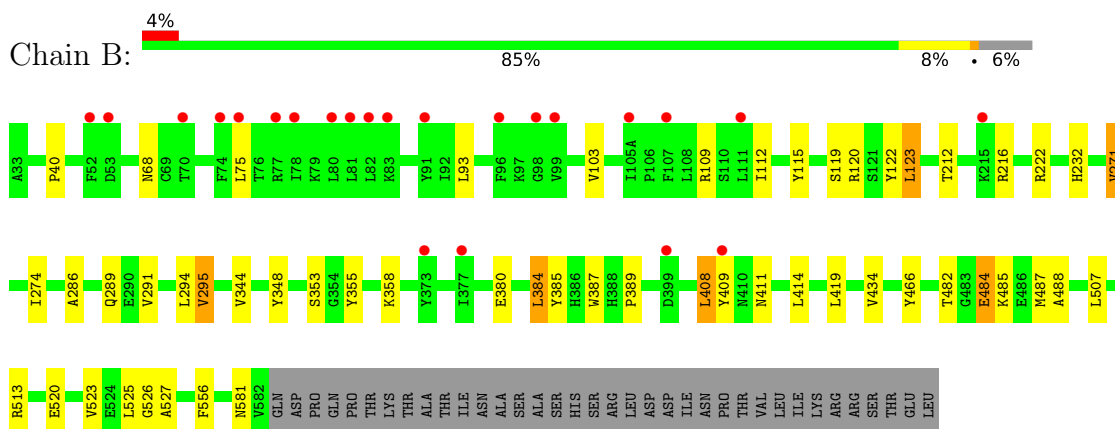
### 3 Residue-property plots [i](#)

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.

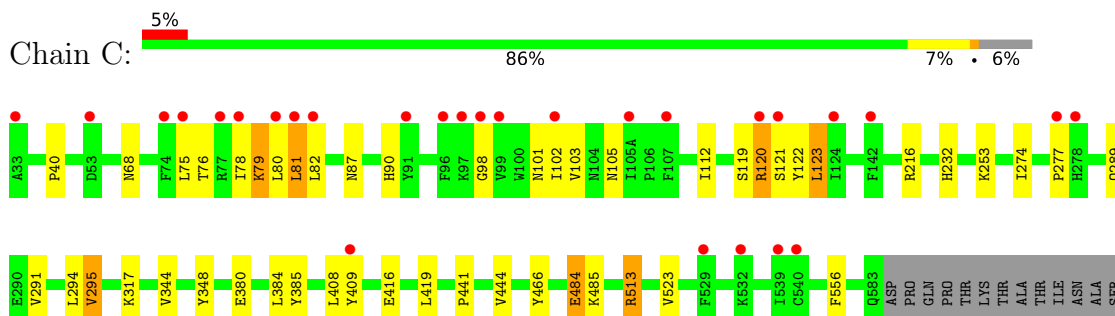
- Molecule 1: Prostaglandin G/H synthase 2



- Molecule 1: Prostaglandin G/H synthase 2

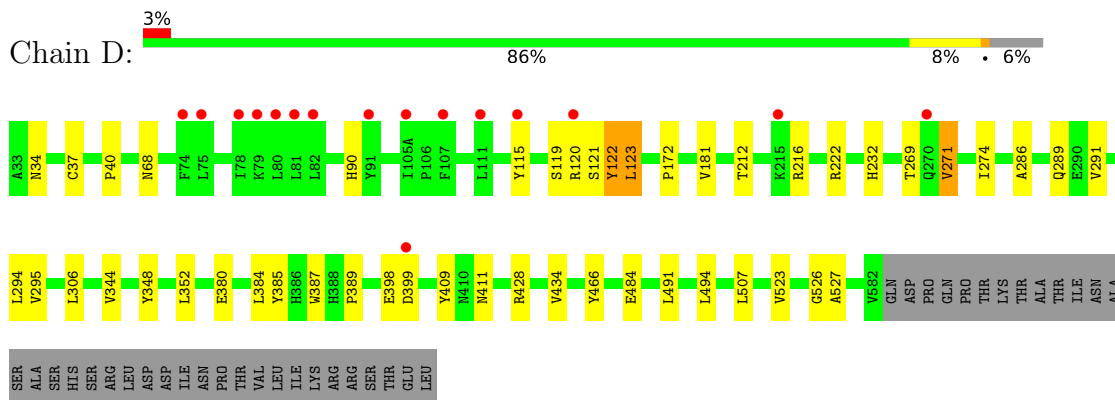


- Molecule 1: Prostaglandin G/H synthase 2

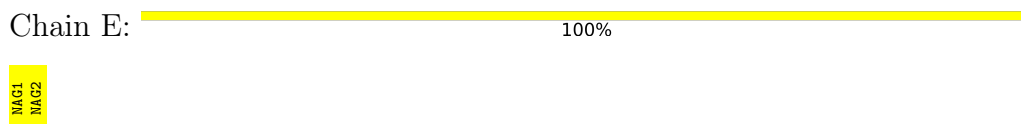


ALA  
SER  
HIS  
SER  
SER  
ARG  
LEU  
ASP  
ASP  
ILE  
ASN  
PRO  
THR  
VAL  
LEU  
LEU  
LYS  
LYS  
ARG  
ARG  
SER  
THR  
GLU  
LEU

- 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



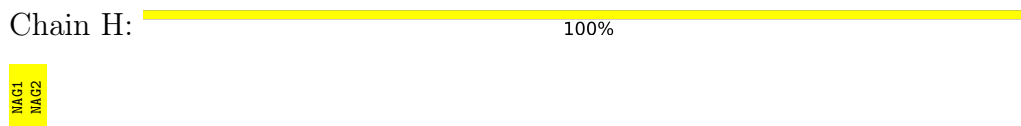
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.71Å 133.94Å 122.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.11 – 2.11 50.11 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.11-2.11) 99.6 (50.11-2.11)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.177 , 0.199 0.177 , 0.199	Depositor DCC
$R_{free}$ test set	5135 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtrriage
Anisotropy	0.533	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20131	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3388e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, BOG, NAG, IXP

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	0.33	0/4612	0.50	0/6253
1	B	0.36	0/4592	0.50	0/6227
1	C	0.34	0/4612	0.51	0/6253
1	D	0.36	0/4601	0.51	0/6239
All	All	0.35	0/18417	0.51	0/24972

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4482	0	4386	29	0
1	B	4465	0	4365	46	0
1	C	4482	0	4386	35	0
1	D	4471	0	4371	34	0
2	E	28	0	25	1	0
2	F	28	0	25	1	0
2	G	28	0	25	1	0
2	H	28	0	25	1	0
3	A	28	0	26	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	26	1	0
3	C	28	0	26	2	0
3	D	28	0	26	2	0
4	A	43	0	30	2	0
4	B	43	0	30	2	0
4	C	43	0	30	2	0
4	D	43	0	30	2	0
5	A	66	0	50	7	0
5	B	66	0	50	13	0
5	C	66	0	50	7	0
5	D	66	0	50	13	0
6	B	20	0	25	4	0
6	D	20	0	25	1	0
7	A	340	0	0	7	0
7	B	336	0	0	3	0
7	C	406	0	0	7	0
7	D	449	0	0	4	0
All	All	20131	0	18082	177	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 5.

All (177) 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:D:115:TYR:O	1:D:119:SER:HB3	1.53	1.07
1:D:523:VAL:CG2	5:D:707:IXP:H44	1.85	1.06
1:D:523:VAL:HG21	5:D:707:IXP:H44	1.36	1.06
1:A:120:ARG:NH2	5:A:706:IXP:H33	1.76	0.99
6:B:701:BOG:H5'2	6:B:701:BOG:H1'2	1.51	0.92
1:B:482:THR:OG1	1:B:484:GLU:HG3	1.72	0.89
1:C:384:LEU:HD13	5:C:706:IXP:CL	2.20	0.79
1:B:115:TYR:O	1:B:119:SER:HB3	1.84	0.78
1:A:384:LEU:HD23	1:A:507:LEU:HD11	1.69	0.74
1:B:212:THR:O	1:B:222:ARG:NH2	2.24	0.71
1:A:120:ARG:HH21	5:A:706:IXP:H33	1.57	0.70
1:C:75:LEU:O	1:C:79:LYS:HD3	1.92	0.69
1:C:523:VAL:HG21	5:C:706:IXP:H43	1.75	0.69
1:C:384:LEU:CD1	5:C:706:IXP:CL	2.79	0.68
1:D:523:VAL:HG21	5:D:707:IXP:CCN	2.18	0.67
1:B:222:ARG:NH1	7:B:947:HOH:O	2.22	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:LEU:HD12	1:B:507:LEU:HD11	1.78	0.65
1:C:294:LEU:HA	1:C:409:TYR:CE1	2.33	0.64
1:C:90:HIS:HE1	7:C:1178:HOH:O	1.81	0.64
1:A:216:ARG:NH1	2:E:2:NAG:O7	2.31	0.63
4:C:705:HEM:HBC2	4:C:705:HEM:HHD	1.78	0.63
1:C:484:GLU:HG2	1:C:485:LYS:H	1.65	0.62
1:C:523:VAL:CG2	5:C:706:IXP:H43	2.30	0.62
1:D:222:ARG:NH1	7:D:1133:HOH:O	2.33	0.62
1:D:523:VAL:HG22	5:D:707:IXP:H44	1.77	0.62
1:C:78:ILE:O	1:C:82:LEU:HG	2.01	0.60
1:D:526:GLY:HA3	5:D:707:IXP:H49	1.82	0.60
1:D:120:ARG:NH2	5:D:707:IXP:H33	2.16	0.59
6:B:701:BOG:H5'2	6:B:701:BOG:C1'	2.29	0.59
1:B:484:GLU:OE1	1:B:488:ALA:N	2.36	0.59
1:D:212:THR:O	1:D:222:ARG:NH2	2.36	0.59
1:B:484:GLU:CD	1:B:487:MET:HB2	2.24	0.58
5:C:706:IXP:H44	7:C:1119:HOH:O	2.02	0.58
1:A:122:TYR:CE2	1:A:123:LEU:HD13	2.38	0.58
1:D:274:ILE:HD12	1:D:291:VAL:HG12	1.86	0.57
4:A:705:HEM:HBC2	4:A:705:HEM:HHD	1.86	0.57
1:B:482:THR:CB	1:B:484:GLU:HG3	2.34	0.57
1:B:523:VAL:HG21	5:B:707:IXP:H44	1.86	0.57
1:A:384:LEU:HD23	1:A:507:LEU:CD1	2.35	0.56
4:A:705:HEM:HBB2	4:A:705:HEM:HHC	1.86	0.56
5:D:707:IXP:H39	5:D:707:IXP:OCA	2.05	0.56
1:C:485:LYS:HD2	7:C:1161:HOH:O	2.07	0.55
1:A:267:LYS:HD2	1:A:281:GLU:OE1	2.07	0.54
1:B:523:VAL:CG2	5:B:707:IXP:H44	2.36	0.54
1:A:46:GLU:HG2	7:A:1125:HOH:O	2.07	0.54
1:B:109:ARG:NH2	1:B:358:LYS:HG2	2.22	0.54
1:B:109:ARG:HH21	1:B:358:LYS:HG2	1.72	0.54
1:C:253:LYS:NZ	7:C:1027:HOH:O	2.40	0.54
1:B:484:GLU:OE1	1:B:487:MET:HB2	2.07	0.54
6:B:701:BOG:C1'	6:B:701:BOG:C5'	2.85	0.54
1:D:120:ARG:CZ	5:D:707:IXP:H33	2.37	0.53
5:D:707:IXP:CBQ	5:D:707:IXP:H46	2.37	0.53
1:A:116:VAL:O	1:A:120:ARG:HD3	2.08	0.53
1:C:120:ARG:NH2	5:C:706:IXP:OCA	2.41	0.53
1:A:222:ARG:HD3	7:A:1109:HOH:O	2.06	0.53
1:B:274:ILE:HD12	1:B:291:VAL:HG12	1.90	0.53
4:C:705:HEM:HHC	4:C:705:HEM:HBB2	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:ARG:HG3	7:D:918:HOH:O	2.09	0.53
1:B:216:ARG:NH1	2:F:2:NAG:O7	2.41	0.52
5:C:706:IXP:OBW	5:C:706:IXP:H38	2.09	0.52
1:C:103:VAL:HG11	1:C:112:ILE:HD12	1.92	0.52
4:D:705:HEM:HBC2	4:D:705:HEM:HHD	1.91	0.52
1:C:295:VAL:HG13	1:C:408:LEU:HD23	1.91	0.51
1:A:274:ILE:HD12	1:A:291:VAL:HG12	1.93	0.50
1:C:274:ILE:HD12	1:C:291:VAL:HG12	1.93	0.50
1:B:581:ASN:ND2	7:B:881:HOH:O	2.42	0.50
1:A:115:TYR:O	1:A:119:SER:HB3	2.11	0.50
1:A:122:TYR:CE1	1:A:123:LEU:HD22	2.47	0.49
4:D:705:HEM:HHC	4:D:705:HEM:HBB2	1.94	0.49
1:B:112:ILE:O	1:B:115:TYR:HB3	2.12	0.49
1:C:119:SER:OG	1:C:120:ARG:N	2.45	0.49
1:B:294:LEU:HG	1:B:295:VAL:HG22	1.95	0.49
1:B:384:LEU:HD21	1:B:525:LEU:HB3	1.96	0.48
1:C:98:GLY:O	1:C:102:ILE:HD12	2.13	0.48
1:A:103:VAL:HG11	1:A:112:ILE:HD12	1.95	0.48
1:D:526:GLY:HA3	5:D:707:IXP:CBU	2.43	0.48
4:B:706:HEM:HBC2	4:B:706:HEM:HHD	1.96	0.48
1:D:294:LEU:HA	1:D:409:TYR:CE1	2.48	0.48
1:C:87:ASN:OD1	1:C:513:ARG:NH1	2.47	0.48
1:C:380:GLU:HG2	1:C:466:TYR:CE1	2.49	0.48
5:B:707:IXP:CBV	5:B:707:IXP:H46	2.44	0.47
5:D:707:IXP:CBQ	5:D:707:IXP:CBI	2.92	0.47
3:A:701:NAG:O7	3:A:701:NAG:H3	2.13	0.47
1:A:171:LEU:O	7:A:1030:HOH:O	2.20	0.47
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.50	0.47
1:D:122:TYR:CE2	1:D:123:LEU:HD13	2.50	0.47
6:B:701:BOG:H1'2	6:B:701:BOG:C5'	2.24	0.47
1:A:315:ILE:HG13	7:A:991:HOH:O	2.15	0.47
4:B:706:HEM:HBB2	4:B:706:HEM:HHC	1.97	0.47
1:C:484:GLU:HG2	1:C:485:LYS:N	2.29	0.47
1:D:172:PRO:HG3	1:D:494:LEU:O	2.15	0.47
1:B:294:LEU:HA	1:B:409:TYR:CE1	2.49	0.46
5:A:706:IXP:H38	5:A:706:IXP:OBW	2.15	0.46
1:B:353:SER:HA	5:B:707:IXP:OCM	2.15	0.46
1:C:76:THR:O	1:C:80:LEU:HD13	2.15	0.46
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.51	0.46
5:B:707:IXP:CBV	5:B:707:IXP:CBI	2.94	0.46
5:B:707:IXP:OBW	5:B:707:IXP:H38	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:701:NAG:O7	3:C:701:NAG:H3	2.16	0.45
1:D:387:TRP:HZ2	5:D:707:IXP:CL	2.36	0.45
5:A:706:IXP:CBI	5:A:706:IXP:CBV	2.94	0.45
1:B:484:GLU:OE2	1:B:487:MET:HB2	2.16	0.45
1:B:120:ARG:CZ	5:B:707:IXP:H33	2.47	0.45
1:C:101:ASN:O	1:C:105:ASN:ND2	2.45	0.45
1:A:75:LEU:O	1:A:79:LYS:HG3	2.16	0.45
1:C:295:VAL:CG1	1:C:408:LEU:HD23	2.47	0.45
1:A:176:GLU:OE1	1:A:180:LYS:HE2	2.17	0.45
1:A:382:ASN:O	1:A:386:HIS:HD2	1.99	0.45
1:D:269:THR:OG1	1:D:271:VAL:HG13	2.16	0.45
1:B:527:ALA:HB1	5:B:707:IXP:OCA	2.17	0.45
1:C:294:LEU:HA	1:C:409:TYR:CD1	2.52	0.45
1:D:216:ARG:NH1	2:H:2:NAG:O7	2.50	0.45
1:D:90:HIS:HE1	7:D:964:HOH:O	1.99	0.45
1:D:527:ALA:CA	5:D:707:IXP:H50	2.47	0.44
1:A:120:ARG:HB3	1:A:528:PRO:HG3	1.98	0.44
1:B:353:SER:HA	5:B:707:IXP:CBG	2.47	0.44
1:C:81:LEU:HB3	1:C:82:LEU:HD23	1.99	0.44
1:B:271:VAL:HG22	1:B:286:ALA:HB1	1.98	0.44
1:D:120:ARG:HE	1:D:120:ARG:HB2	1.60	0.44
1:B:484:GLU:HB2	1:B:485:LYS:H	1.63	0.44
1:D:380:GLU:HG2	1:D:466:TYR:CE1	2.52	0.44
1:B:384:LEU:HD12	1:B:507:LEU:CD1	2.46	0.44
1:D:344:VAL:HA	1:D:348:TYR:HB3	2.00	0.44
1:C:82:LEU:HD23	1:C:82:LEU:N	2.32	0.44
1:B:526:GLY:HA3	5:B:707:IXP:CBU	2.47	0.44
1:D:389:PRO:HB2	1:D:434:VAL:HA	2.00	0.44
1:B:295:VAL:HG13	1:B:408:LEU:HD22	2.00	0.43
1:B:414:LEU:HD11	1:B:419:LEU:HD23	2.01	0.43
3:D:701:NAG:O7	3:D:701:NAG:H3	2.19	0.43
1:D:34:ASN:HB3	1:D:37:CYS:SG	2.59	0.43
1:D:384:LEU:HD23	1:D:507:LEU:HD11	2.01	0.43
1:A:120:ARG:NH2	5:A:706:IXP:CCC	2.66	0.43
1:A:399:ASP:OD1	7:A:892:HOH:O	2.21	0.43
1:B:122:TYR:CE2	1:B:123:LEU:HD13	2.53	0.43
1:B:120:ARG:HD3	5:B:707:IXP:H28	1.99	0.43
1:A:40:PRO:O	1:A:68:ASN:HB3	2.19	0.43
1:C:40:PRO:O	1:C:68:ASN:HB3	2.19	0.43
1:C:122:TYR:CE2	1:C:123:LEU:HD13	2.54	0.42
1:D:40:PRO:O	1:D:68:ASN:HB3	2.18	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:TRP:HZ2	5:B:707:IXP:CL	2.40	0.42
1:D:384:LEU:HD23	1:D:507:LEU:CD1	2.49	0.42
3:D:701:NAG:O7	3:D:701:NAG:C3	2.66	0.42
5:A:706:IXP:CBV	5:A:706:IXP:H46	2.50	0.42
1:D:271:VAL:HG22	1:D:286:ALA:HB1	2.00	0.42
1:A:344:VAL:HA	1:A:348:TYR:HB3	2.01	0.42
3:A:701:NAG:O7	3:A:701:NAG:C3	2.66	0.42
3:B:702:NAG:O7	3:B:702:NAG:C3	2.67	0.42
1:A:39:ASN:HA	7:A:999:HOH:O	2.20	0.42
1:B:411:ASN:ND2	7:B:1086:HOH:O	2.52	0.42
1:B:484:GLU:C	1:B:485:LYS:HG2	2.39	0.42
1:C:344:VAL:O	1:C:348:TYR:HB3	2.20	0.42
1:C:277:PRO:HA	7:C:1145:HOH:O	2.18	0.42
1:D:123:LEU:HD12	1:D:123:LEU:HA	1.93	0.42
1:B:389:PRO:HB2	1:B:434:VAL:HA	2.00	0.42
1:B:484:GLU:OE2	1:B:487:MET:HE2	2.20	0.42
1:C:317:LYS:NZ	7:C:892:HOH:O	2.39	0.42
1:C:216:ARG:NH1	2:G:2:NAG:O7	2.51	0.41
1:C:419:LEU:HD23	1:C:419:LEU:HA	1.90	0.41
1:D:398:GLU:HB3	1:D:399:ASP:H	1.66	0.41
1:C:441:PRO:HG2	1:C:444:VAL:HG22	2.02	0.41
1:C:484:GLU:HG2	7:C:1130:HOH:O	2.21	0.41
1:B:344:VAL:O	1:B:348:TYR:HB3	2.20	0.41
5:A:706:IXP:H39	5:A:706:IXP:OCA	2.20	0.41
1:A:147:TYR:HB2	7:A:853:HOH:O	2.21	0.41
6:D:706:BOG:H2'1	6:D:706:BOG:H5'2	1.80	0.41
1:B:40:PRO:O	1:B:68:ASN:HB3	2.21	0.41
1:B:93:LEU:HD13	1:B:355:TYR:CZ	2.56	0.41
1:B:120:ARG:HB3	1:B:123:LEU:HD23	2.03	0.41
1:A:172:PRO:HG3	1:A:494:LEU:O	2.20	0.40
1:B:513:ARG:HH21	1:B:520:GLU:HG3	1.86	0.40
3:C:701:NAG:O7	3:C:701:NAG:C3	2.69	0.40
1:B:482:THR:HB	1:B:484:GLU:CG	2.52	0.40
1:A:289:GLN:OE1	1:A:291:VAL:HG22	2.21	0.40
1:B:103:VAL:HG11	1:B:112:ILE:HD12	2.02	0.40
5:B:707:IXP:H46	5:B:707:IXP:CBQ	2.52	0.40
1:D:181:VAL:HG21	1:D:491:LEU:HD21	2.03	0.40
1:D:411:ASN:ND2	7:D:1044:HOH:O	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/587 (94%)	536 (97%)	15 (3%)	0	100	100
1	B	549/587 (94%)	531 (97%)	18 (3%)	0	100	100
1	C	551/587 (94%)	535 (97%)	16 (3%)	0	100	100
1	D	550/587 (94%)	533 (97%)	16 (3%)	1 (0%)	47	48
All	All	2201/2348 (94%)	2135 (97%)	65 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	122	TYR

