



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:42 PM UTC

PDB ID : 6BL3 / pdb_00006bl3
Title : Crystal Complex of Cyclooxygenase-2 with indomethacin-butyldiamine-dans
yl conjugate
Authors : Xu, S.; Uddin, M.J.; Banerjee, S.; Marnett, L.J.
Deposited on : 2017-11-09
Resolution : 2.22 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

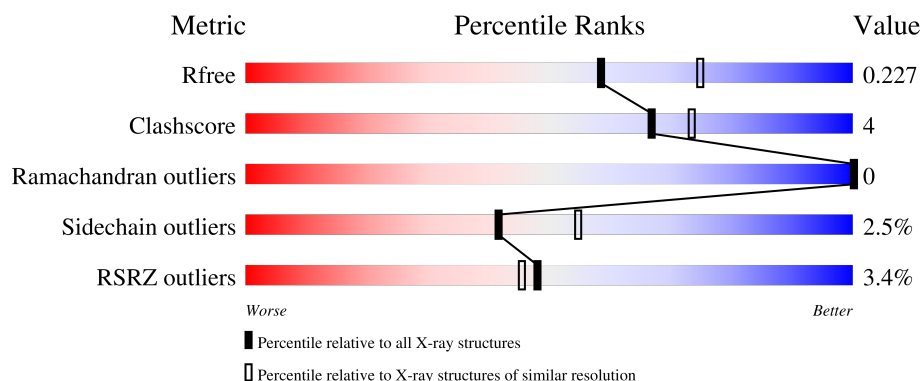
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	587	2% 85% 8% 6%
1	B	587	4% 86% 7% 6%
1	C	587	4% 86% 7% 6%
1	D	587	3% 84% 9% 6%
2	E	2	50% 50%

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

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
6	BOG	A	708	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 19452 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	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			

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



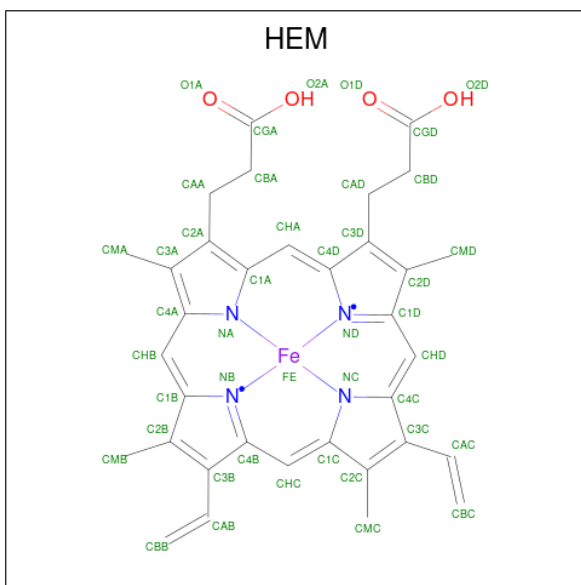
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



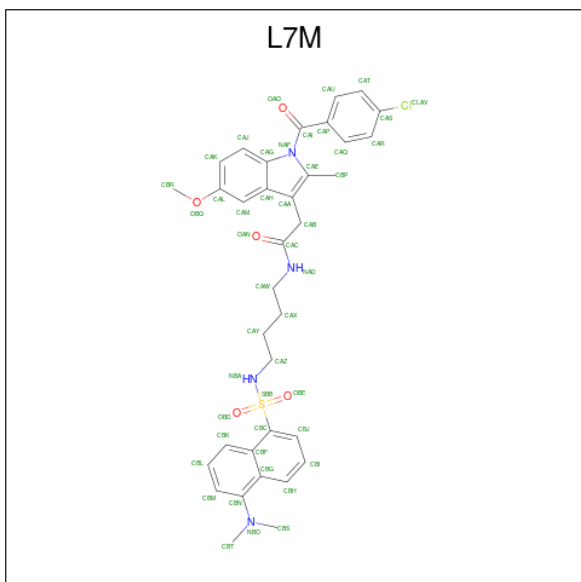
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1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

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



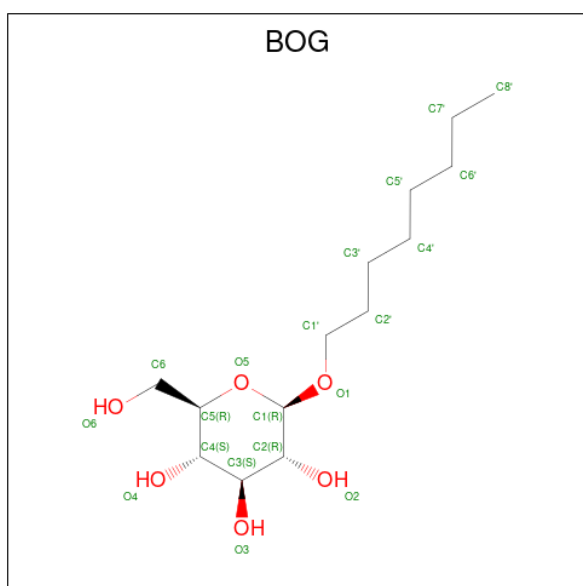
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is 2-[1-(4-chlorobenzene-1-carbonyl)-5-methoxy-2-methyl-1H-indol-3-yl]-N-[4-(5-(dimethylamino)naphthalen-1-yl)sulfonyl]amino]butyl]acetamide (CCD ID: L7M) (formula: C₃₅H₃₇ClN₄O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	S	
			46	35	1	4	5	1	
5	B	1	Total	C	Cl	N	O	S	
			46	35	1	4	5	1	
5	C	1	Total	C	Cl	N	O	S	
			46	35	1	4	5	1	
5	D	1	Total	C	Cl	N	O	S	
			46	35	1	4	5	1	

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



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		
6	B	1	Total	C O	0	0
			20	14 6		
6	C	1	Total	C O	0	0
			20	14 6		
6	C	1	Total	C O	0	0
			20	14 6		
6	D	1	Total	C O	0	0
			20	14 6		

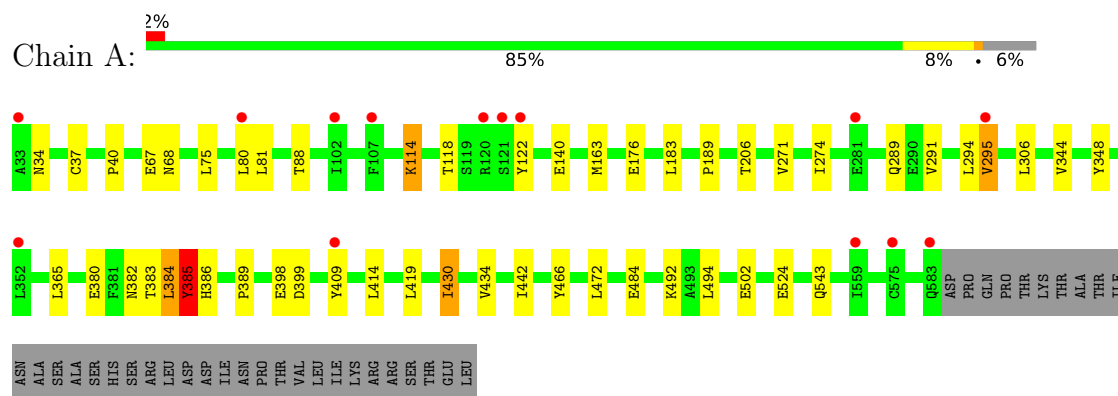
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	226	Total 226	O 226	0	0
7	B	198	Total 198	O 198	0	0
7	C	201	Total 201	O 201	0	0
7	D	231	Total 231	O 231	0	0

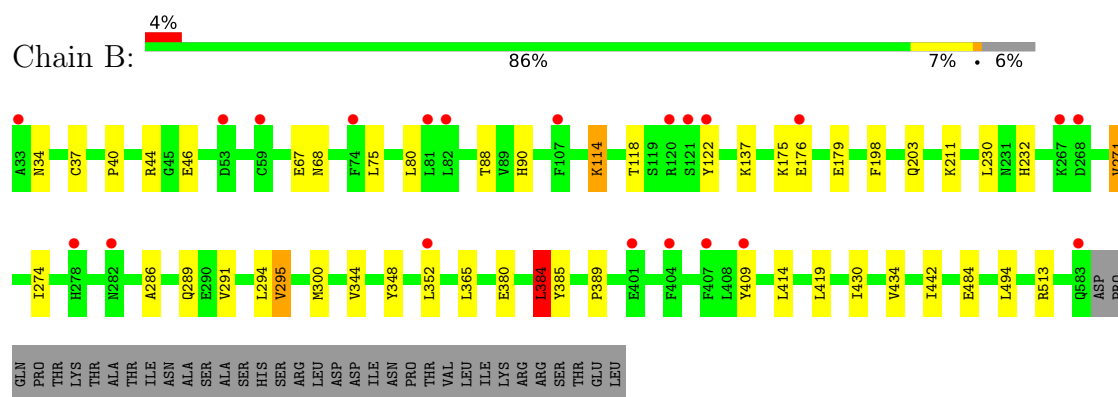
3 Residue-property plots [i](#)

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.