### 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	494/525 (94%)	486 (98%)	8 (2%)	62	68
1	B	492/525 (94%)	481 (98%)	11 (2%)	52	55
1	C	494/525 (94%)	481 (97%)	13 (3%)	46	49
1	D	493/525 (94%)	483 (98%)	10 (2%)	55	59
All	All	1973/2100 (94%)	1931 (98%)	42 (2%)	53	57

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ARG
1	A	121	SER
1	A	123	LEU
1	A	232	HIS
1	A	289	GLN
1	A	385	TYR
1	A	484	GLU
1	A	556	PHE
1	B	75	LEU
1	B	123	LEU
1	B	232	HIS
1	B	271	VAL
1	B	289	GLN
1	B	295	VAL
1	B	384	LEU
1	B	385	TYR
1	B	408	LEU
1	B	484	GLU
1	B	556	PHE
1	C	79	LYS
1	C	81	LEU
1	C	120	ARG
1	C	121	SER
1	C	123	LEU
1	C	232	HIS
1	C	289	GLN
1	C	295	VAL
1	C	385	TYR
1	C	416	GLU
1	C	484	GLU
1	C	513	ARG
1	C	556	PHE
1	D	121	SER
1	D	123	LEU
1	D	232	HIS
1	D	271	VAL
1	D	289	GLN
1	D	295	VAL
1	D	306	LEU
1	D	352	LEU
1	D	385	TYR
1	D	484	GLU

Sometimes 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](#)

8 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	E	1	2,1	14,14,15	0.20	0	17,19,21	0.70	1 (5%)
2	NAG	E	2	2	14,14,15	0.41	0	17,19,21	0.45	0
2	NAG	F	1	2,1	14,14,15	0.33	0	17,19,21	0.50	0
2	NAG	F	2	2	14,14,15	0.50	0	17,19,21	0.45	0
2	NAG	G	1	2,1	14,14,15	0.16	0	17,19,21	0.61	0
2	NAG	G	2	2	14,14,15	0.63	1 (7%)	17,19,21	0.56	0
2	NAG	H	1	2,1	14,14,15	0.31	0	17,19,21	0.67	1 (5%)
2	NAG	H	2	2	14,14,15	0.50	0	17,19,21	0.40	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
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	1/6/23/26	0/1/1/1

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	NAG	C1-C2	2.06	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-O5-C5	2.36	115.39	112.19
2	H	1	NAG	C1-O5-C5	2.18	115.15	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

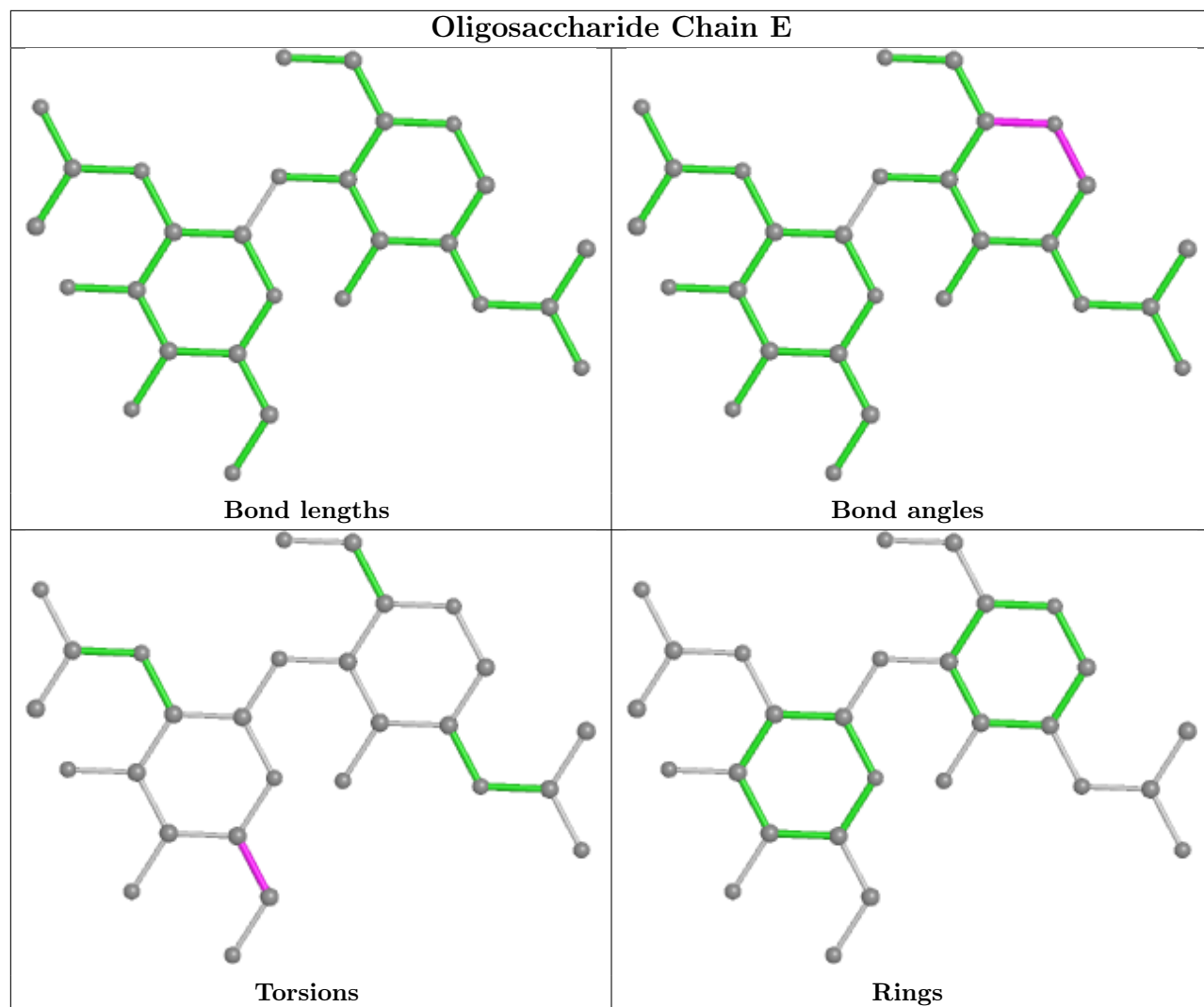
Mol	Chain	Res	Type	Atoms
2	H	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6

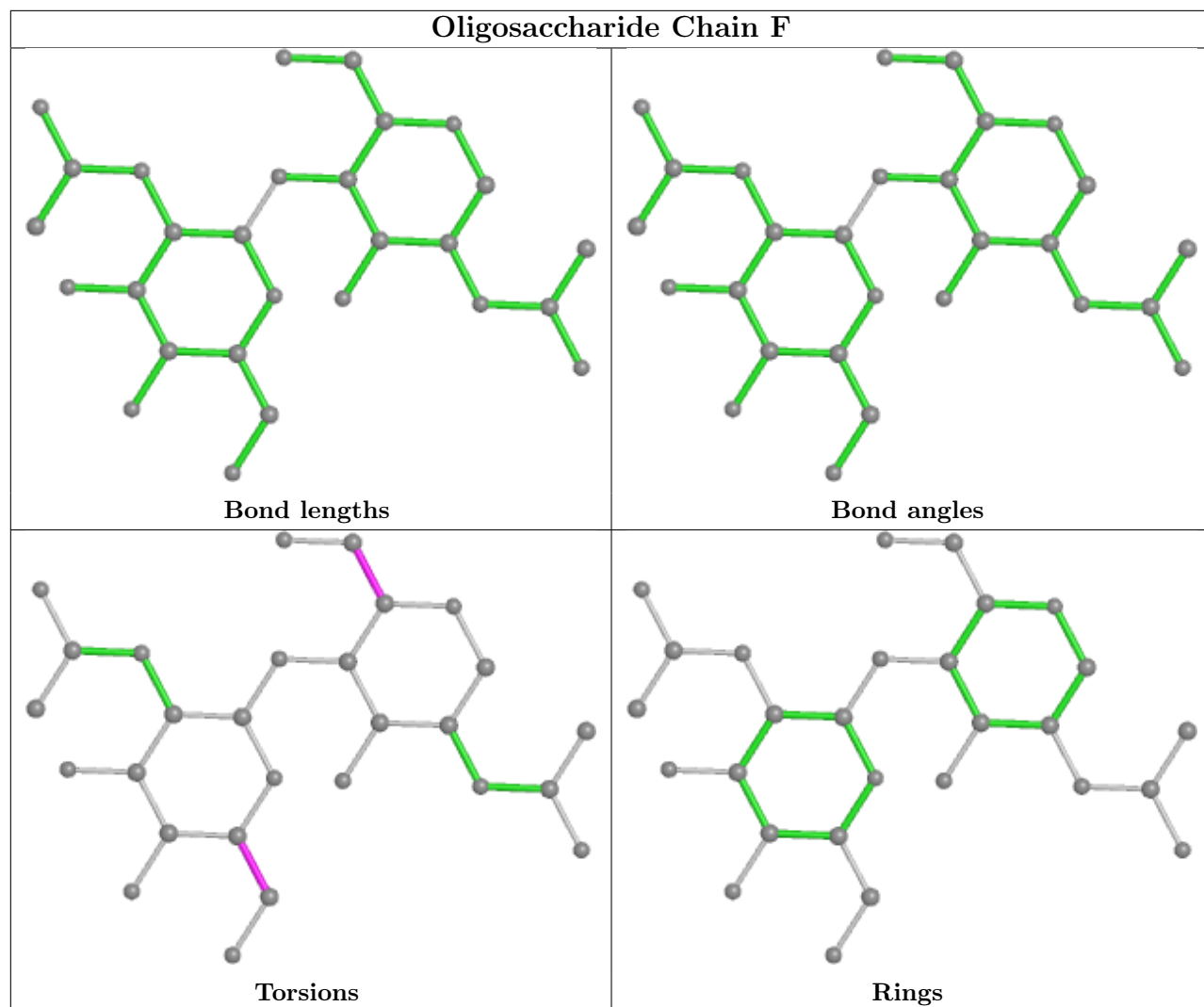
There are no ring outliers.