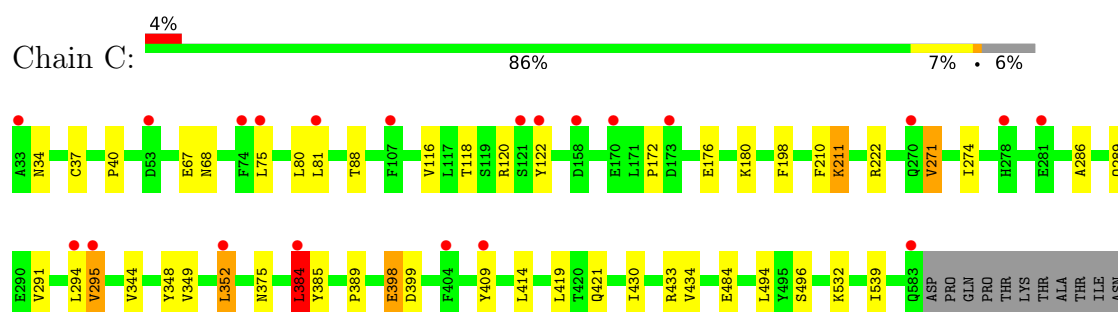
• Molecule 1: Prostaglandin G/H synthase 2



• Molecule 1: Prostaglandin G/H synthase 2

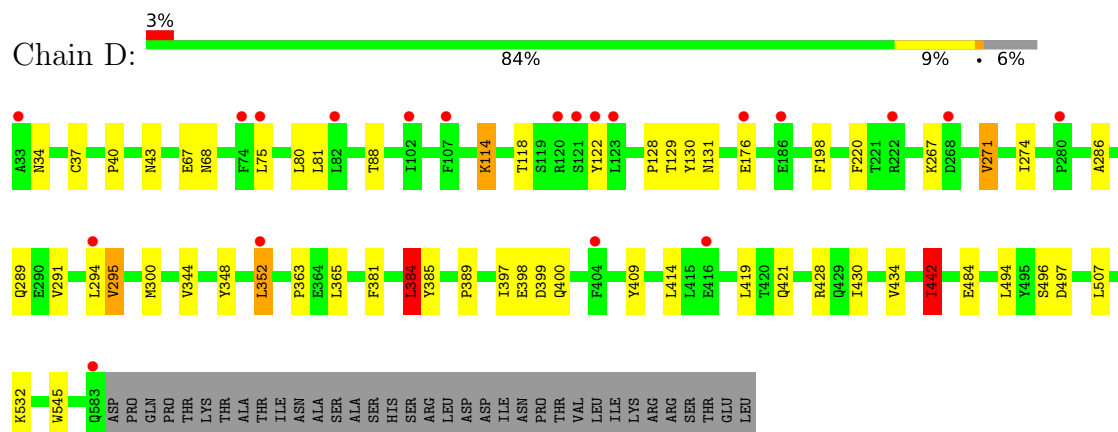


• Molecule 1: Prostaglandin G/H synthase 2



ALA
SER
ALA
SER
HIS
SER
ARG
LEU
ASP
ASP
ILE
ASN
PRO
THR
VAL
LEU
ILE
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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.47Å 121.78Å 134.80Å 90.00° 123.48° 90.00°	Depositor
Resolution (Å)	112.44 – 2.22 112.43 – 2.22	Depositor EDS
% Data completeness (in resolution range)	97.8 (112.44-2.22) 97.8 (112.43-2.22)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.22Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.205 , 0.229 0.205 , 0.227	Depositor DCC
R_{free} test set	4220 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.000 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19452	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BOG, HEM, L7M, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	6/4601 (0.1%)	0.42	0/6239
1	B	0.23	1/4601 (0.0%)	0.41	0/6239
1	C	0.40	3/4601 (0.1%)	0.44	1/6239 (0.0%)
1	D	0.51	12/4601 (0.3%)	0.48	1/6239 (0.0%)
All	All	0.38	22/18404 (0.1%)	0.44	2/24956 (0.0%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	ASN	C-O	-6.88	1.16	1.24
1	D	442	ILE	C-O	-6.82	1.15	1.24
1	D	129	THR	C-O	-6.80	1.15	1.24
1	D	400	GLN	C-O	-6.69	1.16	1.23
1	A	386	HIS	C-O	-6.65	1.16	1.23
1	C	210	PHE	C-O	-6.65	1.16	1.23
1	D	130	TYR	C-O	-6.65	1.14	1.23
1	A	384	LEU	C-O	-6.64	1.16	1.24
1	D	128	PRO	C-O	-6.51	1.16	1.23
1	C	384	LEU	C-O	-6.27	1.16	1.24
1	D	384	LEU	C-O	-6.20	1.16	1.24
1	D	131	ASN	C-O	-5.84	1.16	1.23
1	B	384	LEU	C-O	-5.83	1.16	1.24
1	D	220	PHE	C-O	-5.73	1.16	1.24
1	D	397	ILE	C-O	-5.71	1.18	1.24
1	C	398	GLU	C-O	-5.61	1.19	1.24
1	D	352	LEU	C-O	-5.48	1.17	1.24
1	A	383	THR	C-O	-5.47	1.17	1.24
1	A	385	TYR	C-O	-5.39	1.16	1.24
1	D	400	GLN	CA-C	-5.26	1.46	1.52
1	D	497	ASP	C-O	-5.25	1.17	1.24
1	A	384	LEU	N-CA	-5.21	1.40	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	130	TYR	N-CA-C	7.10	119.69	110.53
1	C	398	GLU	CB-CA-C	-5.55	109.69	117.23

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	4474	0	4373	32	0
1	B	4474	0	4373	26	0
1	C	4474	0	4373	34	0
1	D	4474	0	4373	32	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
3	A	28	0	26	2	0
3	B	28	0	26	1	0
3	C	28	0	26	1	0
3	D	28	0	26	1	0
4	A	43	0	30	2	0
4	B	43	0	30	3	0
4	C	43	0	30	3	0
4	D	43	0	30	2	0
5	A	46	0	0	0	0
5	B	46	0	0	0	0
5	C	46	0	0	2	0
5	D	46	0	0	0	0
6	A	40	0	56	11	0
6	B	20	0	28	1	0
6	C	40	0	56	2	0
6	D	20	0	28	1	0
7	A	226	0	0	2	0
7	B	198	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	201	0	0	5	0
7	D	231	0	0	4	0
All	All	19452	0	17984	135	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 4.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ILE:HD12	6:A:708:BOG:H8'1	1.05	1.04
1:A:442:ILE:CD1	6:A:708:BOG:H8'1	1.90	1.01
1:A:442:ILE:HD12	6:A:708:BOG:C8'	1.96	0.96
1:D:398:GLU:HG3	1:D:421:GLN:CG	1.99	0.92
1:C:176:GLU:HG2	1:C:494:LEU:HD21	1.62	0.81
1:D:398:GLU:HG3	1:D:421:GLN:HG2	1.62	0.81
1:A:183:LEU:CD1	6:A:708:BOG:H8'3	2.12	0.79
1:D:384:LEU:HD23	1:D:507:LEU:HD11	1.75	0.68
1:C:116:VAL:O	1:C:120:ARG:HG2	1.92	0.68
1:D:398:GLU:HG3	1:D:421:GLN:CD	2.17	0.68
1:C:118:THR:O	1:C:122:TYR:CD1	2.47	0.67
1:A:183:LEU:HD13	6:A:708:BOG:H8'3	1.79	0.64
1:C:211:LYS:NZ	7:C:801:HOH:O	2.20	0.64
1:C:294:LEU:HG	1:C:295:VAL:HG22	1.80	0.64
1:A:294:LEU:HG	1:A:295:VAL:HG22	1.79	0.63
1:B:294:LEU:HG	1:B:295:VAL:HG22	1.81	0.62
1:D:88:THR:HG23	6:D:707:BOG:H4'1	1.81	0.62
1:C:88:THR:HG23	6:C:707:BOG:H4'1	1.82	0.62
1:B:274:ILE:HD12	1:B:291:VAL:HG12	1.82	0.62
1:B:380:GLU:O	1:B:384:LEU:HD12	2.01	0.61
1:A:183:LEU:HD13	6:A:708:BOG:C8'	2.31	0.61
1:B:198:PHE:CZ	1:B:352:LEU:HD21	2.37	0.60
1:A:183:LEU:HD12	6:A:708:BOG:H8'3	1.84	0.60
1:D:274:ILE:HD12	1:D:291:VAL:HG12	1.83	0.60
4:D:705:HEM:HBC2	4:D:705:HEM:HMC2	1.85	0.59
1:A:88:THR:HG23	6:A:707:BOG:H4'1	1.83	0.59
1:A:492:LYS:HE2	7:A:1008:HOH:O	2.01	0.59
4:C:705:HEM:HMC2	4:C:705:HEM:HBC2	1.85	0.59
1:B:88:THR:HG23	6:B:707:BOG:H4'1	1.85	0.59
1:B:198:PHE:HZ	1:B:352:LEU:HD21	1.68	0.58
1:D:532:LYS:NZ	7:D:809:HOH:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:THR:O	1:C:122:TYR:HD1	1.86	0.58
1:A:274:ILE:HD12	1:A:291:VAL:HG12	1.85	0.57
1:D:294:LEU:HG	1:D:295:VAL:HG22	1.85	0.57
4:A:705:HEM:HBC2	4:A:705:HEM:HMC2	1.87	0.57
1:C:222:ARG:NE	7:C:812:HOH:O	2.37	0.56
3:A:701:NAG:O7	3:A:701:NAG:O3	2.21	0.55
1:C:274:ILE:HD12	1:C:291:VAL:HG12	1.89	0.54
1:C:198:PHE:CZ	1:C:352:LEU:HD23	2.43	0.54
1:D:428:ARG:HG3	7:D:901:HOH:O	2.08	0.54
1:B:176:GLU:HG2	1:B:494:LEU:HD21	1.89	0.53
1:D:398:GLU:CG	1:D:421:GLN:CD	2.82	0.52
1:C:399:ASP:OD1	1:C:399:ASP:N	2.38	0.52
1:D:381:PHE:HA	1:D:384:LEU:HD12	1.91	0.52
1:D:176:GLU:HG2	1:D:494:LEU:HD21	1.92	0.52
1:A:176:GLU:HG2	1:A:494:LEU:HD21	1.93	0.51
1:C:384:LEU:HD23	5:C:706:L7M:CLAV	2.47	0.51
1:A:118:THR:O	1:A:122:TYR:HD1	1.94	0.51
1:C:122:TYR:CD1	1:C:122:TYR:N	2.79	0.50
3:D:701:NAG:O7	3:D:701:NAG:O3	2.19	0.50
1:A:344:VAL:HA	1:A:348:TYR:HB3	1.93	0.50
1:B:211:LYS:NZ	7:B:809:HOH:O	2.44	0.50
1:C:398:GLU:HG3	1:C:421:GLN:CD	2.36	0.49
1:D:267:LYS:HD3	7:D:1023:HOH:O	2.12	0.49
1:B:389:PRO:HB2	1:B:434:VAL:HA	1.93	0.49
1:C:67:GLU:HG2	1:C:68:ASN:OD1	2.13	0.49
1:C:198:PHE:HZ	1:C:352:LEU:HD23	1.78	0.49
1:A:442:ILE:CD1	6:A:708:BOG:C8'	2.74	0.49
3:B:701:NAG:O7	3:B:701:NAG:O3	2.19	0.49
4:B:705:HEM:HMC1	4:B:705:HEM:HBC2	1.95	0.48
1:B:118:THR:O	1:B:122:TYR:HD1	1.96	0.48
1:C:34:ASN:HB3	1:C:37:CYS:SG	2.53	0.48
1:D:389:PRO:HB2	1:D:434:VAL:HA	1.95	0.48
1:B:344:VAL:HA	1:B:348:TYR:HB3	1.94	0.48
1:D:118:THR:O	1:D:122:TYR:HD1	1.96	0.48
1:C:294:LEU:HA	1:C:409:TYR:CE1	2.49	0.48
1:A:294:LEU:HA	1:A:409:TYR:CE1	2.49	0.48
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.54	0.48
1:D:414:LEU:HD11	1:D:419:LEU:HD23	1.96	0.47
1:B:414:LEU:HD11	1:B:419:LEU:HD23	1.96	0.47
1:C:176:GLU:HG2	1:C:494:LEU:CD2	2.40	0.47
1:A:183:LEU:CD1	6:A:708:BOG:C8'	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:VAL:HA	1:C:348:TYR:HB3	1.96	0.47
4:C:705:HEM:HBB2	4:C:705:HEM:HMB2	1.96	0.47
1:B:46:GLU:OE1	1:B:137:LYS:NZ	2.45	0.47
1:C:349:VAL:HA	1:C:352:LEU:HD11	1.96	0.46
1:D:442:ILE:CD1	1:D:442:ILE:N	2.77	0.46
1:D:384:LEU:HD23	1:D:507:LEU:CD1	2.43	0.46
1:C:352:LEU:HD13	5:C:706:L7M:CAJ	2.45	0.46
1:D:300:MET:HG3	1:D:419:LEU:HD22	1.97	0.46
1:C:122:TYR:HD1	1:C:122:TYR:H	1.62	0.46
1:A:206:THR:HG21	1:A:385:TYR:CE1	2.50	0.45
1:B:40:PRO:O	1:B:68:ASN:HB3	2.17	0.45
1:B:90:HIS:CD2	1:B:513:ARG:HG2	2.51	0.45
1:C:389:PRO:HB2	1:C:434:VAL:HA	1.98	0.45
1:D:271:VAL:HG22	1:D:286:ALA:HB1	1.98	0.45
1:A:67:GLU:HG2	1:A:68:ASN:OD1	2.17	0.45
1:A:389:PRO:HB2	1:A:434:VAL:HA	1.97	0.45
1:B:67:GLU:HG2	1:B:68:ASN:OD1	2.16	0.44
1:D:198:PHE:HZ	1:D:352:LEU:HD21	1.81	0.44
1:C:122:TYR:HD1	1:C:122:TYR:N	2.15	0.44
1:C:271:VAL:HG22	1:C:286:ALA:HB1	2.00	0.44
1:C:414:LEU:HD11	1:C:419:LEU:HD23	2.00	0.44
1:C:532:LYS:NZ	7:C:818:HOH:O	2.50	0.44
1:D:398:GLU:HB3	1:D:399:ASP:H	1.60	0.43
1:C:172:PRO:HG3	1:C:494:LEU:O	2.18	0.43
1:D:363:PRO:HG2	1:D:545:TRP:CD2	2.54	0.43
1:A:398:GLU:HB3	1:A:399:ASP:H	1.63	0.43
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.57	0.43
1:A:114:LYS:HE3	1:A:365:LEU:O	2.18	0.43
1:B:300:MET:HG3	1:B:419:LEU:HD22	1.99	0.43
1:D:34:ASN:HB3	1:D:37:CYS:SG	2.59	0.43
1:D:67:GLU:HG2	1:D:68:ASN:OD1	2.19	0.43
1:C:295:VAL:HG11	4:C:705:HEM:CBB	2.49	0.43
1:B:114:LYS:HE3	1:B:365:LEU:O	2.18	0.42
3:C:701:NAG:O7	3:C:701:NAG:O3	2.19	0.42
1:D:344:VAL:HA	1:D:348:TYR:HB3	2.01	0.42
1:C:375:ASN:O	7:C:802:HOH:O	2.21	0.42
1:D:399:ASP:OD1	1:D:399:ASP:N	2.50	0.42
1:D:295:VAL:HG11	4:D:705:HEM:CBB	2.50	0.42
1:A:189:PRO:HB2	1:A:430:ILE:HD12	2.02	0.42
1:D:40:PRO:O	1:D:68:ASN:HB3	2.19	0.42
1:B:295:VAL:HG11	4:B:705:HEM:CBB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:LEU:HD11	1:A:419:LEU:HD23	2.02	0.42
1:A:472:LEU:HD11	1:A:524:GLU:HB2	2.01	0.42
1:A:543:GLN:HB2	7:B:928:HOH:O	2.18	0.42
4:A:705:HEM:HMB2	4:A:705:HEM:HBB2	2.02	0.42
1:C:40:PRO:O	1:C:68:ASN:HB3	2.20	0.42
1:A:183:LEU:CB	6:A:708:BOG:H8'3	2.50	0.41
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.55	0.41
1:C:180:LYS:HG2	6:C:708:BOG:H1'2	2.01	0.41
1:D:294:LEU:HA	1:D:409:TYR:CE1	2.56	0.41
1:A:40:PRO:O	1:A:68:ASN:HB3	2.20	0.41
1:A:140:GLU:OE2	7:A:801:HOH:O	2.22	0.41
1:B:294:LEU:HA	1:B:409:TYR:CE1	2.55	0.41
1:D:114:LYS:HE3	1:D:365:LEU:O	2.21	0.41
1:B:230:LEU:HA	1:B:232:HIS:CE1	2.55	0.41
1:B:271:VAL:HG22	1:B:286:ALA:HB1	2.03	0.41
1:A:163:MET:CE	1:A:502:GLU:HG2	2.51	0.41
1:B:203:GLN:HB2	4:B:705:HEM:HMC3	2.03	0.41
1:B:175:LYS:O	1:B:179:GLU:HG3	2.21	0.41
1:C:433:ARG:NH1	7:C:822:HOH:O	2.48	0.41
1:D:43:ASN:O	7:D:801:HOH:O	2.22	0.41
3:A:701:NAG:O7	3:A:701:NAG:C3	2.69	0.40
1:B:44:ARG:HG3	7:B:986:HOH:O	2.20	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	550/587 (94%)	535 (97%)	15 (3%)	0	100	100
1	B	550/587 (94%)	536 (98%)	14 (2%)	0	100	100
1	C	550/587 (94%)	536 (98%)	14 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	550/587 (94%)	537 (98%)	13 (2%)	0	100	100
All	All	2200/2348 (94%)	2144 (98%)	56 (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	493/525 (94%)	481 (98%)	12 (2%)	43	56
1	B	493/525 (94%)	482 (98%)	11 (2%)	45	59
1	C	493/525 (94%)	479 (97%)	14 (3%)	38	50
1	D	493/525 (94%)	480 (97%)	13 (3%)	40	53
All	All	1972/2100 (94%)	1922 (98%)	50 (2%)	42	55

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LEU
1	A	80	LEU
1	A	81	LEU
1	A	114	LYS
1	A	271	VAL
1	A	289	GLN
1	A	295	VAL
1	A	306	LEU
1	A	384	LEU
1	A	385	TYR
1	A	430	ILE
1	A	484	GLU
1	B	75	LEU
1	B	80	LEU
1	B	114	LYS
1	B	271	VAL

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Mol	Chain	Res	Type
1	B	289	GLN
1	B	295	VAL
1	B	384	LEU
1	B	385	TYR
1	B	430	ILE
1	B	442	ILE
1	B	484	GLU
1	C	75	LEU
1	C	80	LEU
1	C	81	LEU
1	C	211	LYS
1	C	271	VAL
1	C	289	GLN
1	C	295	VAL
1	C	352	LEU
1	C	384	LEU
1	C	385	TYR
1	C	430	ILE
1	C	484	GLU
1	C	496	SER
1	C	539	ILE
1	D	75	LEU
1	D	80	LEU
1	D	81	LEU
1	D	114	LYS
1	D	271	VAL
1	D	289	GLN
1	D	295	VAL
1	D	384	LEU
1	D	385	TYR
1	D	430	ILE
1	D	442	ILE
1	D	484	GLU
1	D	496	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	396	ASN
1	A	571	ASN
1	B	284	GLN

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Mol	Chain	Res	Type
1	B	396	ASN
1	B	571	ASN
1	C	204	HIS
1	C	241	GLN
1	C	396	ASN
1	C	571	ASN
1	D	204	HIS
1	D	284	GLN
1	D	396	ASN
1	D	461	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	1,2	14,14,15	0.36	0	17,19,21	0.60	0
2	NAG	E	2	2	14,14,15	0.70	1 (7%)	17,19,21	0.57	0
2	NAG	F	1	1,2	14,14,15	0.38	0	17,19,21	0.53	0
2	NAG	F	2	2	14,14,15	0.71	1 (7%)	17,19,21	0.60	0
2	NAG	G	1	1,2	14,14,15	0.42	0	17,19,21	0.56	0
2	NAG	G	2	2	14,14,15	0.66	1 (7%)	17,19,21	0.54	0
2	NAG	H	1	1,2	14,14,15	0.36	0	17,19,21	0.48	0
2	NAG	H	2	2	14,14,15	0.72	1 (7%)	17,19,21	0.56	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	1,2	-	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	NAG	C1-C2	2.54	1.55	1.52
2	F	2	NAG	C1-C2	2.43	1.55	1.52
2	E	2	NAG	C1-C2	2.32	1.55	1.52
2	G	2	NAG	C1-C2	2.16	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