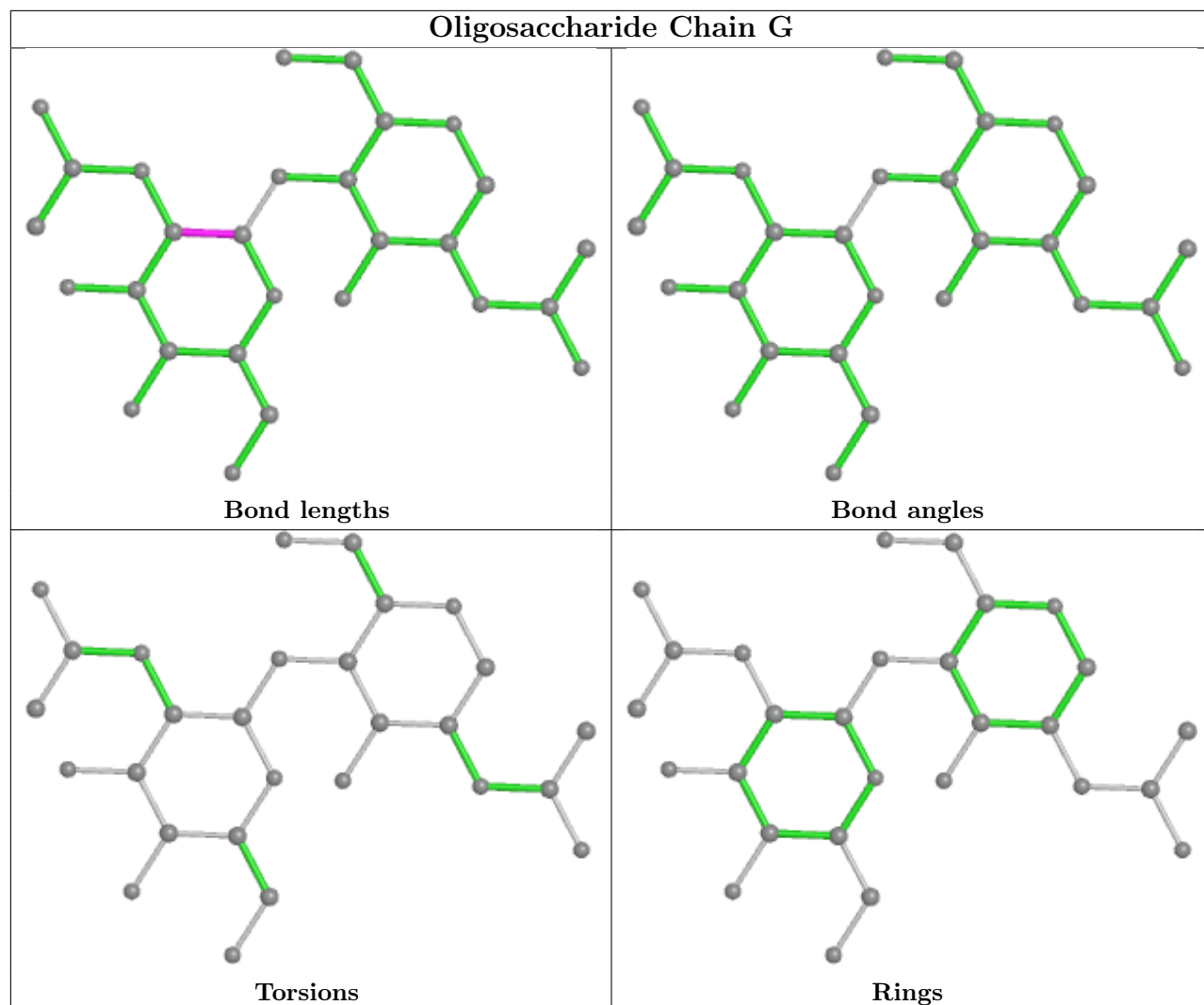
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	NAG	1	0
2	E	2	NAG	1	0
2	F	2	NAG	1	0
2	H	2	NAG	1	0

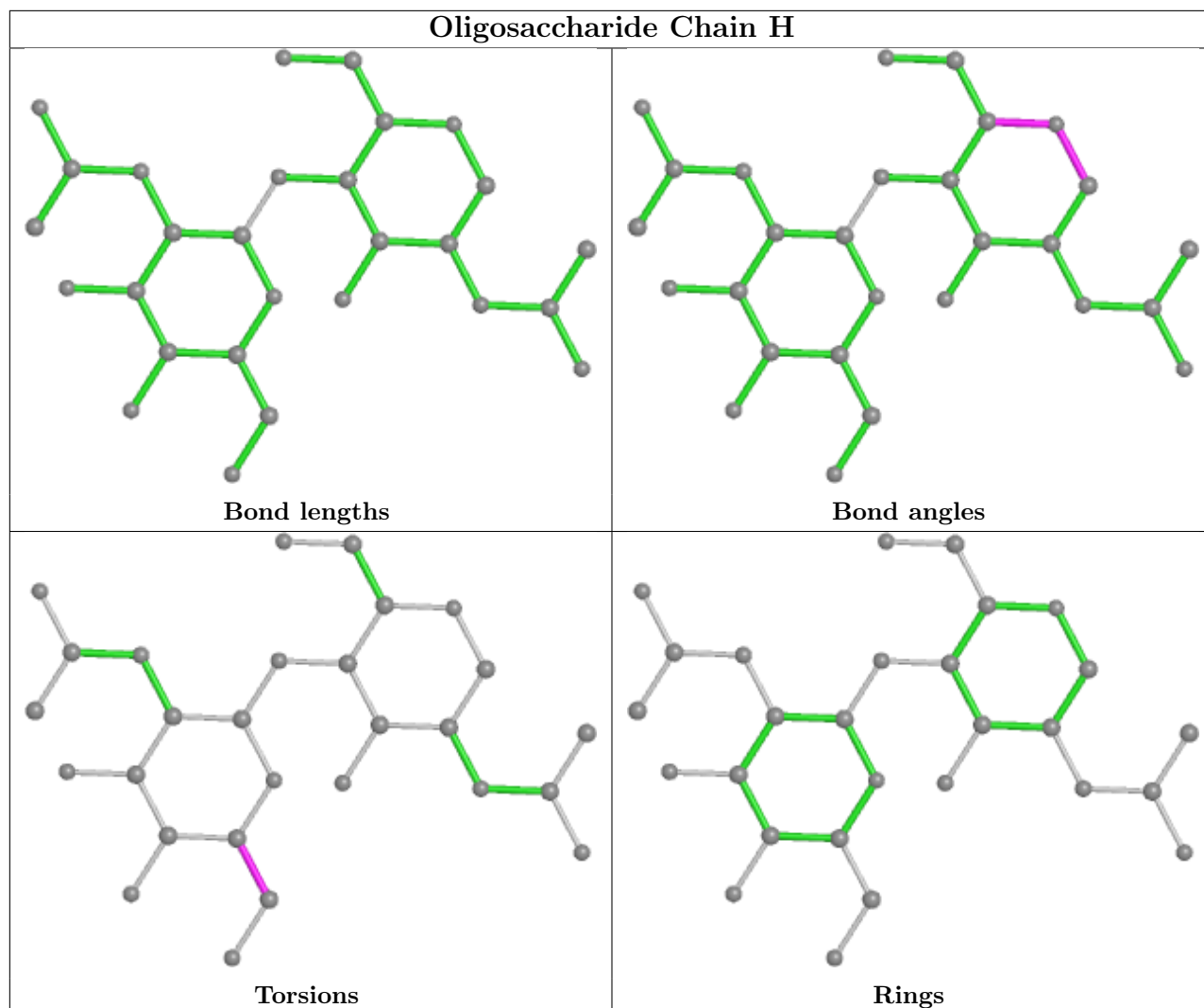
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

18 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	$\# Z  > 2$
5	IXP	D	707	-	70,73,73	2.43	13 (18%)	95,105,105	1.85	16 (16%)
3	NAG	B	702	1	14,14,15	0.71	1 (7%)	17,19,21	1.14	1 (5%)
3	NAG	A	704	1	14,14,15	0.38	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	701	1	14,14,15	0.75	1 (7%)	17,19,21	1.09	1 (5%)
3	NAG	C	704	1	14,14,15	0.35	0	17,19,21	0.43	0
3	NAG	A	701	1	14,14,15	0.87	1 (7%)	17,19,21	1.19	1 (5%)
5	IXP	A	706	-	70,73,73	2.45	14 (20%)	95,105,105	1.88	18 (18%)
5	IXP	B	707	-	70,73,73	2.41	14 (20%)	95,105,105	1.90	18 (18%)
4	HEM	A	705	7,1	41,50,50	2.00	7 (17%)	45,82,82	1.80	7 (15%)
5	IXP	C	706	-	70,73,73	2.51	14 (20%)	95,105,105	2.04	25 (26%)
4	HEM	B	706	7,1	41,50,50	1.98	7 (17%)	45,82,82	1.84	9 (20%)
4	HEM	D	705	7,1	41,50,50	1.99	6 (14%)	45,82,82	1.85	8 (17%)
6	BOG	D	706	-	20,20,20	1.65	7 (35%)	25,25,25	1.45	1 (4%)
4	HEM	C	705	7,1	41,50,50	2.02	6 (14%)	45,82,82	1.83	8 (17%)
3	NAG	D	704	1	14,14,15	0.42	0	17,19,21	0.47	0
3	NAG	B	705	1	14,14,15	0.36	0	17,19,21	0.51	0
3	NAG	D	701	1	14,14,15	0.82	1 (7%)	17,19,21	1.17	1 (5%)
6	BOG	B	701	-	20,20,20	1.67	5 (25%)	25,25,25	1.84	6 (24%)

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
5	IXP	D	707	-	-	12/38/77/77	0/8/8/8
3	NAG	B	702	1	-	1/6/23/26	0/1/1/1
3	NAG	A	704	1	-	0/6/23/26	0/1/1/1
3	NAG	C	701	1	-	1/6/23/26	0/1/1/1
3	NAG	C	704	1	-	0/6/23/26	0/1/1/1
3	NAG	A	701	1	-	1/6/23/26	0/1/1/1
5	IXP	A	706	-	-	10/38/77/77	0/8/8/8
5	IXP	B	707	-	-	12/38/77/77	0/8/8/8
4	HEM	A	705	7,1	-	1/12/54/54	-
5	IXP	C	706	-	-	15/38/77/77	0/8/8/8
4	HEM	B	706	7,1	-	0/12/54/54	-
4	HEM	D	705	7,1	-	0/12/54/54	-
6	BOG	D	706	-	-	5/11/31/31	0/1/1/1
4	HEM	C	705	7,1	-	0/12/54/54	-
3	NAG	D	704	1	-	1/6/23/26	0/1/1/1
3	NAG	B	705	1	-	0/6/23/26	0/1/1/1
3	NAG	D	701	1	-	1/6/23/26	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BOG	B	701	-	-	7/11/31/31	0/1/1/1

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	707	IXP	CAZ-CAL	-10.50	1.39	1.52
5	A	706	IXP	CAZ-CAL	-10.49	1.39	1.52
5	D	707	IXP	CAZ-CAL	-10.48	1.39	1.52
5	A	706	IXP	CAK-CAX	-10.06	1.38	1.51
5	B	707	IXP	CAK-CAX	-10.02	1.38	1.51
5	D	707	IXP	CAK-CAX	-9.98	1.38	1.51
5	C	706	IXP	CAK-CAX	-8.79	1.39	1.51
4	C	705	HEM	C3D-C2D	8.09	1.53	1.36
4	A	705	HEM	C3D-C2D	8.04	1.53	1.36
4	D	705	HEM	C3D-C2D	7.94	1.53	1.36
4	B	706	HEM	C3D-C2D	7.88	1.53	1.36
5	C	706	IXP	CAZ-CAL	-7.17	1.43	1.52
5	C	706	IXP	CBQ-CBP	-7.02	1.38	1.50
5	A	706	IXP	CBQ-CBP	-6.48	1.39	1.50
5	C	706	IXP	CAM-CAL	-6.47	1.42	1.51
5	D	707	IXP	CBQ-CBP	-6.43	1.39	1.50
5	C	706	IXP	CBL-CBK	-5.95	1.30	1.42
5	B	707	IXP	CBQ-CBP	-5.90	1.40	1.50
5	D	707	IXP	CAM-CAL	-5.47	1.44	1.51
5	B	707	IXP	CAM-CAL	-5.45	1.44	1.51
5	A	706	IXP	CAM-CAL	-5.44	1.44	1.51
5	C	706	IXP	CBJ-NBM	-5.30	1.31	1.39
5	C	706	IXP	CBN-CBO	-4.97	1.28	1.39
5	C	706	IXP	CBT-CL	-4.66	1.64	1.74
4	C	705	HEM	C3C-C2C	-4.66	1.33	1.40
4	A	705	HEM	C3C-C2C	-4.47	1.34	1.40
5	A	706	IXP	CBL-CBK	-4.44	1.33	1.42
4	D	705	HEM	C3C-C2C	-4.44	1.34	1.40
5	B	707	IXP	CBL-CBK	-4.31	1.33	1.42
4	B	706	HEM	C3C-C2C	-4.28	1.34	1.40
5	D	707	IXP	CBL-CBK	-4.26	1.33	1.42
6	B	701	BOG	O2-C2	-4.23	1.33	1.43
5	A	706	IXP	CBI-CBJ	-3.89	1.33	1.41
5	C	706	IXP	CBI-CBJ	-3.82	1.33	1.41
4	A	705	HEM	C3C-CAC	3.72	1.55	1.47
5	D	707	IXP	CBI-CBJ	-3.70	1.33	1.41
5	D	707	IXP	CBJ-NBM	-3.70	1.34	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	707	IXP	CBI-CBJ	-3.66	1.33	1.41
4	D	705	HEM	C3C-CAC	3.65	1.55	1.47
5	B	707	IXP	CBJ-NBM	-3.58	1.34	1.39
4	B	706	HEM	C3C-CAC	3.55	1.55	1.47
5	C	706	IXP	CBN-NBM	-3.54	1.30	1.36
5	C	706	IXP	CAO-CAP	-3.53	1.32	1.38
4	C	705	HEM	C3C-CAC	3.51	1.55	1.47
5	D	707	IXP	CAN-CAI	-3.50	1.44	1.50
5	B	707	IXP	CAN-CAI	-3.47	1.44	1.50
5	A	706	IXP	CAN-CAI	-3.43	1.44	1.50
5	A	706	IXP	CBJ-NBM	-3.41	1.34	1.39
5	A	706	IXP	CBN-CBO	-3.41	1.32	1.39
5	C	706	IXP	CAN-CAI	-3.39	1.44	1.50
6	D	706	BOG	O2-C2	-3.29	1.35	1.43
5	B	707	IXP	CBN-CBO	-3.25	1.32	1.39
5	D	707	IXP	CBN-CBO	-3.17	1.32	1.39
6	D	706	BOG	O3-C3	-3.00	1.35	1.43
4	B	706	HEM	CAB-C3B	2.91	1.55	1.47
4	C	705	HEM	CAB-C3B	2.89	1.55	1.47
4	D	705	HEM	FE-NB	2.87	2.11	1.96
4	D	705	HEM	CAB-C3B	2.84	1.55	1.47
4	A	705	HEM	CAB-C3B	2.84	1.55	1.47
5	C	706	IXP	CAR-CAQ	-2.83	1.33	1.38
6	B	701	BOG	O3-C3	-2.81	1.36	1.43
3	D	701	NAG	O5-C1	-2.80	1.39	1.43
4	C	705	HEM	FE-ND	2.79	2.10	1.96
4	A	705	HEM	FE-NB	2.76	2.10	1.96
4	B	706	HEM	FE-NB	2.75	2.10	1.96
3	A	701	NAG	O5-C1	-2.74	1.39	1.43
4	B	706	HEM	FE-ND	2.74	2.10	1.96
5	D	707	IXP	CAO-CAP	-2.71	1.33	1.38
5	A	706	IXP	CAO-CAP	-2.70	1.33	1.38
5	A	706	IXP	CAR-CAQ	-2.70	1.33	1.38
5	D	707	IXP	CAR-CAQ	-2.69	1.33	1.38
5	C	706	IXP	CAQ-CAP	-2.68	1.32	1.39
5	B	707	IXP	CAR-CAQ	-2.67	1.33	1.38
5	B	707	IXP	CAO-CAP	-2.66	1.33	1.38
5	D	707	IXP	CAJ-CAI	2.63	1.57	1.53
4	C	705	HEM	FE-NB	2.62	2.09	1.96
5	A	706	IXP	CAJ-CAI	2.61	1.57	1.53
4	D	705	HEM	FE-ND	2.58	2.09	1.96
5	B	707	IXP	CAJ-CAI	2.54	1.56	1.53