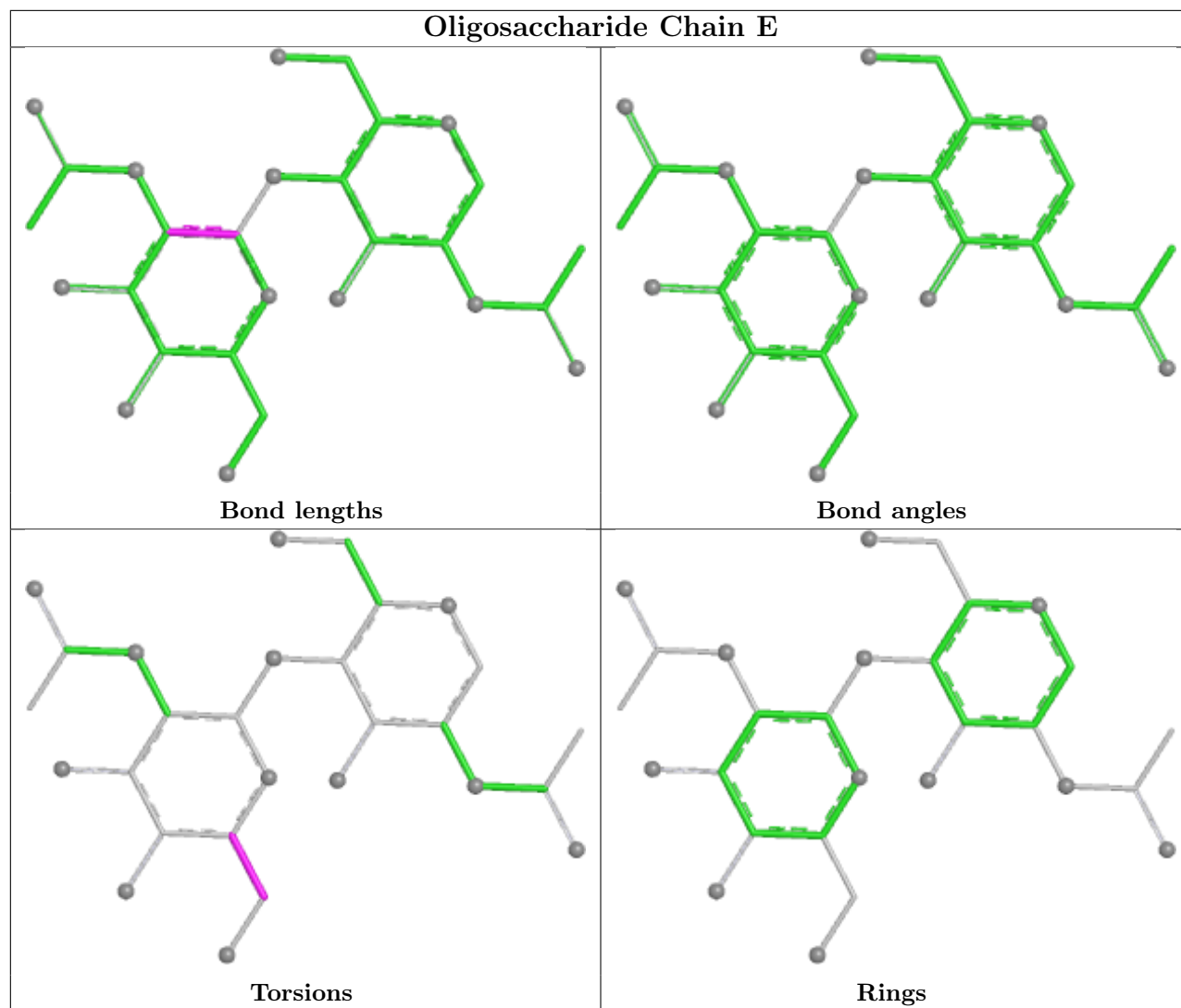
All (9) torsion outliers are listed below:

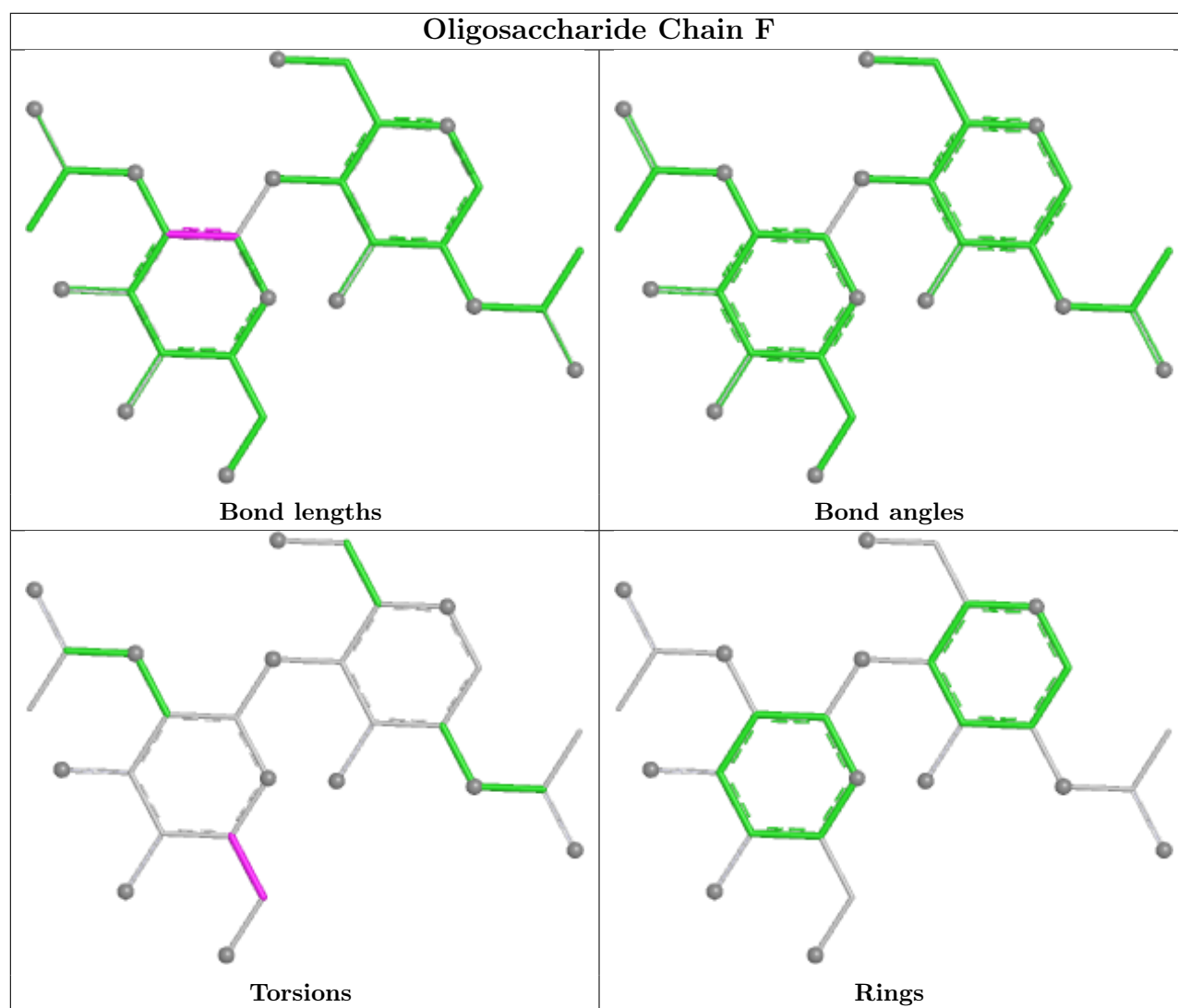
Mol	Chain	Res	Type	Atoms
2	H	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C1-C2-N2-C7

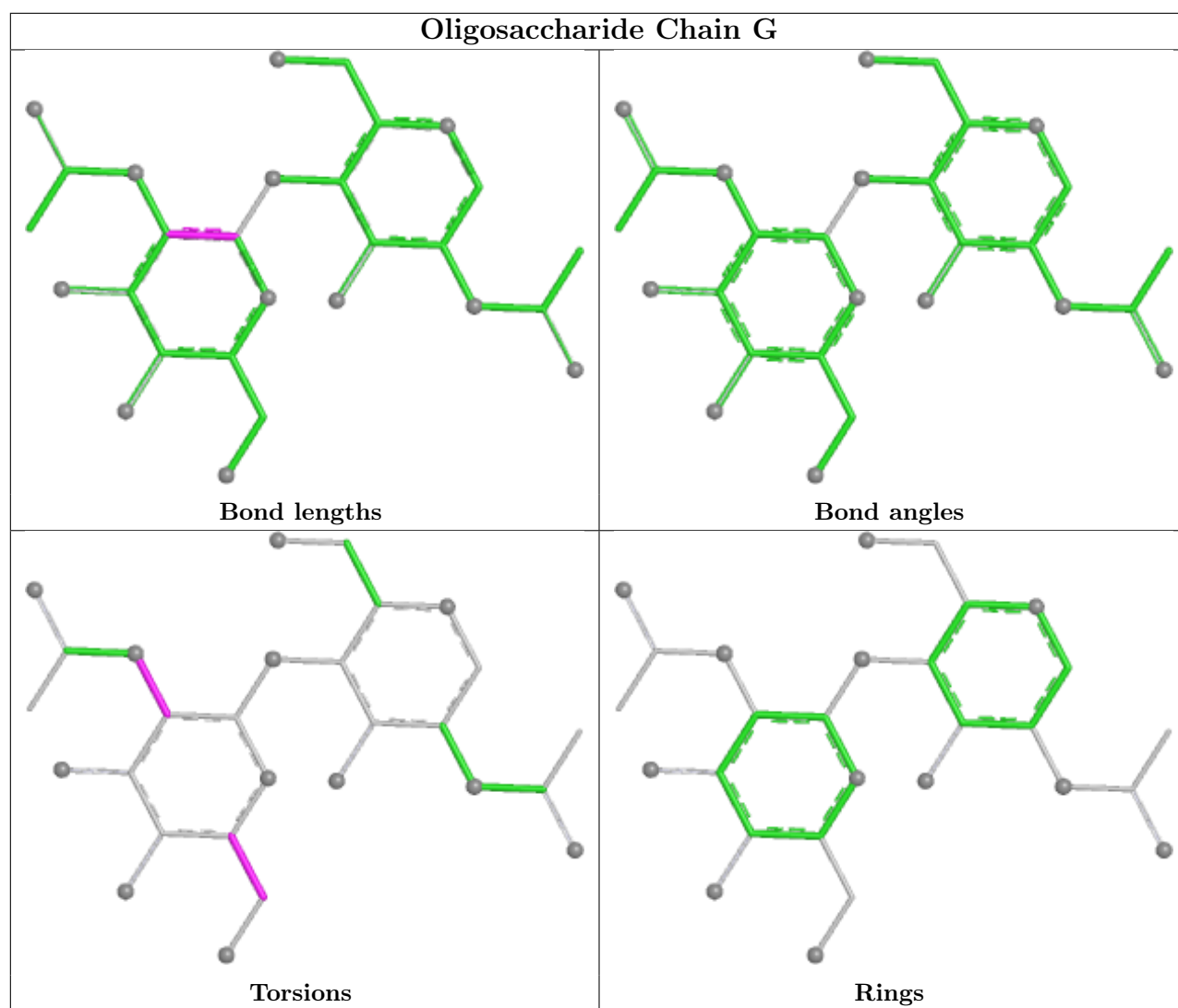
There are no ring outliers.