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	701	NAG	O5-C1	-2.52	1.39	1.43
6	B	701	BOG	O4-C4	-2.51	1.37	1.43
6	D	706	BOG	O1-C1'	-2.46	1.36	1.43
6	D	706	BOG	O4-C4	-2.39	1.37	1.43
6	B	701	BOG	O1-C1'	-2.28	1.36	1.43
6	B	701	BOG	O5-C5	-2.28	1.38	1.44
4	A	705	HEM	FE-ND	2.27	2.08	1.96
3	B	702	NAG	O5-C1	-2.26	1.40	1.43
6	D	706	BOG	O5-C5	-2.24	1.38	1.44
6	D	706	BOG	O5-C1	-2.17	1.36	1.41
6	D	706	BOG	O1-C1	-2.15	1.36	1.40
5	A	706	IXP	CAQ-CAP	-2.11	1.33	1.39
5	D	707	IXP	CAQ-CAP	-2.10	1.33	1.39
5	B	707	IXP	CAQ-CAP	-2.10	1.33	1.39
4	A	705	HEM	CAA-C2A	2.08	1.55	1.52
5	B	707	IXP	CBN-NBM	-2.07	1.32	1.36
5	A	706	IXP	CBN-NBM	-2.05	1.32	1.36
4	B	706	HEM	CMB-C2B	2.03	1.55	1.50

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	706	IXP	CAJ-CAK-CAX	-7.47	93.07	103.07
4	C	705	HEM	C4D-ND-C1D	6.78	112.07	105.07
4	D	705	HEM	C4D-ND-C1D	6.75	112.05	105.07
4	A	705	HEM	C4D-ND-C1D	6.75	112.04	105.07
4	B	706	HEM	C4D-ND-C1D	6.54	111.83	105.07
6	B	701	BOG	C1'-O1-C1	6.50	124.61	113.84
5	A	706	IXP	CAV-OAW-CAX	-6.27	104.56	110.28
5	D	707	IXP	CAV-OAW-CAX	-6.24	104.59	110.28
5	B	707	IXP	CAV-OAW-CAX	-6.23	104.60	110.28
5	D	707	IXP	OAY-CAX-CAK	-5.41	122.42	129.38
5	A	706	IXP	OAY-CAX-CAK	-5.38	122.46	129.38
5	D	707	IXP	CCI-OCH-CBB	-5.35	109.45	117.53
5	B	707	IXP	OAY-CAX-CAK	-5.35	122.50	129.38
5	A	706	IXP	CCI-OCH-CBB	-5.34	109.47	117.53
5	B	707	IXP	CCG-OCF-CBD	-5.33	109.48	117.53
5	B	707	IXP	CCI-OCH-CBB	-5.32	109.50	117.53
5	A	706	IXP	CCG-OCF-CBD	-5.31	109.51	117.53
5	D	707	IXP	CCG-OCF-CBD	-5.31	109.52	117.53
6	D	706	BOG	C1'-O1-C1	5.23	122.51	113.84
5	C	706	IXP	CAV-OAW-CAX	-5.16	105.57	110.28

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	706	IXP	CAD-CAC-CAB	-4.83	104.08	112.56
5	A	706	IXP	CAJ-CAK-CAX	-4.63	96.87	103.07
5	D	707	IXP	CAJ-CAK-CAX	-4.62	96.87	103.07
5	B	707	IXP	CAJ-CAK-CAX	-4.59	96.92	103.07
5	C	706	IXP	OAY-CAX-CAK	-4.54	123.54	129.38
5	C	706	IXP	CBQ-CBP-NBM	4.23	122.89	117.95
5	C	706	IXP	CAZ-CAL-CAM	-4.19	106.54	112.86
5	A	706	IXP	CAM-CAL-CAK	4.08	113.45	106.58
5	B	707	IXP	CAM-CAL-CAK	4.06	113.40	106.58
5	D	707	IXP	CAM-CAL-CAK	4.04	113.37	106.58
5	C	706	IXP	CAM-CAL-CAK	3.99	113.29	106.58
3	B	702	NAG	C2-N2-C7	3.98	128.57	122.90
3	D	701	NAG	C2-N2-C7	3.97	128.56	122.90
3	A	701	NAG	C2-N2-C7	3.94	128.51	122.90
5	D	707	IXP	OAW-CAX-OAY	3.93	125.50	121.42
5	B	707	IXP	OAW-CAX-OAY	3.90	125.46	121.42
5	A	706	IXP	OAW-CAX-OAY	3.89	125.45	121.42
4	A	705	HEM	C4B-CHC-C1C	3.83	127.62	122.56
5	C	706	IXP	CBV-CBU-CBT	3.83	123.28	119.24
4	C	705	HEM	C4B-CHC-C1C	3.75	127.50	122.56
5	B	707	IXP	CCN-OCM-CBG	-3.71	109.45	117.51
5	D	707	IXP	CCN-OCM-CBG	-3.68	109.52	117.51
3	C	701	NAG	C2-N2-C7	3.65	128.10	122.90
5	C	706	IXP	OCM-CBG-CBL	-3.59	114.63	124.43
4	C	705	HEM	C4C-CHD-C1D	3.58	127.28	122.56
4	D	705	HEM	CBA-CAA-C2A	-3.44	106.74	112.62
4	B	706	HEM	C4B-CHC-C1C	3.40	127.05	122.56
5	C	706	IXP	CAN-CAM-CAL	3.31	123.14	114.40
5	C	706	IXP	OAW-CAV-CAJ	-3.30	99.89	104.71
5	C	706	IXP	CCG-OCF-CBD	-3.29	112.57	117.53
5	C	706	IXP	CCL-CBN-NBM	3.27	126.50	122.37
4	D	705	HEM	C1B-NB-C4B	3.26	108.44	105.07
4	B	706	HEM	C4C-CHD-C1D	3.22	126.81	122.56
5	D	707	IXP	CAJ-CAK-CAL	-3.18	107.21	113.21
5	C	706	IXP	OAW-CAX-OAY	3.17	124.70	121.42
4	D	705	HEM	C4B-CHC-C1C	3.16	126.73	122.56
5	A	706	IXP	CAJ-CAK-CAL	-3.15	107.27	113.21
5	B	707	IXP	CAJ-CAK-CAL	-3.14	107.28	113.21
5	C	706	IXP	OAU-CAT-OAS	-3.13	103.08	108.08
4	C	705	HEM	CBD-CAD-C3D	-3.10	104.02	112.63
5	D	707	IXP	OAW-CAV-CAJ	-3.07	100.23	104.71
5	B	707	IXP	OAW-CAV-CAJ	-3.07	100.23	104.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	706	HEM	CBD-CAD-C3D	-3.06	104.12	112.63
5	A	706	IXP	OAW-CAV-CAJ	-3.06	100.25	104.71
5	B	707	IXP	CBQ-CBP-NBM	3.06	121.52	117.95
4	B	706	HEM	C1B-NB-C4B	3.02	108.19	105.07
4	C	705	HEM	C1B-NB-C4B	3.00	108.18	105.07
4	D	705	HEM	C3B-C2B-C1B	2.95	108.67	106.49
5	A	706	IXP	CBL-CBK-CBJ	2.94	123.17	119.65
4	D	705	HEM	C4C-CHD-C1D	2.88	126.36	122.56
5	C	706	IXP	CAR-CAN-CAM	-2.85	116.51	120.26
5	B	707	IXP	CAN-CAM-CAL	2.83	121.87	114.40
5	D	707	IXP	CAN-CAM-CAL	2.82	121.85	114.40
5	A	706	IXP	CAN-CAM-CAL	2.81	121.81	114.40
4	A	705	HEM	C4C-CHD-C1D	2.79	126.24	122.56
4	D	705	HEM	CBD-CAD-C3D	-2.77	104.92	112.63
4	C	705	HEM	C3B-C2B-C1B	2.75	108.53	106.49
4	B	706	HEM	CBA-CAA-C2A	-2.74	107.94	112.62
4	B	706	HEM	C3B-C2B-C1B	2.74	108.52	106.49
4	A	705	HEM	C3B-C2B-C1B	2.74	108.52	106.49
5	B	707	IXP	CCL-CBN-NBM	2.73	125.82	122.37
4	A	705	HEM	C1B-NB-C4B	2.71	107.87	105.07
5	C	706	IXP	CBU-CBT-CBS	-2.66	117.79	121.24
5	D	707	IXP	CCL-CBN-NBM	2.66	125.72	122.37
5	C	706	IXP	CBH-CBG-CBL	-2.65	117.24	120.81
5	C	706	IXP	CCL-CBN-CBO	-2.65	123.51	129.24
5	A	706	IXP	CCL-CBN-NBM	2.64	125.70	122.37
4	B	706	HEM	CHC-C4B-C3B	2.63	128.60	124.57
4	C	705	HEM	CHC-C4B-C3B	2.57	128.51	124.57
5	C	706	IXP	CCE-NAA-CAB	-2.55	118.11	122.84
5	C	706	IXP	CCI-OCH-CBB	-2.43	113.86	117.53
5	D	707	IXP	CAZ-CAL-CAK	-2.43	109.45	113.31
5	C	706	IXP	CBL-CBK-CBO	-2.42	129.99	134.17
5	C	706	IXP	CAT-OAS-CAP	-2.42	102.19	105.34
4	A	705	HEM	CBD-CAD-C3D	-2.41	105.94	112.63
5	B	707	IXP	CAZ-CAL-CAK	-2.41	109.48	113.31
5	A	706	IXP	CAZ-CAL-CAK	-2.39	109.50	113.31
4	A	705	HEM	CHC-C4B-C3B	2.35	128.16	124.57
5	B	707	IXP	CAI-OAF-CAE	-2.34	109.47	116.53
5	A	706	IXP	CAI-OAF-CAE	-2.34	109.47	116.53
4	D	705	HEM	CHC-C4B-C3B	2.32	128.13	124.57
5	B	707	IXP	CAV-CAJ-CAK	-2.31	98.45	101.79
5	D	707	IXP	CAI-OAF-CAE	-2.30	109.59	116.53
5	D	707	IXP	CAV-CAJ-CAK	-2.28	98.49	101.79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	706	IXP	CAV-CAJ-CAK	-2.27	98.50	101.79
5	A	706	IXP	CBL-CBK-CBO	-2.27	130.26	134.17
5	D	707	IXP	CAZ-CAL-CAM	-2.25	109.47	112.86
5	A	706	IXP	CAZ-CAL-CAM	-2.24	109.48	112.86
6	B	701	BOG	C4-C3-C2	2.24	114.72	110.82
5	A	706	IXP	CCE-NAA-CAB	-2.22	118.72	122.84
5	B	707	IXP	CAZ-CAL-CAM	-2.21	109.52	112.86
6	B	701	BOG	C1-C2-C3	-2.17	105.48	110.00
6	B	701	BOG	O2-C2-C3	-2.16	105.34	110.35
4	C	705	HEM	CAA-CBA-CGA	-2.16	107.71	113.76
5	B	707	IXP	CBL-CBK-CBJ	2.16	122.23	119.65
5	C	706	IXP	CBS-CBT-CL	2.06	122.57	119.35
6	B	701	BOG	C3'-C2'-C1'	-2.05	104.41	113.49
6	B	701	BOG	O4-C4-C3	-2.04	105.63	110.35
5	C	706	IXP	CAT-OAU-CAQ	-2.03	102.70	105.34
4	B	706	HEM	CAB-C3B-C2B	-2.02	121.95	128.60

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	NAG	C3-C2-N2-C7
3	B	702	NAG	C3-C2-N2-C7
3	C	701	NAG	C3-C2-N2-C7
3	D	701	NAG	C3-C2-N2-C7
5	A	706	IXP	CAD-CAE-OAF-CAI
5	B	707	IXP	CAD-CAE-OAF-CAI
5	C	706	IXP	CAD-CAE-OAF-CAI
5	D	707	IXP	CAD-CAE-OAF-CAI
6	B	701	BOG	O5-C1-O1-C1'
6	B	701	BOG	C2'-C1'-O1-C1
5	D	707	IXP	CBL-CBG-OCM-CCN
5	A	706	IXP	OAH-CAE-OAF-CAI
5	B	707	IXP	OAH-CAE-OAF-CAI
5	C	706	IXP	OAH-CAE-OAF-CAI
5	D	707	IXP	OAH-CAE-OAF-CAI
5	B	707	IXP	CBH-CBG-OCM-CCN
5	D	707	IXP	CBH-CBG-OCM-CCN
5	B	707	IXP	CBL-CBG-OCM-CCN
5	D	707	IXP	CBC-CBB-OCH-CCI
6	B	701	BOG	C4-C5-C6-O6
5	A	706	IXP	CBC-CBB-OCH-CCI

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	D	707	IXP	NCB-CCC-CCD-CBF
6	B	701	BOG	O5-C5-C6-O6
5	B	707	IXP	CBC-CBB-OCH-CCI
5	B	707	IXP	CBA-CBB-OCH-CCI
5	D	707	IXP	CBE-CBD-OCF-CCG
5	D	707	IXP	CBA-CBB-OCH-CCI
5	C	706	IXP	NCB-CCC-CCD-CBF
5	A	706	IXP	CBA-CBB-OCH-CCI
5	D	707	IXP	CBC-CBD-OCF-CCG
5	C	706	IXP	CCD-CBF-CCE-NAA
5	A	706	IXP	NCB-CCC-CCD-CBF
5	C	706	IXP	CBA-CBB-OCH-CCI
5	C	706	IXP	CBE-CBD-OCF-CCG
5	C	706	IXP	CBC-CBB-OCH-CCI
5	A	706	IXP	CBE-CBD-OCF-CCG
5	B	707	IXP	CBE-CBD-OCF-CCG
6	D	706	BOG	O1-C1'-C2'-C3'
6	B	701	BOG	C2-C1-O1-C1'
6	D	706	BOG	C2-C1-O1-C1'
6	D	706	BOG	O5-C1-O1-C1'
5	C	706	IXP	CBC-CBD-OCF-CCG
6	B	701	BOG	C4'-C5'-C6'-C7'
5	C	706	IXP	CAK-CAL-CAZ-CBE
5	B	707	IXP	CCE-CBF-CCD-CCC
5	D	707	IXP	CCE-CBF-CCD-CCC
5	A	706	IXP	CBC-CBD-OCF-CCG
5	B	707	IXP	CBC-CBD-OCF-CCG
5	C	706	IXP	CAK-CAL-CAZ-CBA
5	C	706	IXP	CCE-CBF-CCD-CCC
5	B	707	IXP	CAB-CAC-CAD-CAE
5	D	707	IXP	CAB-CAC-CAD-CAE
5	C	706	IXP	CAM-CAL-CAZ-CBE
5	C	706	IXP	CAM-CAL-CAZ-CBA
6	D	706	BOG	C2'-C1'-O1-C1
6	B	701	BOG	C2'-C3'-C4'-C5'
5	A	706	IXP	NBM-CBP-CBQ-CBR
5	A	706	IXP	NBM-CBP-CBQ-CBV
5	B	707	IXP	NBM-CBP-CBQ-CBR
5	B	707	IXP	NBM-CBP-CBQ-CBV
5	C	706	IXP	NBM-CBP-CBQ-CBV
6	D	706	BOG	C5'-C6'-C7'-C8'
3	D	704	NAG	C4-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

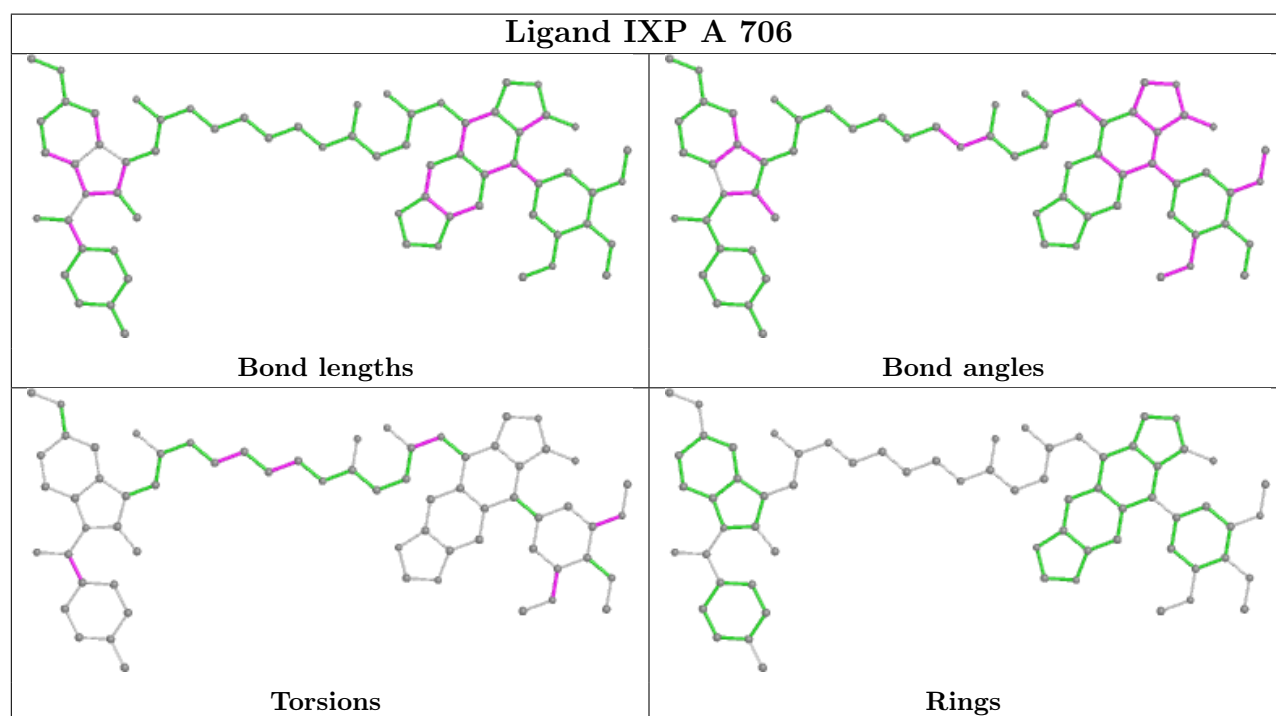
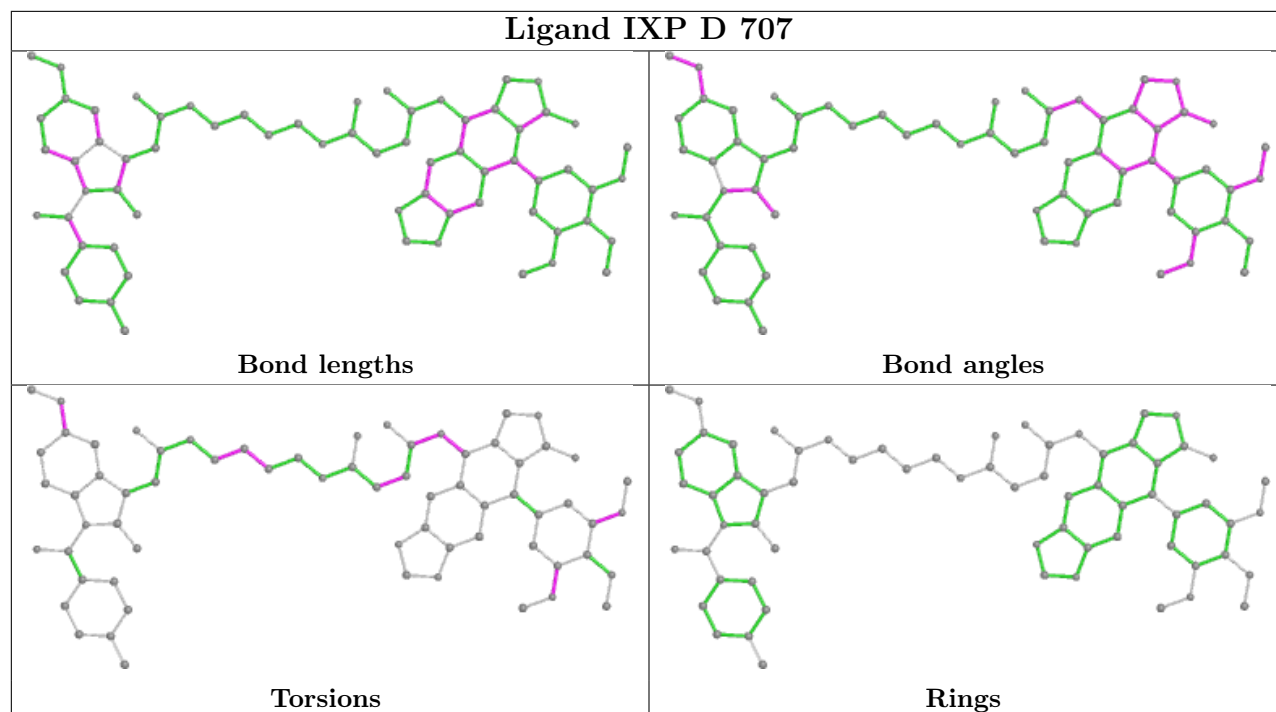
Mol	Chain	Res	Type	Atoms
5	C	706	IXP	NBM-CBP-CBQ-CBR
5	A	706	IXP	CCD-CBF-CCE-NAA
4	A	705	HEM	C4B-C3B-CAB-CBB
5	D	707	IXP	CAJ-CAI-OAF-CAE

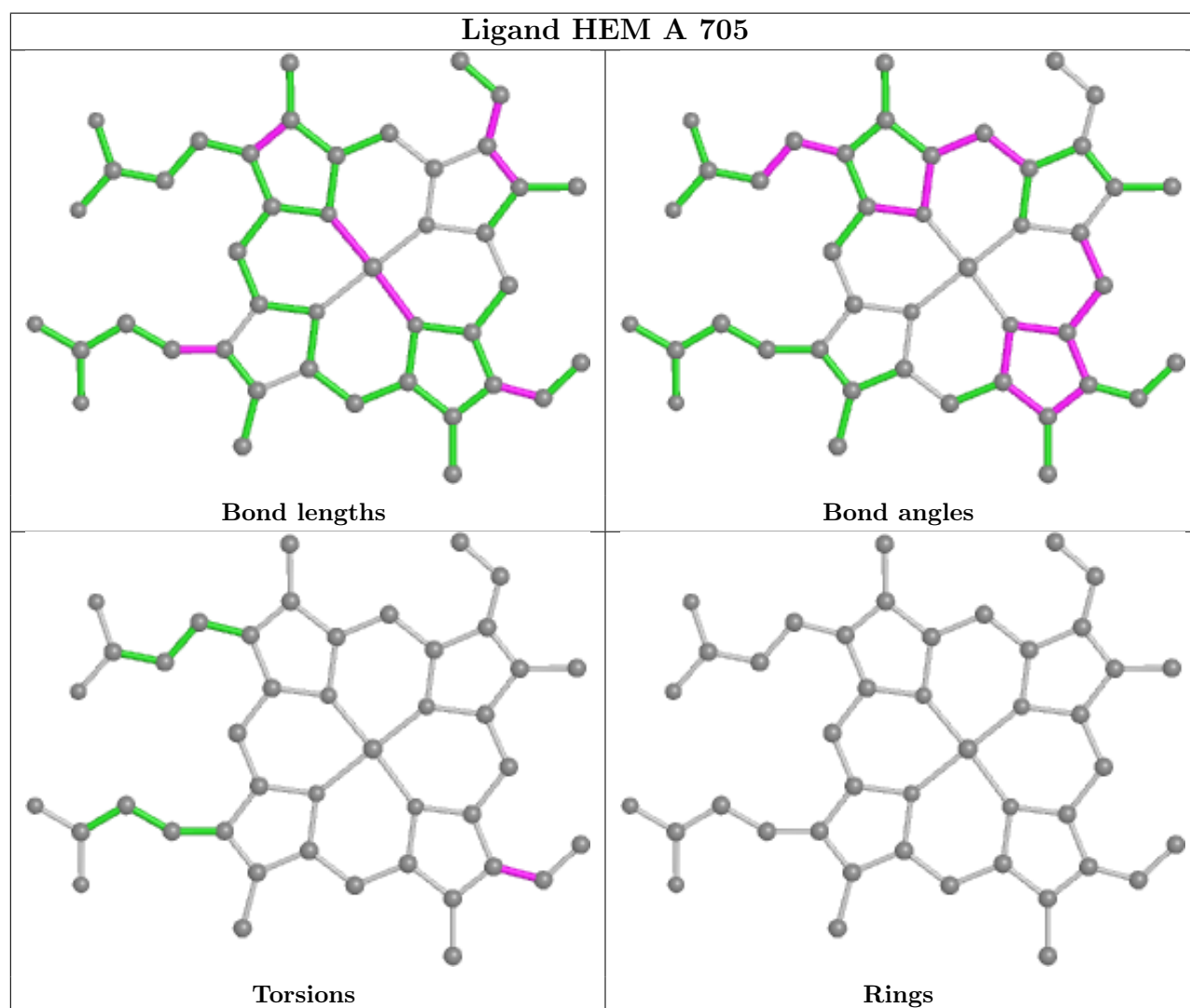
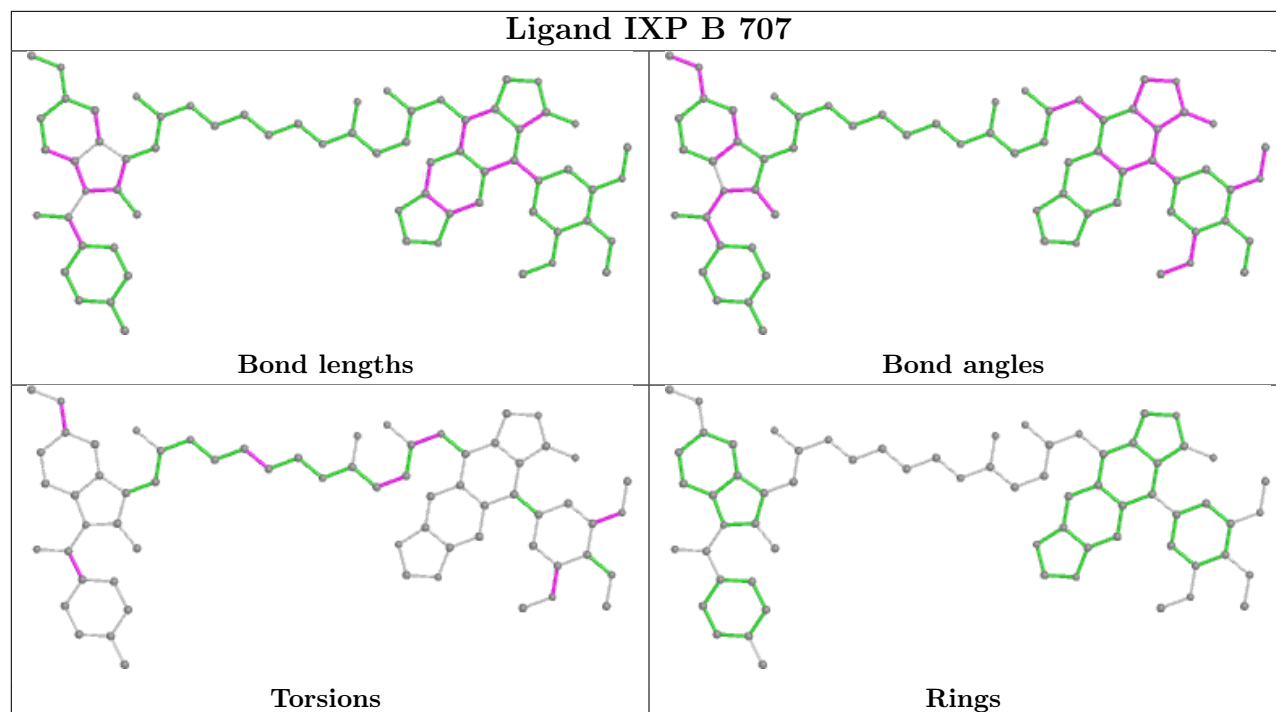
There are no ring outliers.

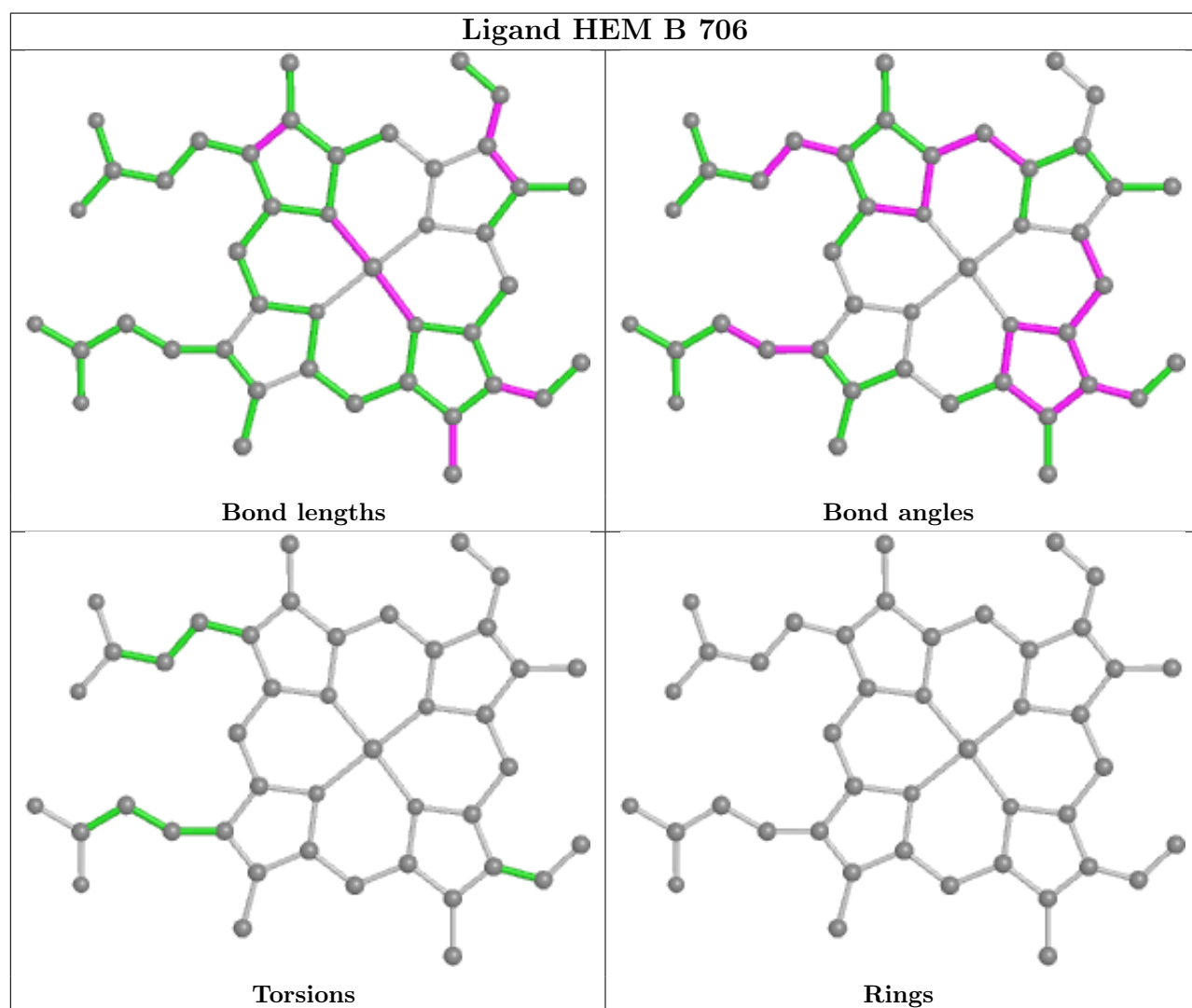
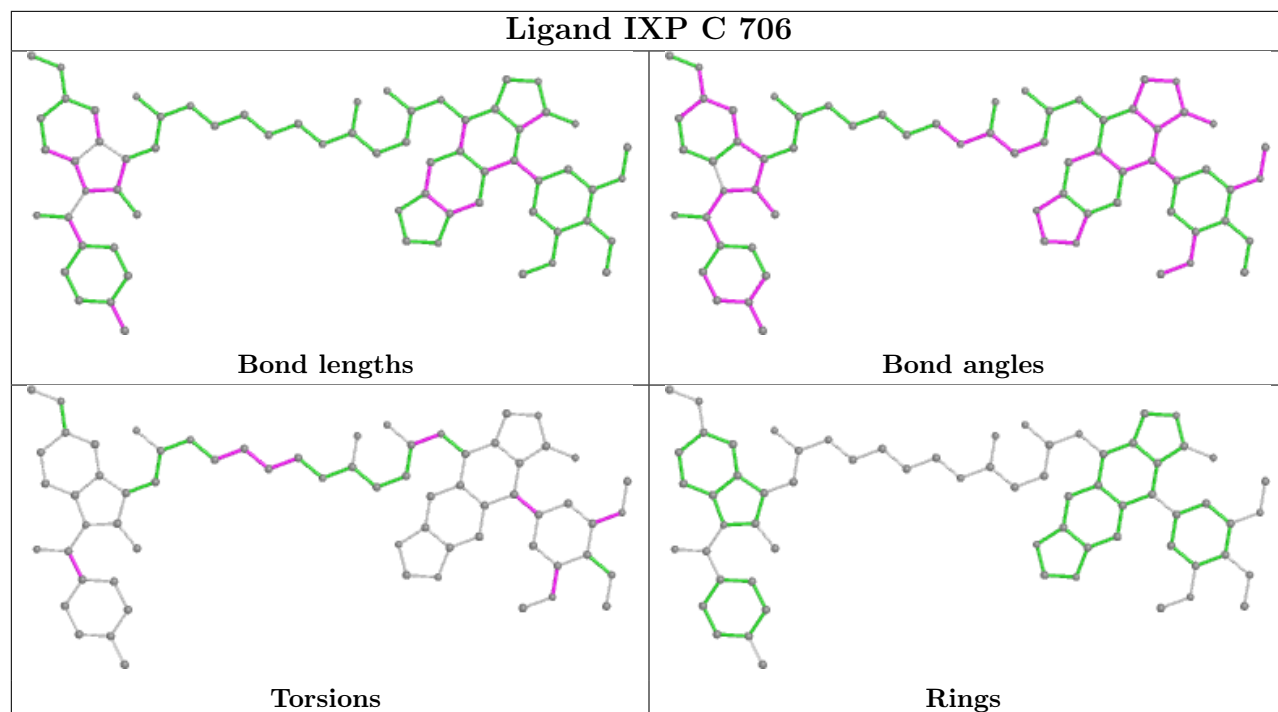
14 monomers are involved in 60 short contacts:

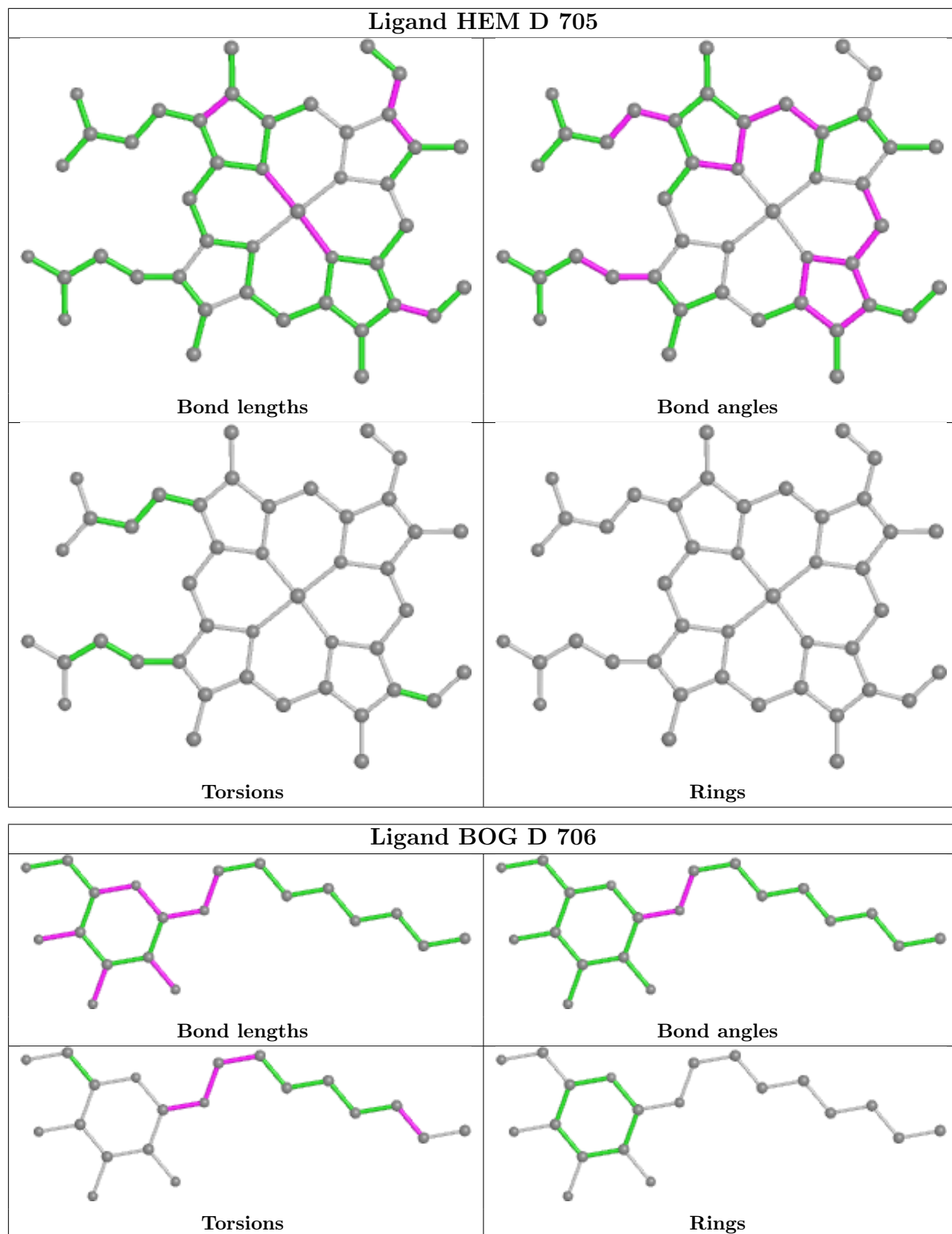
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	707	IXP	13	0
3	B	702	NAG	1	0
3	C	701	NAG	2	0
3	A	701	NAG	2	0
5	A	706	IXP	7	0
5	B	707	IXP	13	0
4	A	705	HEM	2	0
5	C	706	IXP	7	0
4	B	706	HEM	2	0
4	D	705	HEM	2	0
6	D	706	BOG	1	0
4	C	705	HEM	2	0
3	D	701	NAG	2	0
6	B	701	BOG	4	0

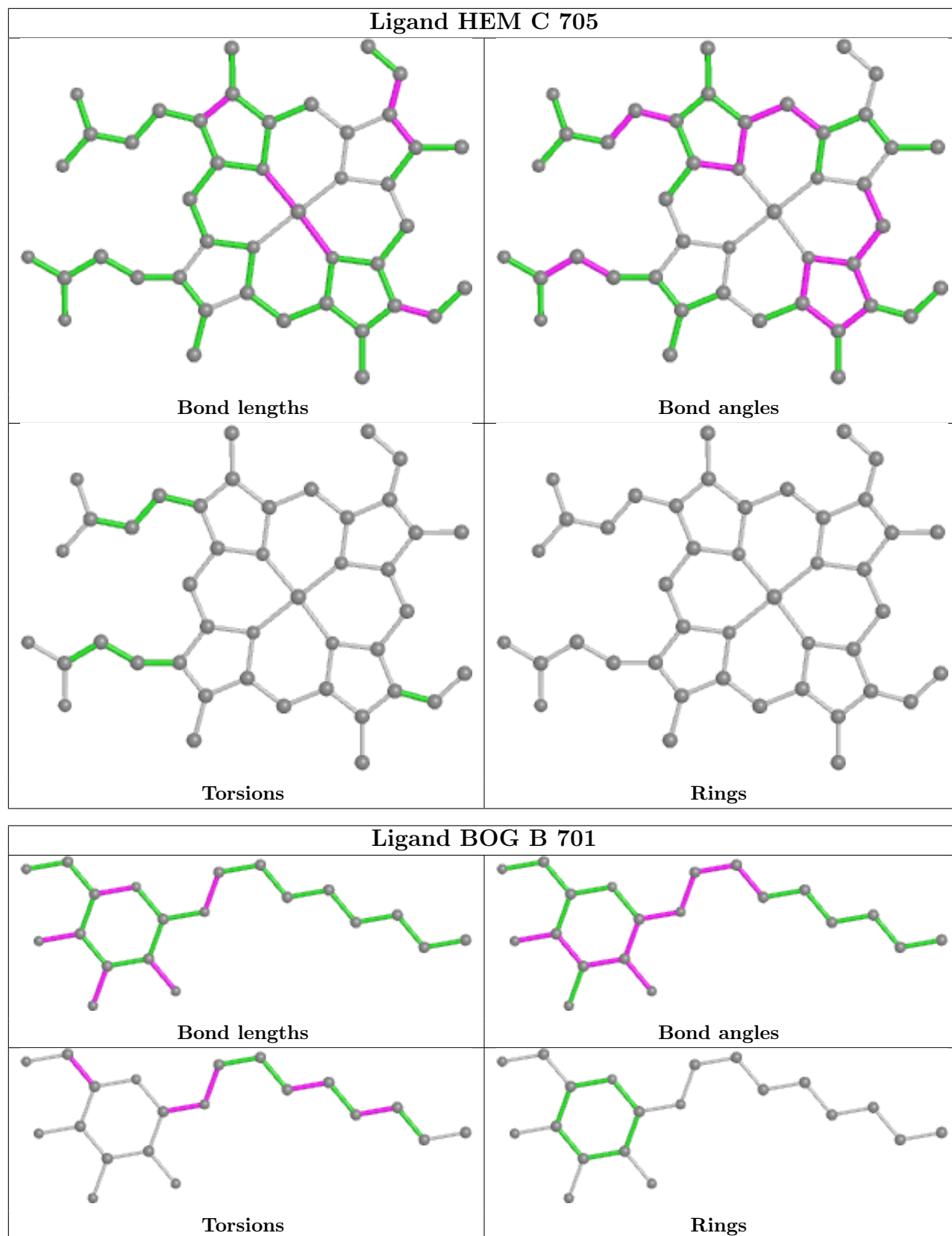
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	552/587 (94%)	-0.07	25 (4%) 33 38	19, 32, 63, 86	0
1	B	551/587 (93%)	-0.07	23 (4%) 36 42	20, 36, 69, 97	0
1	C	552/587 (94%)	-0.11	28 (5%) 28 33	17, 28, 58, 88	0
1	D	551/587 (93%)	-0.24	16 (2%) 51 57	18, 29, 54, 82	0
All	All	2206/2348 (93%)	-0.12	92 (4%) 36 42	17, 31, 62, 97	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	LEU	6.7
1	B	74	PHE	6.7
1	B	81	LEU	5.6
1	A	81	LEU	5.4
1	B	105(A)	ILE	5.2
1	C	74	PHE	4.6
1	D	81	LEU	4.6
1	D	82	LEU	4.4
1	B	409	TYR	4.4
1	D	75	LEU	4.3
1	C	81	LEU	4.3
1	D	107	PHE	4.3
1	D	74	PHE	4.2
1	B	215	LYS	4.1
1	C	82	LEU	3.9
1	A	108	LEU	3.9
1	A	80	LEU	3.8
1	A	122	TYR	3.8
1	A	77	ARG	3.5
1	A	107	PHE	3.5
1	A	78	ILE	3.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	99	VAL	3.4
1	A	82	LEU	3.4
1	D	78	ILE	3.3
1	A	96	PHE	3.3
1	B	111	LEU	3.3
1	C	91	TYR	3.2
1	A	494	LEU	3.2
1	A	74	PHE	3.1
1	C	107	PHE	3.1
1	B	78	ILE	3.1
1	C	97	LYS	3.1
1	A	91	TYR	3.1
1	C	96	PHE	3.0
1	D	270	GLN	2.9
1	B	80	LEU	2.9
1	C	98	GLY	2.9
1	D	80	LEU	2.9
1	D	115	TYR	2.8
1	C	75	LEU	2.8
1	B	107	PHE	2.8
1	A	99	VAL	2.8
1	C	99	VAL	2.8
1	D	79	LYS	2.8
1	C	102	ILE	2.8
1	B	75	LEU	2.8
1	B	53	ASP	2.7
1	B	399	ASP	2.7
1	C	120	ARG	2.7
1	C	121	SER	2.7
1	A	277	PRO	2.7
1	D	399	ASP	2.7
1	A	98	GLY	2.6
1	A	105(A)	ILE	2.6
1	B	83	LYS	2.6
1	D	215	LYS	2.5
1	C	142	PHE	2.5
1	C	78	ILE	2.5
1	C	277	PRO	2.5
1	A	529	PHE	2.5
1	C	105(A)	ILE	2.4
1	C	124	ILE	2.4
1	A	94	THR	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	70	THR	2.4
1	C	80	LEU	2.4
1	B	98	GLY	2.4
1	D	111	LEU	2.4
1	A	33	ALA	2.4
1	C	409	TYR	2.3
1	A	103	VAL	2.3
1	B	96	PHE	2.3
1	C	53	ASP	2.3
1	B	91	TYR	2.2
1	D	105(A)	ILE	2.2
1	B	77	ARG	2.2
1	D	120	ARG	2.2
1	C	539	ILE	2.2
1	A	83	LYS	2.2
1	C	33	ALA	2.2
1	C	278	HIS	2.1
1	A	124	ILE	2.1
1	B	377	ILE	2.1
1	D	91	TYR	2.1
1	C	540	CYS	2.1
1	B	52	PHE	2.0
1	C	529	PHE	2.0
1	B	373	TYR	2.0
1	A	142	PHE	2.0
1	A	280	PRO	2.0
1	A	525	LEU	2.0
1	C	77	ARG	2.0
1	C	532	LYS	2.0

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

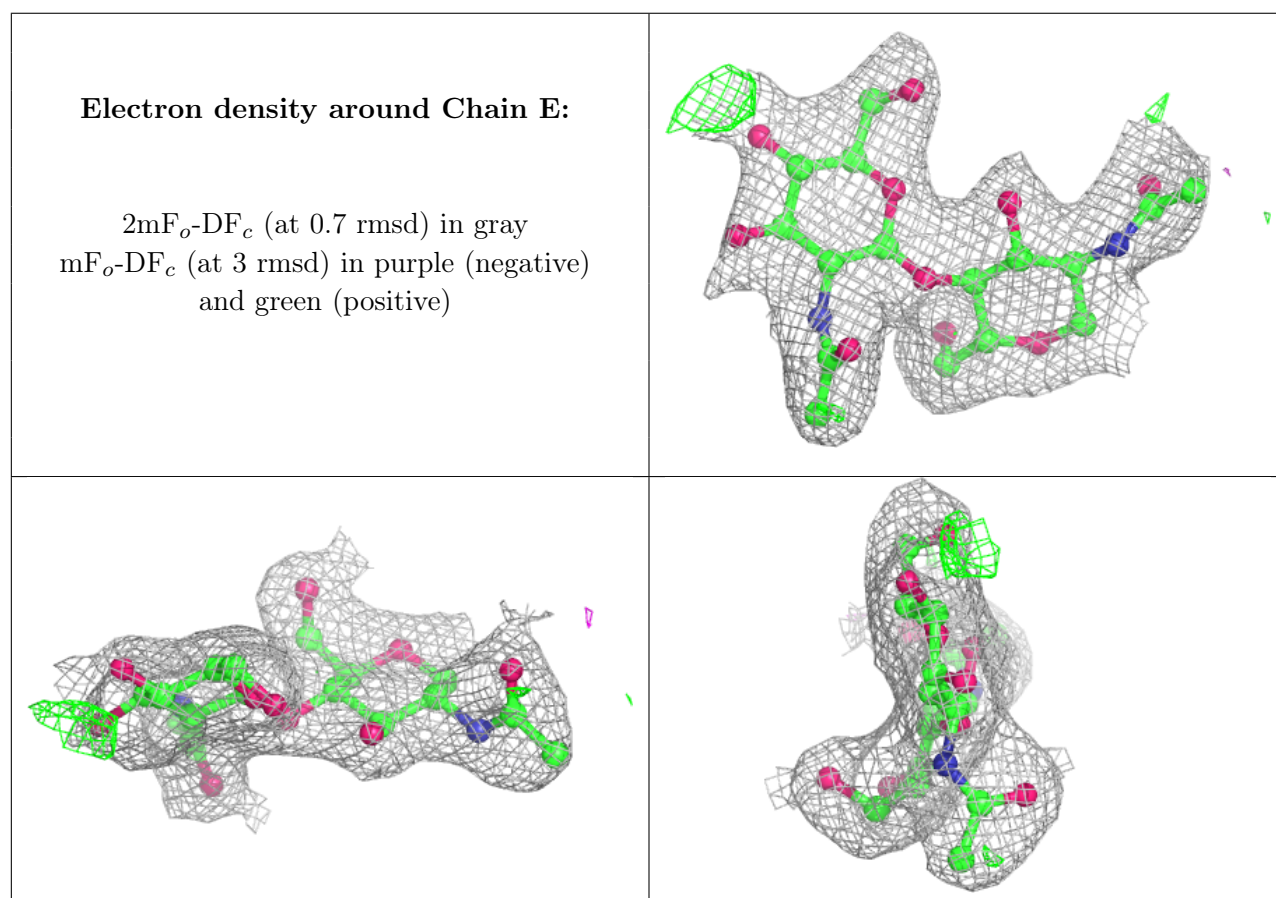
There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