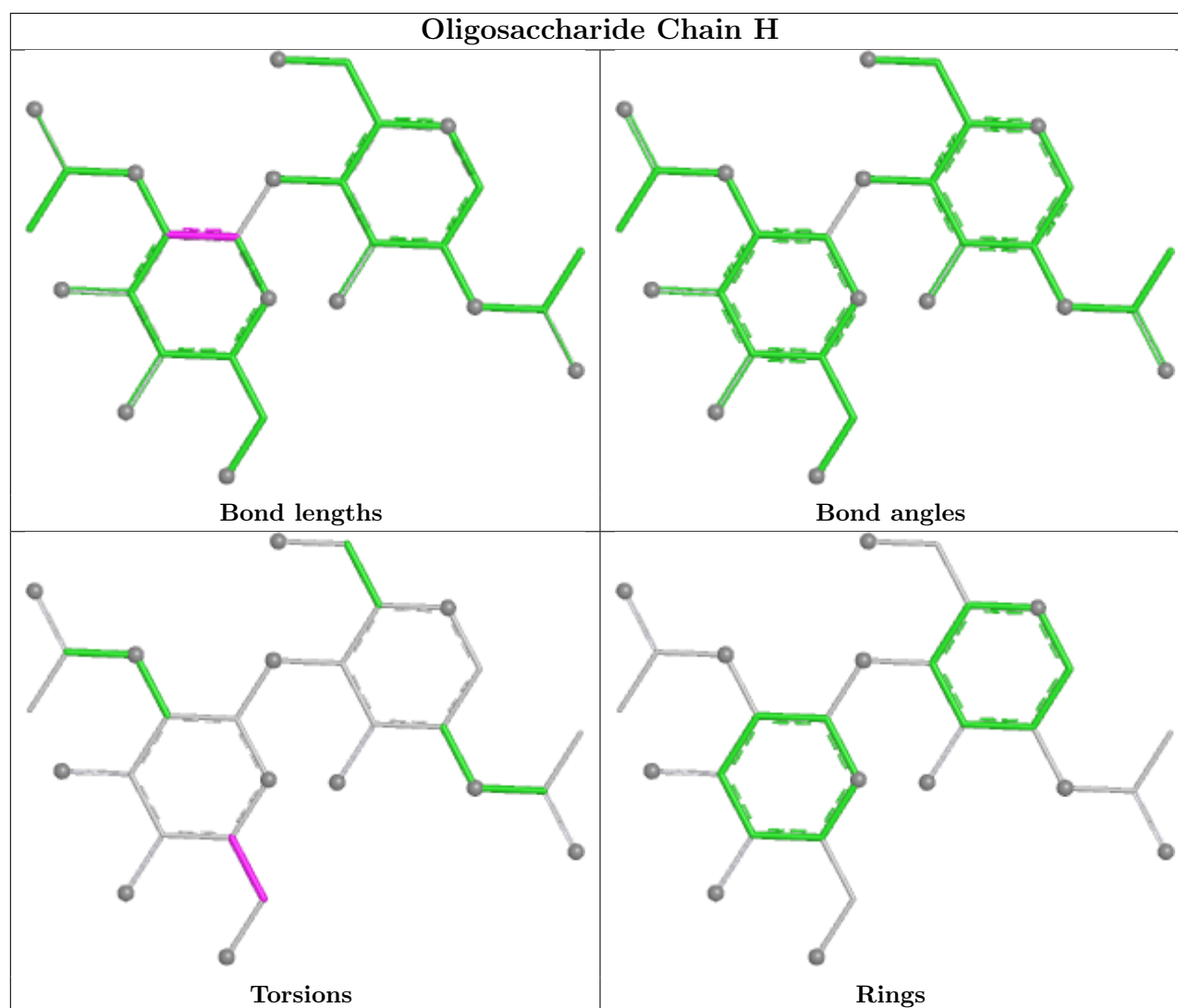
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	BOG	D	707	-	20,20,20	1.04	1 (5%)	25,25,25	1.11	3 (12%)
6	BOG	B	707	-	20,20,20	1.04	1 (5%)	25,25,25	1.12	3 (12%)
3	NAG	D	701	1	14,14,15	0.61	0	17,19,21	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BOG	C	707	-	20,20,20	1.02	1 (5%)	25,25,25	1.11	3 (12%)
3	NAG	B	701	1	14,14,15	0.62	0	17,19,21	1.05	1 (5%)
3	NAG	B	704	1	14,14,15	0.32	0	17,19,21	0.53	0
5	L7M	D	706	-	50,50,50	2.69	14 (28%)	71,72,72	1.63	15 (21%)
3	NAG	C	704	1	14,14,15	0.28	0	17,19,21	0.51	0
5	L7M	A	706	-	50,50,50	2.72	14 (28%)	71,72,72	1.59	12 (16%)
3	NAG	A	704	1	14,14,15	0.31	0	17,19,21	0.51	0
4	HEM	B	705	1	50,50,50	1.45	10 (20%)	67,82,82	1.14	6 (8%)
4	HEM	D	705	1	50,50,50	1.46	9 (18%)	67,82,82	1.14	4 (5%)
6	BOG	A	708	-	20,20,20	0.58	0	25,25,25	1.39	2 (8%)
3	NAG	A	701	1	14,14,15	0.61	0	17,19,21	1.06	1 (5%)
4	HEM	A	705	1	50,50,50	1.48	10 (20%)	67,82,82	1.14	5 (7%)
3	NAG	D	704	1	14,14,15	0.41	0	17,19,21	0.53	0
6	BOG	A	707	-	20,20,20	1.03	1 (5%)	25,25,25	1.16	3 (12%)
5	L7M	C	706	-	50,50,50	2.74	14 (28%)	71,72,72	1.61	15 (21%)
3	NAG	C	701	1	14,14,15	0.62	0	17,19,21	1.04	1 (5%)
5	L7M	B	706	-	50,50,50	2.75	13 (26%)	71,72,72	1.59	14 (19%)
6	BOG	C	708	-	20,20,20	1.09	1 (5%)	25,25,25	1.25	2 (8%)
4	HEM	C	705	1,7	50,50,50	1.45	10 (20%)	67,82,82	1.14	6 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BOG	D	707	-	-	1/11/31/31	0/1/1/1
6	BOG	B	707	-	-	1/11/31/31	0/1/1/1
3	NAG	D	701	1	-	1/6/23/26	0/1/1/1
6	BOG	C	707	-	-	2/11/31/31	0/1/1/1
3	NAG	B	701	1	-	1/6/23/26	0/1/1/1
3	NAG	B	704	1	-	0/6/23/26	0/1/1/1
5	L7M	D	706	-	-	7/34/34/34	0/5/5/5
3	NAG	C	704	1	-	0/6/23/26	0/1/1/1
5	L7M	A	706	-	-	7/34/34/34	0/5/5/5
3	NAG	A	704	1	-	0/6/23/26	0/1/1/1
4	HEM	B	705	1	-	0/14/54/54	-
4	HEM	D	705	1	-	0/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BOG	A	708	-	-	4/11/31/31	0/1/1/1
3	NAG	A	701	1	-	1/6/23/26	0/1/1/1
4	HEM	A	705	1	-	0/14/54/54	-
3	NAG	D	704	1	-	0/6/23/26	0/1/1/1
6	BOG	A	707	-	-	2/11/31/31	0/1/1/1
5	L7M	C	706	-	-	7/34/34/34	0/5/5/5
3	NAG	C	701	1	-	1/6/23/26	0/1/1/1
5	L7M	B	706	-	-	7/34/34/34	0/5/5/5
6	BOG	C	708	-	-	5/11/31/31	0/1/1/1
4	HEM	C	705	1,7	-	0/14/54/54	-