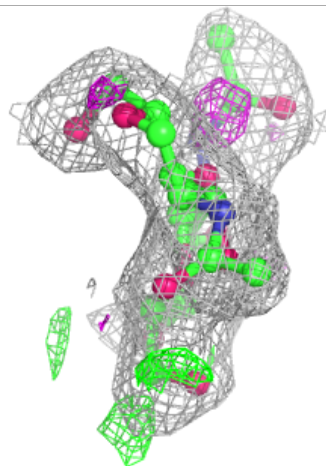
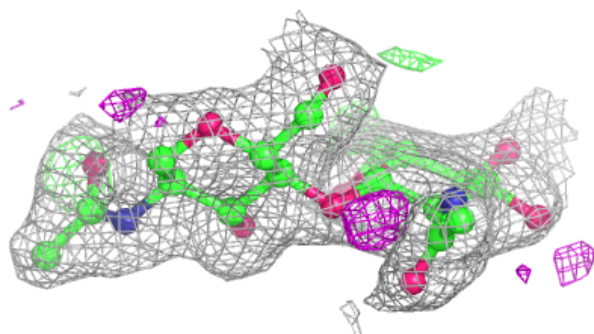
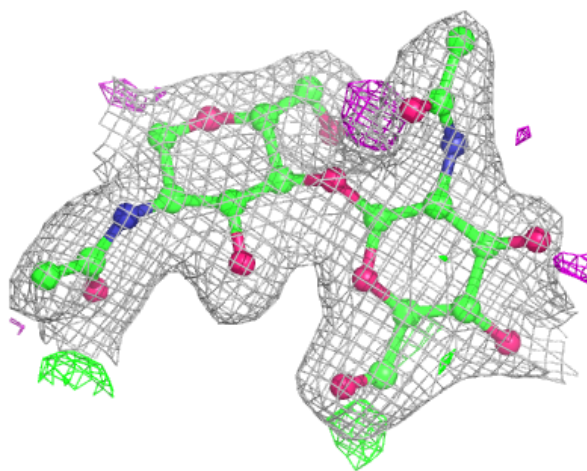
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	E	2	14/15	0.88	0.13	46,54,61,63	0
2	NAG	F	2	14/15	0.88	0.16	47,51,61,65	0
2	NAG	H	2	14/15	0.88	0.16	51,57,62,63	0
2	NAG	G	2	14/15	0.89	0.13	43,50,60,61	0
2	NAG	F	1	14/15	0.94	0.09	30,34,38,43	0
2	NAG	H	1	14/15	0.95	0.09	21,31,38,45	0
2	NAG	G	1	14/15	0.95	0.10	23,32,36,41	0
2	NAG	E	1	14/15	0.96	0.10	23,37,43,45	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.



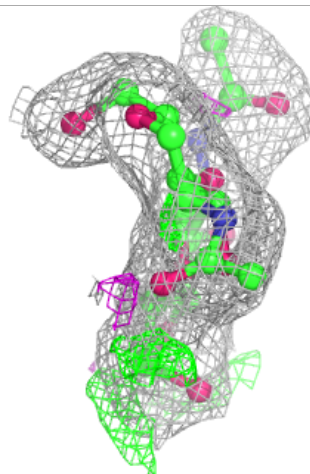
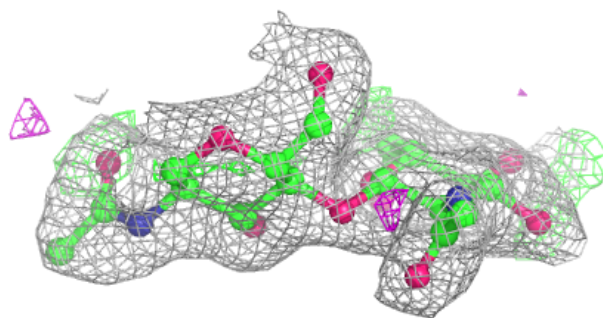
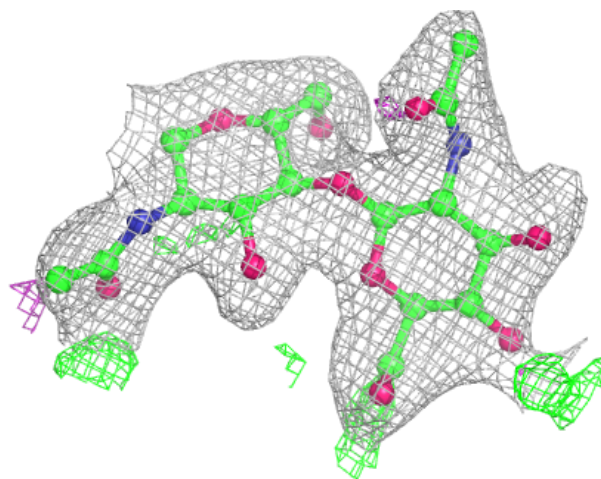
**Electron density around Chain F:**

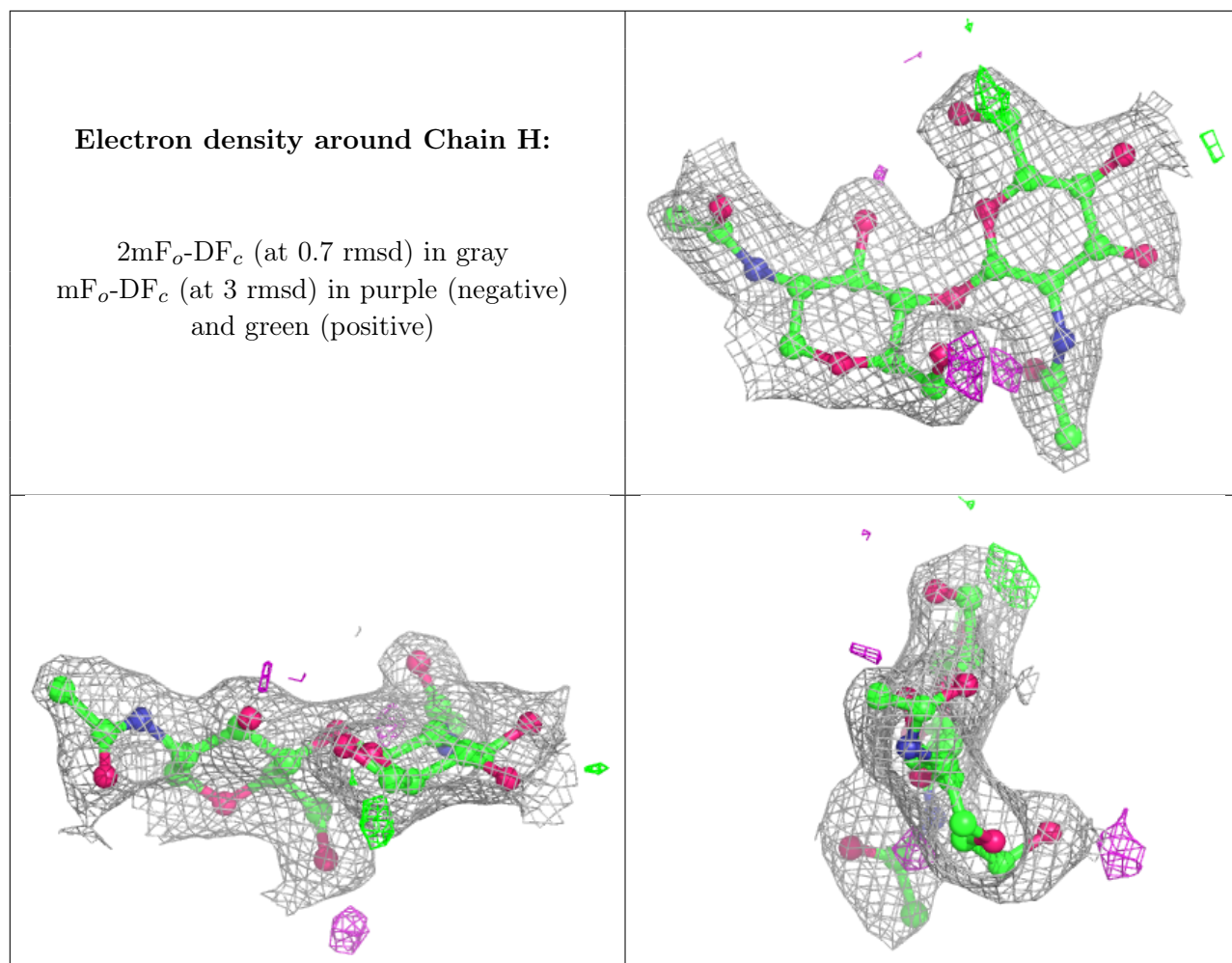
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain G:**

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





## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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.

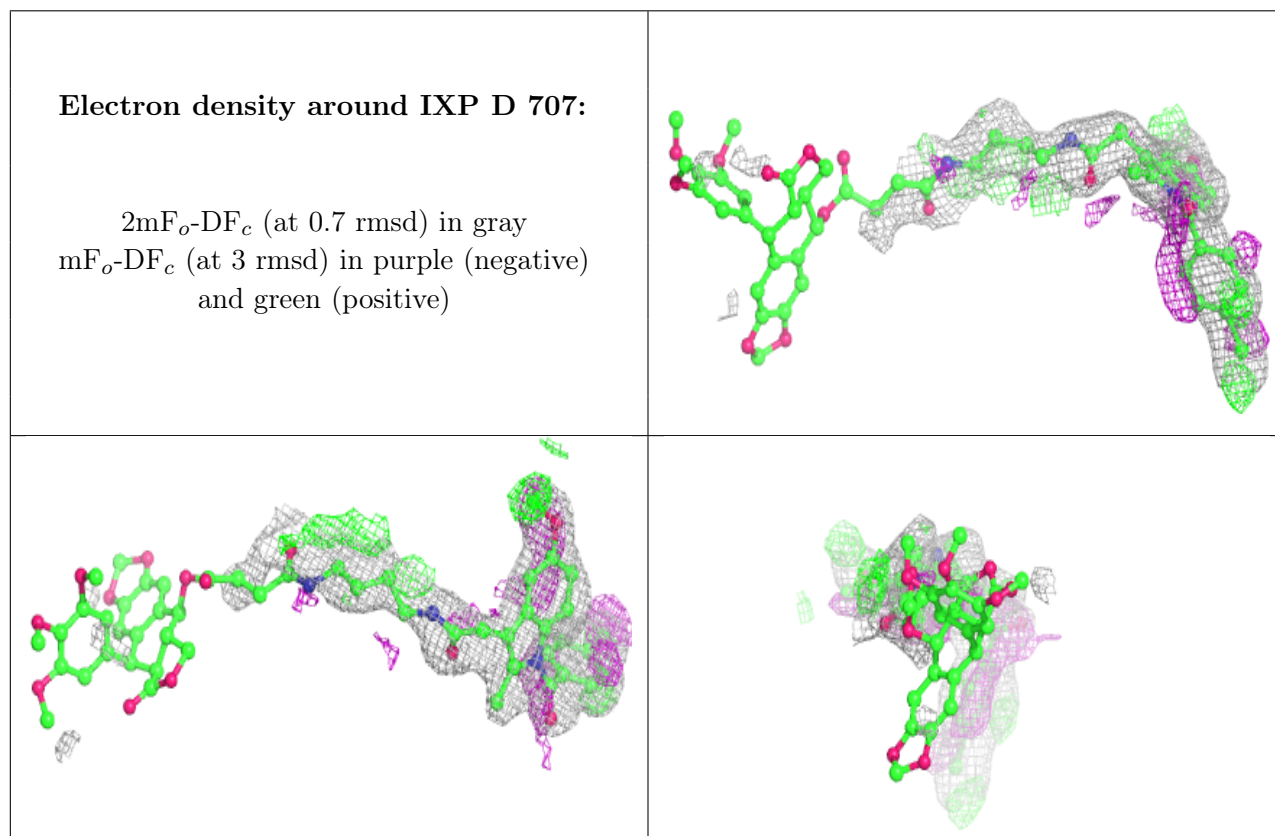
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	701	14/15	0.78	0.23	57,65,75,77	0
3	NAG	B	702	14/15	0.78	0.26	70,74,76,80	0
3	NAG	D	701	14/15	0.79	0.21	49,59,62,64	0
3	NAG	C	701	14/15	0.81	0.27	52,64,69,70	0
5	IXP	D	707	66/66	0.82	0.21	25,35,78,83	34
6	BOG	B	701	20/20	0.86	0.17	42,49,55,55	0
3	NAG	B	705	14/15	0.87	0.21	53,58,63,66	0
5	IXP	B	707	66/66	0.88	0.17	30,32,48,60	41
5	IXP	C	706	66/66	0.88	0.14	30,30,44,55	41
3	NAG	A	704	14/15	0.89	0.10	42,50,57,61	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	IXP	A	706	66/66	0.89	0.15	30,37,62,71	34
3	NAG	D	704	14/15	0.91	0.22	39,50,54,59	0
3	NAG	C	704	14/15	0.91	0.10	35,44,49,55	0
6	BOG	D	706	20/20	0.94	0.09	29,39,54,54	0
4	HEM	D	705	43/43	0.95	0.11	19,25,45,52	0
4	HEM	B	706	43/43	0.96	0.11	26,31,55,66	0
4	HEM	C	705	43/43	0.96	0.13	17,22,44,55	0
4	HEM	A	705	43/43	0.96	0.12	22,27,52,64	0

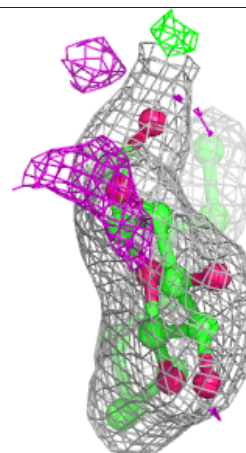
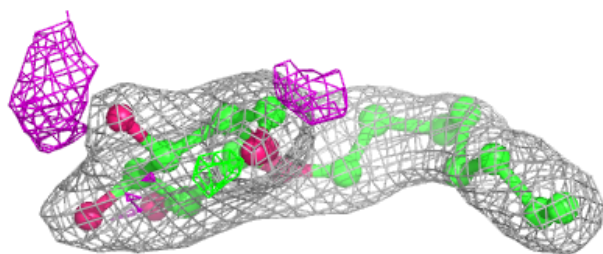
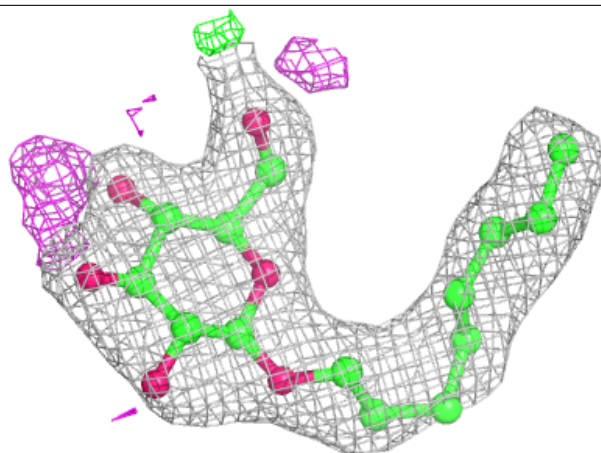
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