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	706	L7M	OBE-SBB	8.97	1.53	1.43
5	C	706	L7M	OBE-SBB	8.91	1.53	1.43
5	D	706	L7M	OBE-SBB	8.87	1.53	1.43
5	B	706	L7M	OBE-SBB	8.86	1.53	1.43
5	B	706	L7M	OBD-SBB	8.77	1.53	1.43
5	C	706	L7M	OBD-SBB	8.74	1.53	1.43
5	A	706	L7M	OBD-SBB	8.68	1.53	1.43
5	D	706	L7M	OBD-SBB	8.62	1.53	1.43
5	B	706	L7M	CAH-CAA	-6.04	1.33	1.44
5	A	706	L7M	CAH-CAA	-5.86	1.33	1.44
5	B	706	L7M	SBB-NBA	5.85	1.70	1.61
5	D	706	L7M	CAH-CAA	-5.80	1.33	1.44
5	C	706	L7M	CAH-CAA	-5.78	1.33	1.44
5	B	706	L7M	CAP-CAI	-5.65	1.40	1.50
5	D	706	L7M	CAP-CAI	-5.63	1.40	1.50
5	C	706	L7M	CAP-CAI	-5.56	1.40	1.50
5	A	706	L7M	CAP-CAI	-5.51	1.40	1.50
5	C	706	L7M	SBB-NBA	5.33	1.69	1.61
5	A	706	L7M	SBB-NBA	5.06	1.69	1.61
4	A	705	HEM	FE-ND	5.00	2.10	1.94
5	C	706	L7M	CAH-CAG	-4.83	1.34	1.41
5	A	706	L7M	CAH-CAG	-4.83	1.34	1.41
5	B	706	L7M	CAH-CAG	-4.78	1.34	1.41
4	B	705	HEM	FE-ND	4.75	2.09	1.94
4	D	705	HEM	FE-ND	4.74	2.09	1.94
4	C	705	HEM	FE-ND	4.73	2.09	1.94
5	D	706	L7M	CAH-CAG	-4.71	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	706	L7M	SBB-NBA	4.54	1.68	1.61
5	A	706	L7M	CAJ-CAG	-3.64	1.33	1.39
5	C	706	L7M	CAG-NAF	-3.61	1.35	1.41
5	C	706	L7M	CAJ-CAG	-3.57	1.34	1.39
5	B	706	L7M	CAJ-CAG	-3.55	1.34	1.39
5	A	706	L7M	CAG-NAF	-3.46	1.35	1.41
5	B	706	L7M	CAM-CAH	-3.45	1.34	1.39
5	D	706	L7M	CAJ-CAG	-3.41	1.34	1.39
4	D	705	HEM	FE-NB	3.39	2.05	1.94
5	D	706	L7M	CAG-NAF	-3.39	1.35	1.41
5	D	706	L7M	CAM-CAH	-3.39	1.34	1.39
5	A	706	L7M	CAM-CAH	-3.34	1.34	1.39
5	B	706	L7M	CAG-NAF	-3.32	1.35	1.41
4	A	705	HEM	FE-NB	3.32	2.05	1.94
5	C	706	L7M	CAM-CAH	-3.29	1.34	1.39
5	C	706	L7M	CAE-NAF	-3.24	1.34	1.40
5	D	706	L7M	CAE-NAF	-3.21	1.34	1.40
5	A	706	L7M	CAE-NAF	-3.17	1.34	1.40
5	B	706	L7M	CAE-NAF	-3.13	1.34	1.40
5	A	706	L7M	CBP-CAE	3.12	1.54	1.49
5	C	706	L7M	CBP-CAE	3.11	1.54	1.49
4	B	705	HEM	FE-NB	3.09	2.04	1.94
4	C	705	HEM	CAB-C3B	3.06	1.55	1.47
4	A	705	HEM	CAC-C3C	3.04	1.55	1.47
4	A	705	HEM	CAB-C3B	3.03	1.55	1.47
4	B	705	HEM	CAC-C3C	3.00	1.55	1.47
4	C	705	HEM	CAC-C3C	2.99	1.55	1.47
4	B	705	HEM	CAB-C3B	2.99	1.55	1.47
4	D	705	HEM	CAC-C3C	2.95	1.55	1.47
4	D	705	HEM	CAB-C3B	2.95	1.55	1.47
5	D	706	L7M	CBP-CAE	2.94	1.54	1.49
5	A	706	L7M	CBN-NBO	-2.92	1.34	1.43
5	D	706	L7M	CBN-NBO	-2.90	1.35	1.43
5	C	706	L7M	CBN-NBO	-2.87	1.35	1.43
4	C	705	HEM	FE-NB	2.82	2.03	1.94
5	B	706	L7M	CBN-NBO	-2.78	1.35	1.43
5	B	706	L7M	CBP-CAE	2.76	1.53	1.49
4	B	705	HEM	FE-NA	2.65	2.03	1.95
4	C	705	HEM	FE-NA	2.64	2.03	1.95
4	D	705	HEM	FE-NC	2.60	2.03	1.95
4	D	705	HEM	FE-NA	2.53	2.03	1.95
4	A	705	HEM	FE-NA	2.46	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	707	BOG	O2-C2	-2.39	1.37	1.43
6	B	707	BOG	O2-C2	-2.37	1.37	1.43
4	A	705	HEM	FE-NC	2.34	2.02	1.95
6	C	707	BOG	O2-C2	-2.33	1.37	1.43
6	A	707	BOG	O2-C2	-2.33	1.37	1.43
6	C	708	BOG	O2-C2	-2.31	1.37	1.43
4	B	705	HEM	FE-NC	2.29	2.02	1.95
4	C	705	HEM	FE-NC	2.28	2.02	1.95
5	C	706	L7M	CBJ-CBC	2.17	1.40	1.37
5	D	706	L7M	CBJ-CBC	2.15	1.40	1.37
5	C	706	L7M	CAI-NAF	-2.14	1.36	1.41
4	D	705	HEM	CMB-C2B	2.14	1.55	1.50
5	A	706	L7M	CBJ-CBC	2.13	1.40	1.37
5	A	706	L7M	CAI-NAF	-2.13	1.36	1.41
5	D	706	L7M	CAI-NAF	-2.09	1.36	1.41
4	A	705	HEM	CMD-C2D	2.08	1.55	1.50
4	D	705	HEM	CMC-C2C	2.08	1.55	1.50
4	B	705	HEM	CMC-C2C	2.06	1.55	1.50
4	B	705	HEM	CMD-C2D	2.06	1.55	1.50
4	A	705	HEM	CMB-C2B	2.06	1.55	1.50
4	C	705	HEM	CMB-C2B	2.06	1.55	1.50
4	C	705	HEM	CMA-C3A	2.05	1.55	1.50
4	A	705	HEM	CMC-C2C	2.05	1.55	1.50
4	C	705	HEM	CMC-C2C	2.04	1.54	1.50
5	B	706	L7M	CBJ-CBC	2.03	1.40	1.37
4	B	705	HEM	CMB-C2B	2.03	1.54	1.50
4	C	705	HEM	CMD-C2D	2.02	1.54	1.50
4	A	705	HEM	CMA-C3A	2.02	1.54	1.50
4	D	705	HEM	CMD-C2D	2.01	1.54	1.50
4	B	705	HEM	CMA-C3A	2.00	1.54	1.50

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	706	L7M	OBE-SBB-OB	-7.29	110.67	119.52
5	C	706	L7M	OBE-SBB-OB	-6.91	111.12	119.52
5	A	706	L7M	OBE-SBB-OB	-6.73	111.35	119.52
5	B	706	L7M	OBE-SBB-OB	-6.66	111.44	119.52
6	A	708	BOG	C1'-O1-C1	4.59	121.53	113.68
6	C	708	BOG	C1'-O1-C1	4.01	120.52	113.68
3	A	701	NAG	C2-N2-C7	3.93	128.17	122.90
3	B	701	NAG	C2-N2-C7	3.87	128.09	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	NAG	C2-N2-C7	3.82	128.02	122.90
3	D	701	NAG	C2-N2-C7	3.82	128.01	122.90
6	A	707	BOG	C1'-O1-C1	3.57	119.77	113.68
6	C	707	BOG	C1'-O1-C1	3.42	119.52	113.68
6	B	707	BOG	C1'-O1-C1	3.38	119.45	113.68
5	B	706	L7M	CBP-CAE-NAF	3.25	126.94	122.07
5	A	706	L7M	CBP-CAE-NAF	3.21	126.89	122.07
5	B	706	L7M	CAG-NAF-CAE	-3.00	105.36	107.80
5	D	706	L7M	CBP-CAE-NAF	2.98	126.53	122.07
5	B	706	L7M	CAJ-CAG-CAH	-2.98	118.63	121.95
5	D	706	L7M	CBK-CBF-CBC	-2.97	119.12	123.58
5	C	706	L7M	CBP-CAE-NAF	2.96	126.51	122.07
5	C	706	L7M	CBK-CBF-CBC	-2.93	119.18	123.58
5	B	706	L7M	CBP-CAE-CAA	-2.92	123.50	128.07
6	D	707	BOG	C1'-O1-C1	2.89	118.61	113.68
5	B	706	L7M	CBK-CBF-CBC	-2.88	119.26	123.58
6	C	708	BOG	C6-C5-C4	-2.86	106.00	113.02
5	A	706	L7M	CBK-CBF-CBC	-2.80	119.38	123.58
5	D	706	L7M	CAJ-CAG-CAH	-2.76	118.86	121.95
5	C	706	L7M	CBM-CBN-NBO	-2.76	117.52	121.61
4	A	705	HEM	CBA-CAA-C2A	-2.74	104.96	112.53
6	D	707	BOG	O1-C1-C2	2.72	112.40	108.27
5	C	706	L7M	CAZ-NBA-SBB	-2.68	112.22	120.27
6	A	707	BOG	O1-C1-C2	2.65	112.30	108.27
5	D	706	L7M	CBP-CAE-CAA	-2.63	123.95	128.07
5	A	706	L7M	CBP-CAE-CAA	-2.63	123.96	128.07
5	D	706	L7M	CAG-NAF-CAE	-2.60	105.68	107.80
5	A	706	L7M	CAZ-NBA-SBB	-2.59	112.48	120.27
5	B	706	L7M	CAZ-NBA-SBB	-2.59	112.48	120.27
5	A	706	L7M	CAJ-CAG-CAH	-2.54	119.11	121.95
4	C	705	HEM	CBA-CAA-C2A	-2.54	105.52	112.53
4	C	705	HEM	C1B-NB-C4B	2.53	108.21	105.21
5	C	706	L7M	CBJ-CBC-SBB	2.53	119.87	116.92
4	A	705	HEM	C1B-NB-C4B	2.53	108.20	105.21
6	A	708	BOG	O1-C1'-C2'	2.53	117.94	109.37
6	D	707	BOG	C1-O5-C5	-2.53	108.79	113.72
4	B	705	HEM	CBA-CAA-C2A	-2.52	105.58	112.53
4	D	705	HEM	C2A-C1A-NA	-2.49	107.39	110.15
5	D	706	L7M	CBJ-CBC-SBB	2.47	119.80	116.92
4	B	705	HEM	C1B-NB-C4B	2.45	108.11	105.21
4	D	705	HEM	CBA-CAA-C2A	-2.45	105.76	112.53
4	B	705	HEM	C2A-C1A-NA	-2.44	107.44	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	706	L7M	CBP-CAE-CAA	-2.44	124.26	128.07
5	D	706	L7M	CBC-SBB-NBA	2.41	111.24	106.78
5	C	706	L7M	CAG-NAF-CAE	-2.40	105.84	107.80
5	C	706	L7M	CAJ-CAG-CAH	-2.40	119.27	121.95
4	A	705	HEM	CHD-C4C-NC	2.38	127.05	124.45
5	C	706	L7M	CBS-NBO-CBN	2.38	121.43	114.19
5	A	706	L7M	CAG-NAF-CAE	-2.37	105.86	107.80
4	A	705	HEM	C2A-C1A-NA	-2.37	107.52	110.15
4	D	705	HEM	C1B-NB-C4B	2.35	107.99	105.21
5	B	706	L7M	CBC-SBB-NBA	2.35	111.12	106.78
5	D	706	L7M	CAZ-NBA-SBB	-2.35	113.21	120.27
6	A	707	BOG	C1-O5-C5	-2.35	109.14	113.72
4	C	705	HEM	CHD-C4C-NC	2.34	127.00	124.45
5	A	706	L7M	CBJ-CBC-SBB	2.33	119.64	116.92
4	C	705	HEM	C2A-C1A-NA	-2.32	107.58	110.15
5	A	706	L7M	CAP-CAI-NAF	2.29	122.33	117.92
5	B	706	L7M	CBR-OBQ-CAL	-2.27	112.62	117.50
6	B	707	BOG	O1-C1-C2	2.27	111.72	108.27
6	C	707	BOG	O1-C1-C2	2.27	111.72	108.27
5	C	706	L7M	CBC-SBB-NBA	2.26	110.96	106.78
5	A	706	L7M	CBM-CBN-NBO	-2.25	118.27	121.61
5	B	706	L7M	CBS-NBO-CBN	2.23	120.98	114.19
6	C	707	BOG	C1-O5-C5	-2.23	109.37	113.72
5	C	706	L7M	CAP-CAI-NAF	2.22	122.19	117.92
5	A	706	L7M	CBS-NBO-CBN	2.22	120.94	114.19
5	D	706	L7M	CBR-OBQ-CAL	-2.21	112.76	117.50
4	D	705	HEM	CBD-CAD-C3D	-2.20	106.46	112.53
5	B	706	L7M	CBJ-CBC-SBB	2.19	119.48	116.92
5	D	706	L7M	CAP-CAI-NAF	2.19	122.13	117.92
5	D	706	L7M	CBS-NBO-CBN	2.19	120.85	114.19
5	A	706	L7M	CBC-SBB-NBA	2.18	110.81	106.78
4	C	705	HEM	C3B-C2B-C1B	2.15	108.03	106.41
5	C	706	L7M	CBG-CBN-NBO	2.09	121.56	118.37
4	B	705	HEM	C4D-ND-C1D	2.07	107.65	105.21
5	D	706	L7M	OAO-CAI-CAP	-2.07	116.19	120.29
5	B	706	L7M	CAK-CAL-CAM	-2.06	117.73	120.50
4	A	705	HEM	C3B-C2B-C1B	2.06	107.96	106.41
5	D	706	L7M	CBM-CBN-NBO	-2.05	118.56	121.61
5	C	706	L7M	CBF-CBC-SBB	-2.05	119.25	121.66
5	B	706	L7M	OAO-CAI-CAP	-2.05	116.23	120.29
6	B	707	BOG	C1-O5-C5	-2.04	109.73	113.72
5	B	706	L7M	CAP-CAI-NAF	2.04	121.84	117.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	705	HEM	CBD-CAD-C3D	-2.02	106.94	112.53
4	C	705	HEM	CBD-CAD-C3D	-2.01	106.96	112.53
4	B	705	HEM	C3B-C2B-C1B	2.01	107.92	106.41
5	C	706	L7M	CBC-CBF-CBG	2.01	120.65	117.97
5	D	706	L7M	CAK-CAL-CAM	-2.00	117.81	120.50

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	NAG	C3-C2-N2-C7
3	B	701	NAG	C3-C2-N2-C7
3	C	701	NAG	C3-C2-N2-C7
3	D	701	NAG	C3-C2-N2-C7
5	A	706	L7M	CAX-CAY-CAZ-NBA
5	D	706	L7M	CAX-CAY-CAZ-NBA
6	C	708	BOG	O5-C1-O1-C1'
6	D	707	BOG	O5-C1-O1-C1'
6	C	708	BOG	C2-C1-O1-C1'
6	B	707	BOG	O5-C1-O1-C1'
6	A	707	BOG	O5-C1-O1-C1'
6	C	707	BOG	O5-C1-O1-C1'
6	A	708	BOG	O1-C1'-C2'-C3'
5	D	706	L7M	NAD-CAW-CAX-CAY
5	B	706	L7M	NAD-CAW-CAX-CAY
6	C	708	BOG	C2'-C3'-C4'-C5'
6	A	708	BOG	C5'-C6'-C7'-C8'
6	A	708	BOG	C1'-C2'-C3'-C4'
6	A	708	BOG	C2'-C1'-O1-C1
6	C	708	BOG	C2'-C1'-O1-C1
5	B	706	L7M	CAX-CAY-CAZ-NBA
5	C	706	L7M	CAX-CAY-CAZ-NBA
5	C	706	L7M	OAO-CAI-NAF-CAE
5	D	706	L7M	CAW-CAX-CAY-CAZ
5	B	706	L7M	CAW-CAX-CAY-CAZ
5	C	706	L7M	CAW-CAX-CAY-CAZ
5	C	706	L7M	NAD-CAW-CAX-CAY
5	A	706	L7M	OAO-CAI-NAF-CAE
5	B	706	L7M	OAO-CAI-NAF-CAE
5	D	706	L7M	OAO-CAI-NAF-CAE
5	A	706	L7M	NAD-CAW-CAX-CAY
5	A	706	L7M	CAW-CAX-CAY-CAZ

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Mol	Chain	Res	Type	Atoms
5	C	706	L7M	OAQ-CAI-CAP-CAQ
5	A	706	L7M	OAQ-CAI-CAP-CAQ
6	A	707	BOG	C3'-C4'-C5'-C6'
5	D	706	L7M	OAQ-CAI-CAP-CAQ
5	B	706	L7M	OAQ-CAI-CAP-CAQ
5	D	706	L7M	CAZ-NBA-SBB-OBE
6	C	707	BOG	C3'-C4'-C5'-C6'
5	A	706	L7M	CAA-CAB-CAC-OAN
5	C	706	L7M	CAA-CAB-CAC-OAN
5	D	706	L7M	CAA-CAB-CAC-OAN
5	A	706	L7M	NAF-CAI-CAP-CAQ
5	C	706	L7M	NAF-CAI-CAP-CAQ
5	B	706	L7M	CAA-CAB-CAC-NAD
6	C	708	BOG	C3'-C4'-C5'-C6'
5	B	706	L7M	NAF-CAI-CAP-CAQ

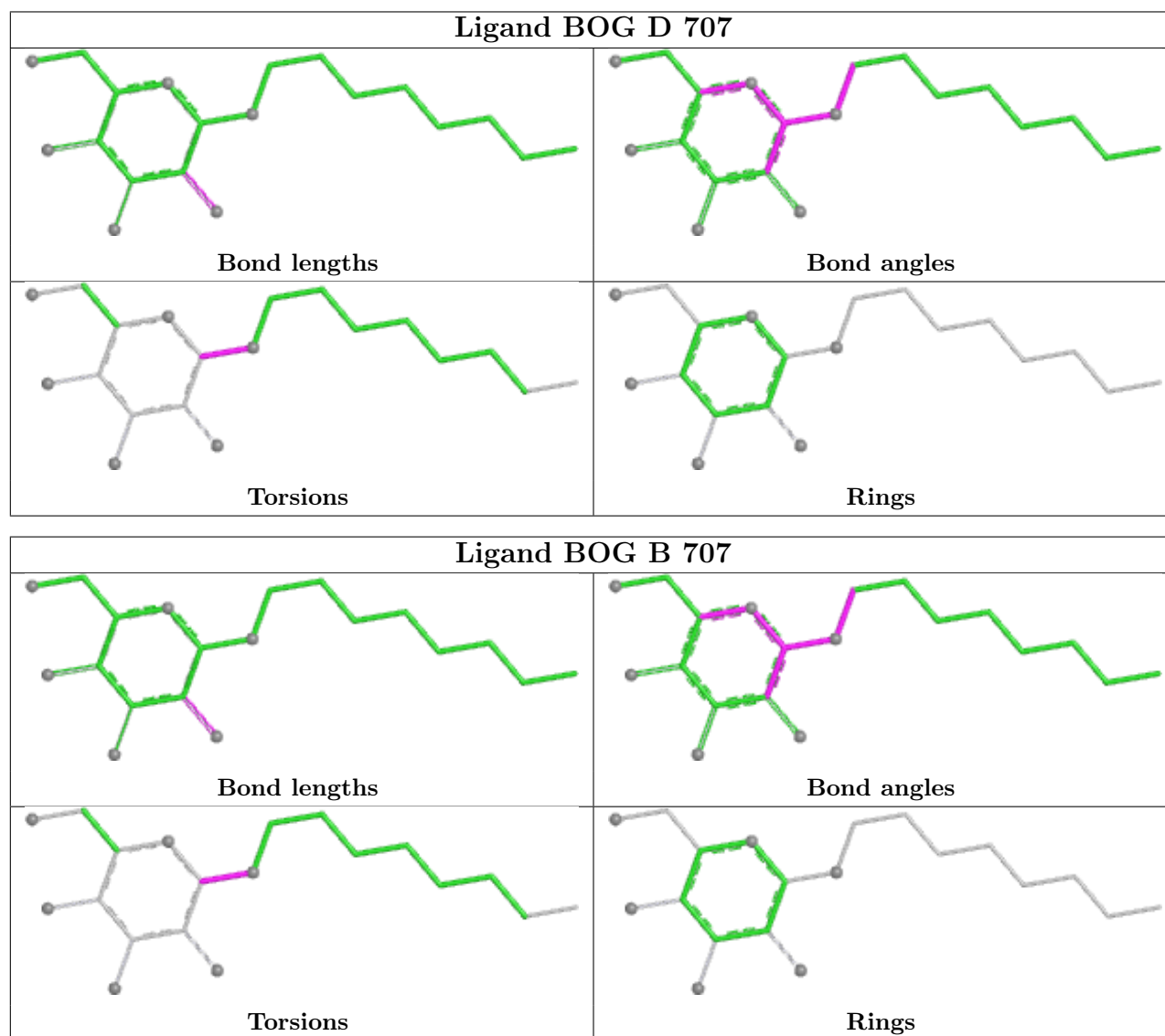
There are no ring outliers.