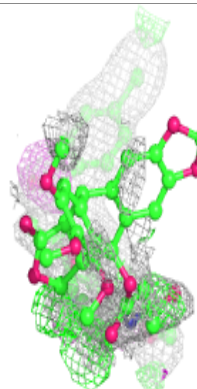
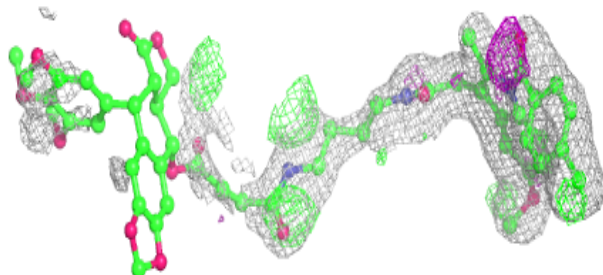
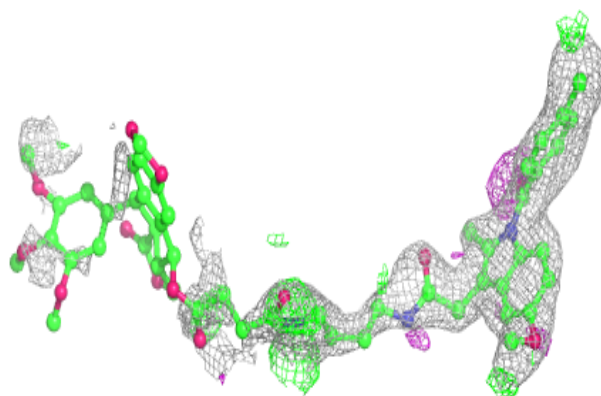


**Electron density around BOG B 701:**

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

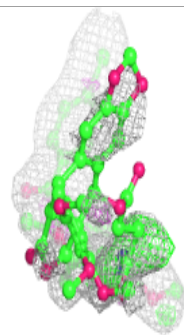
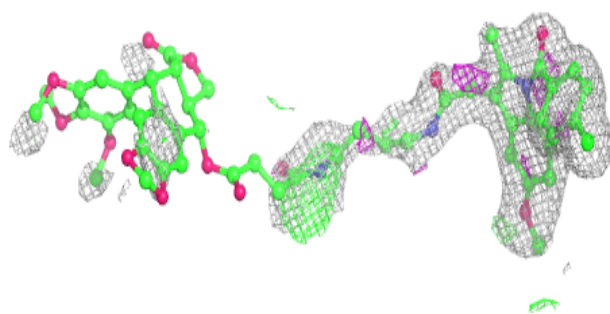
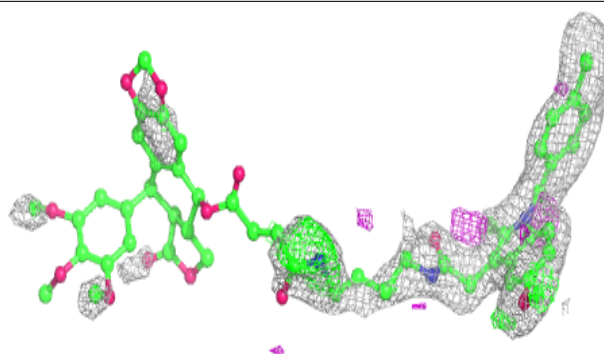
**Electron density around IXP B 707:**

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

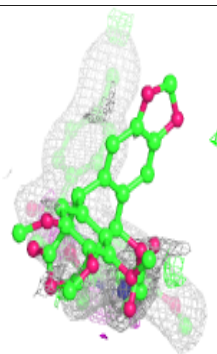
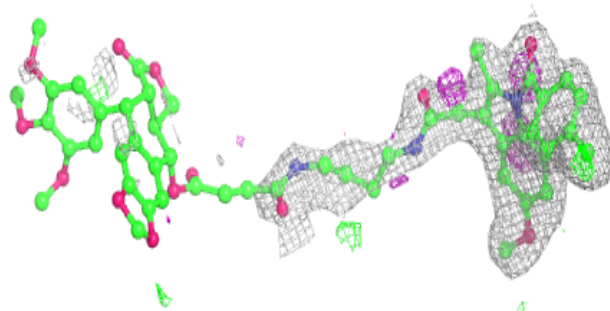
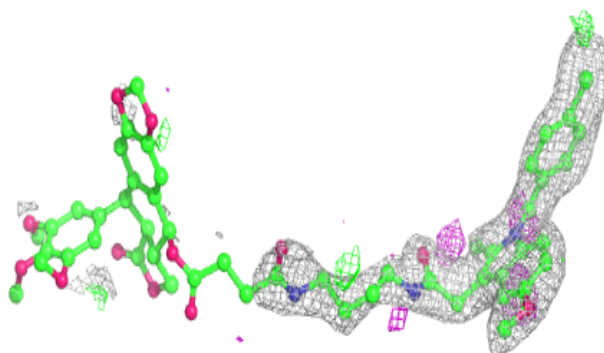


**Electron density around IXP C 706:**

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

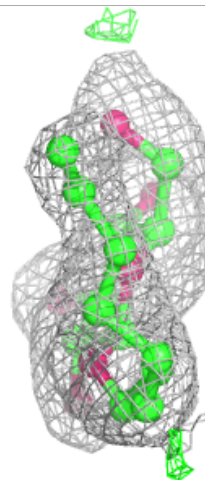
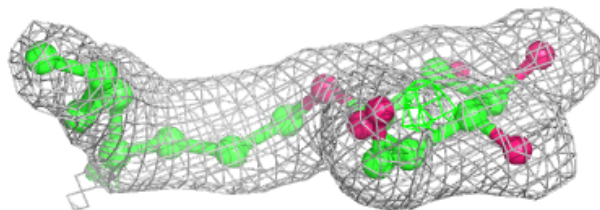
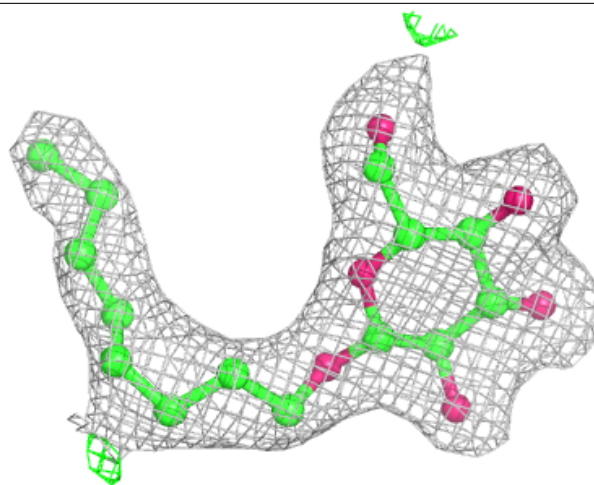
**Electron density around IXP A 706:**

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



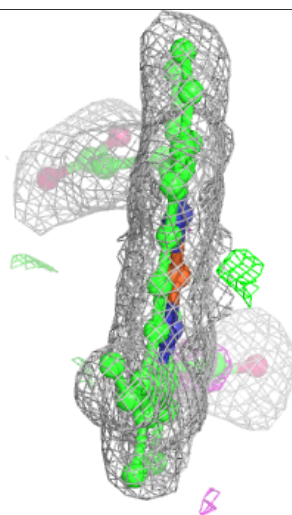
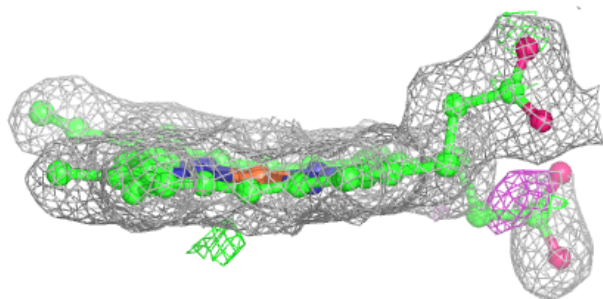
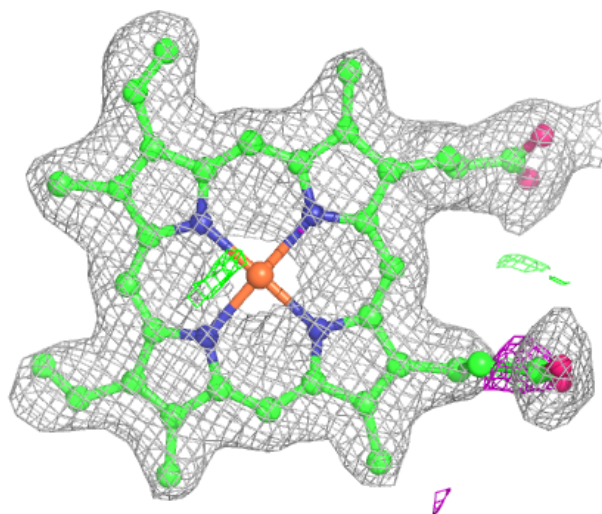
**Electron density around BOG D 706:**

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



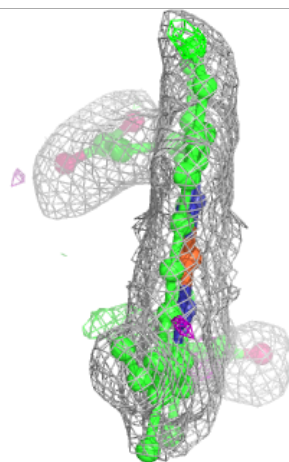
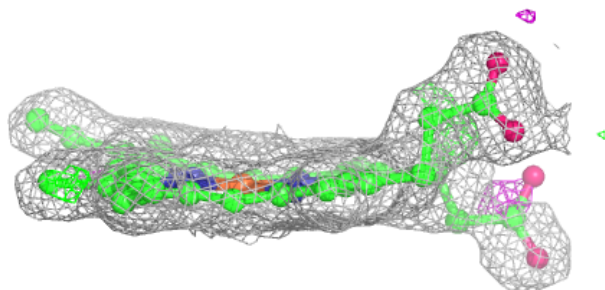
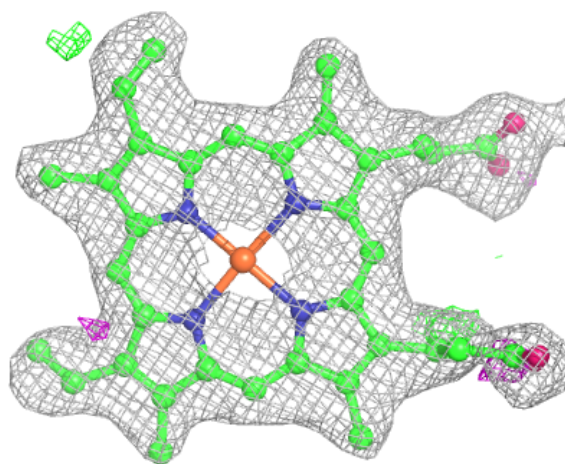
**Electron density around HEM D 705:**

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



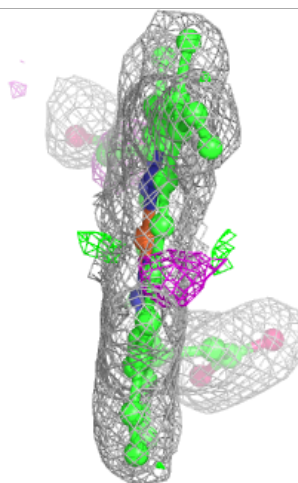
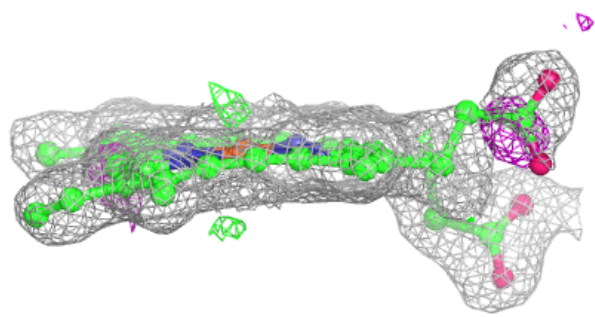
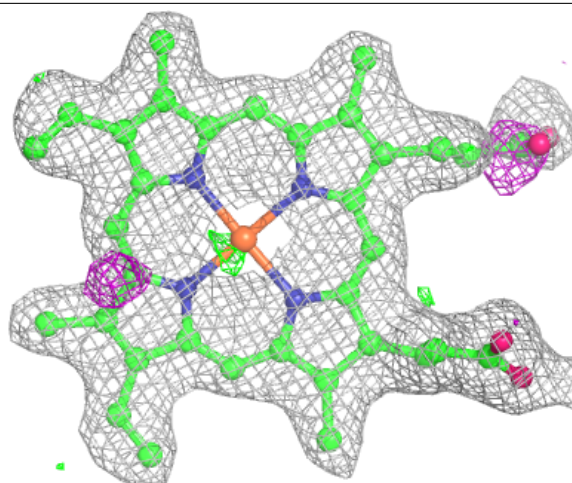
**Electron density around HEM B 706:**

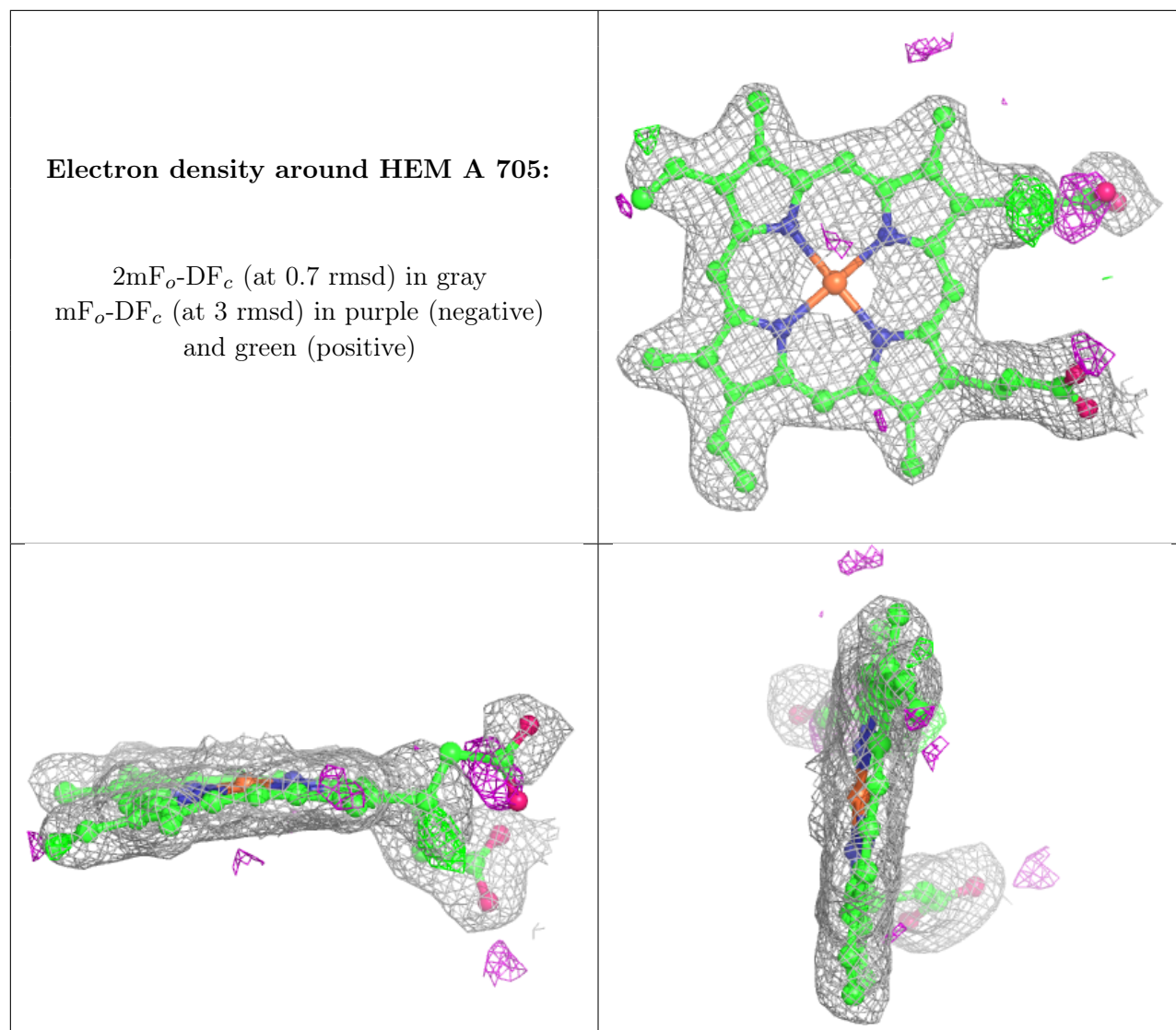
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 705:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.