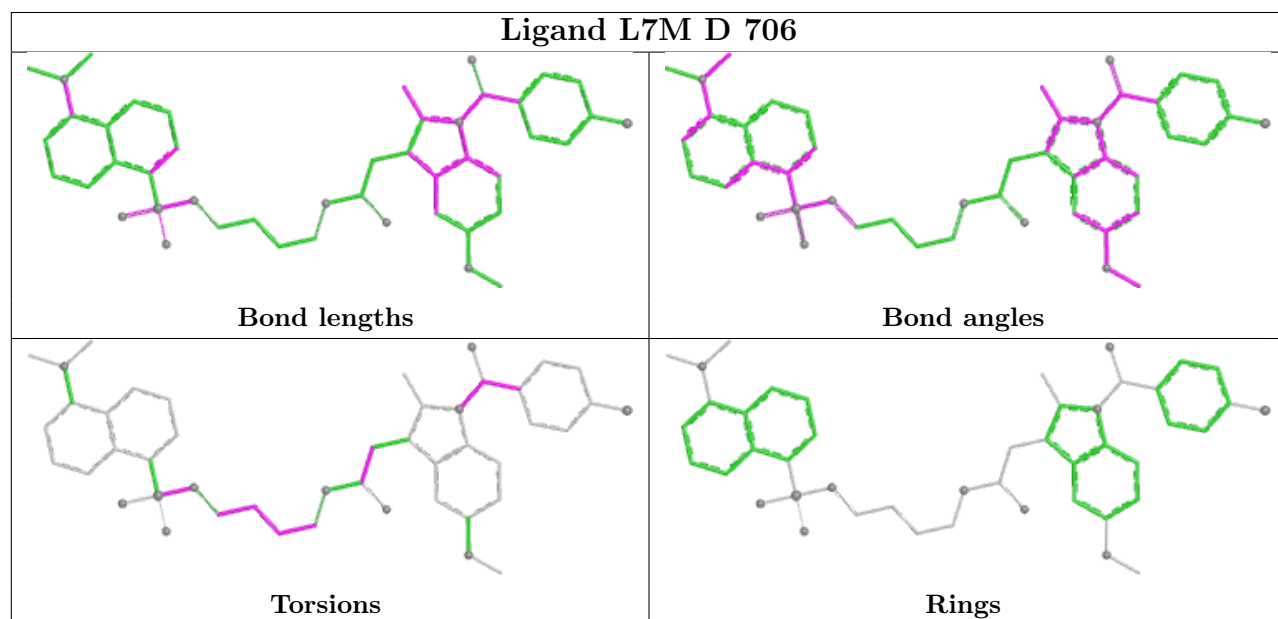
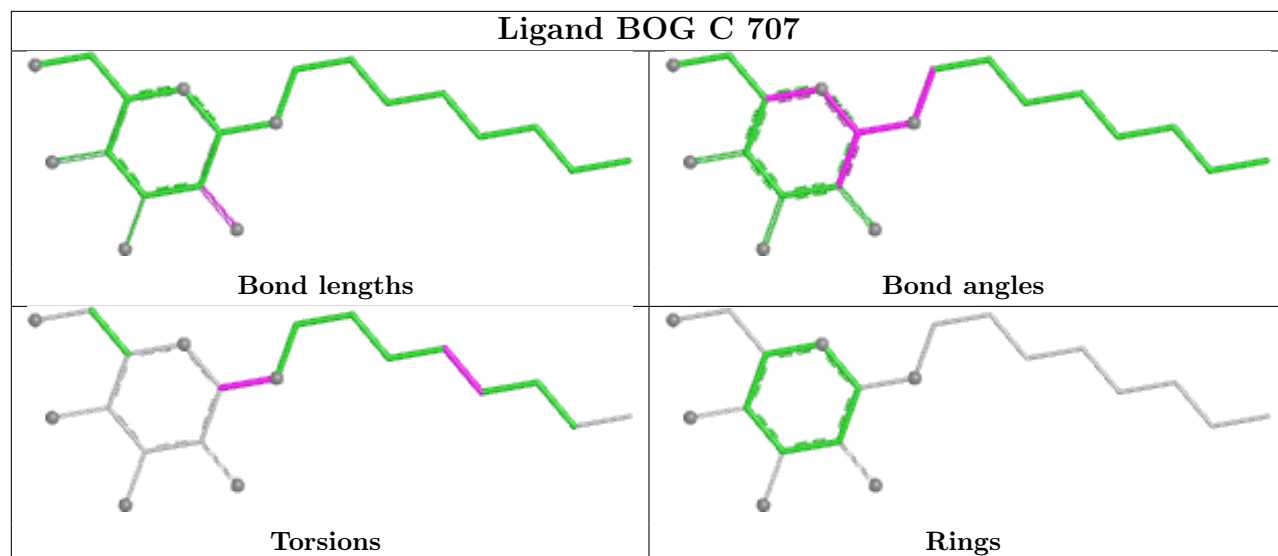
15 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	707	BOG	1	0
6	B	707	BOG	1	0
3	D	701	NAG	1	0
6	C	707	BOG	1	0
3	B	701	NAG	1	0
4	B	705	HEM	3	0
4	D	705	HEM	2	0
6	A	708	BOG	10	0
3	A	701	NAG	2	0
4	A	705	HEM	2	0
6	A	707	BOG	1	0
5	C	706	L7M	2	0
3	C	701	NAG	1	0
6	C	708	BOG	1	0
4	C	705	HEM	3	0

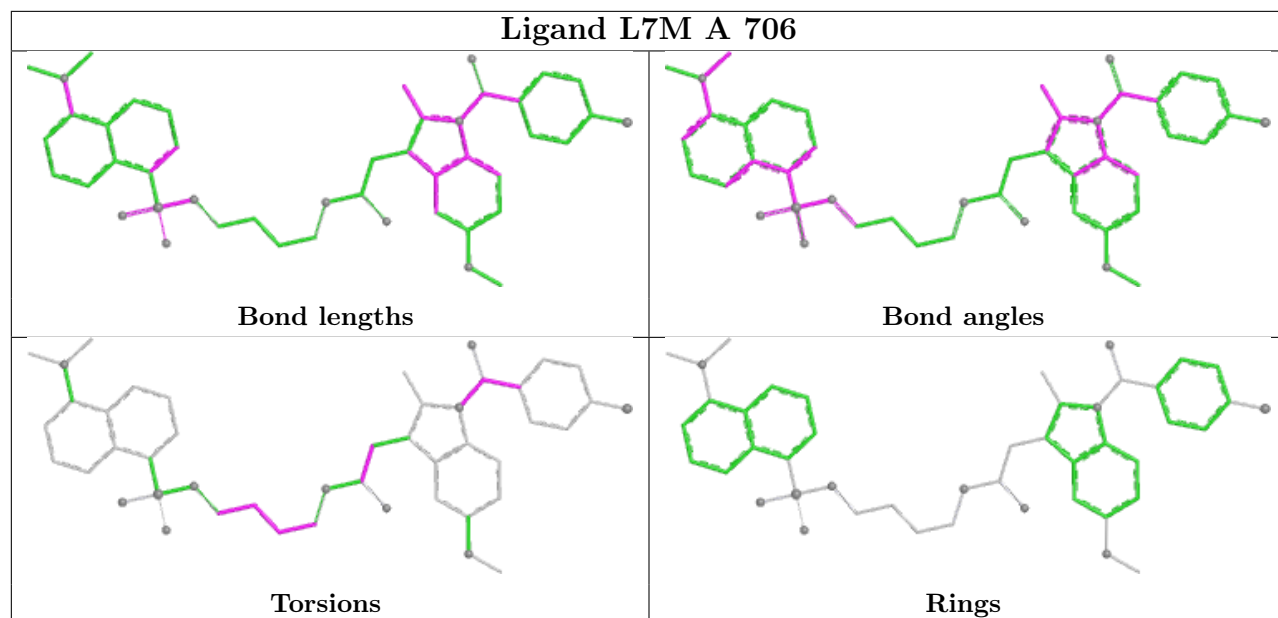
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

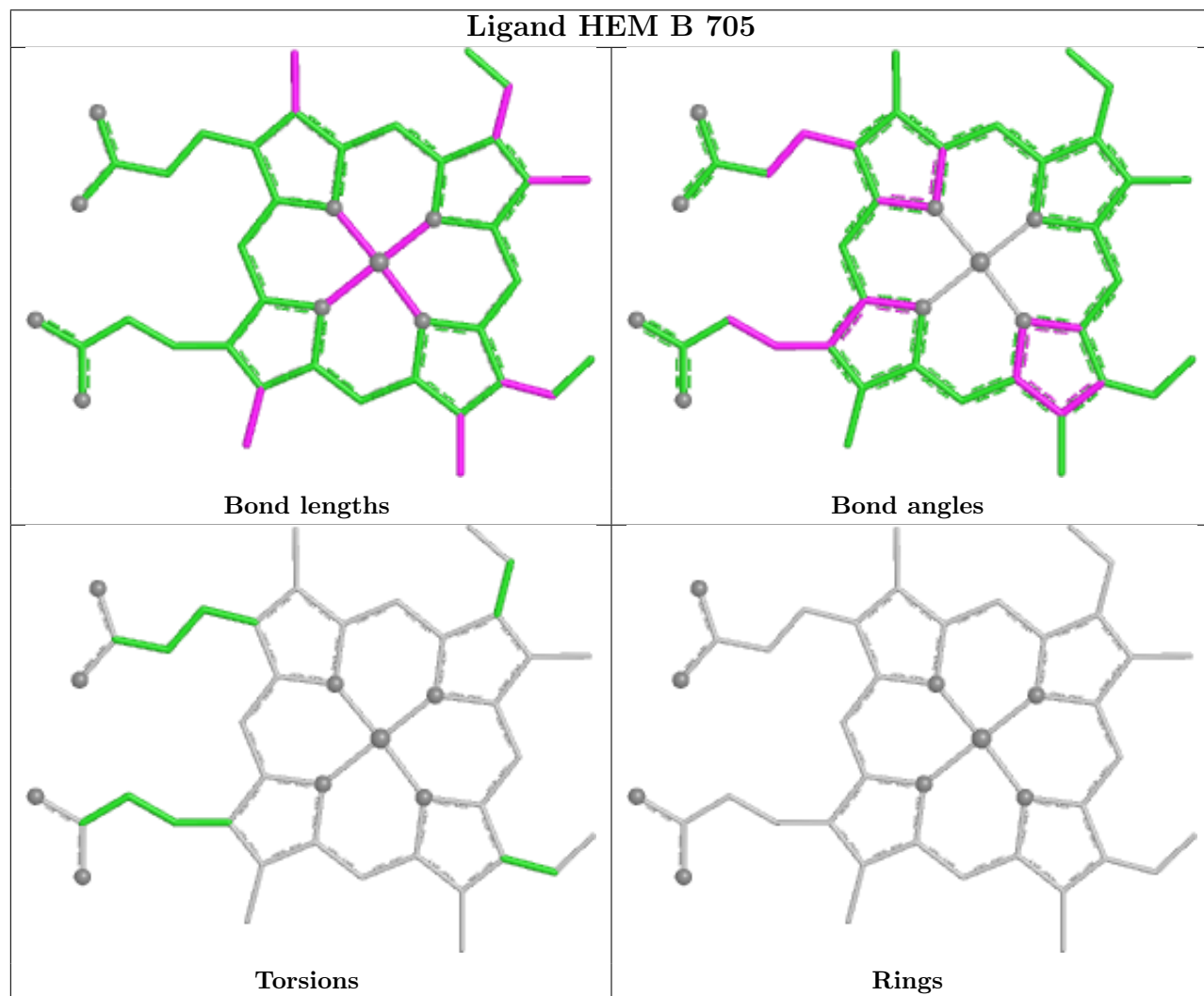




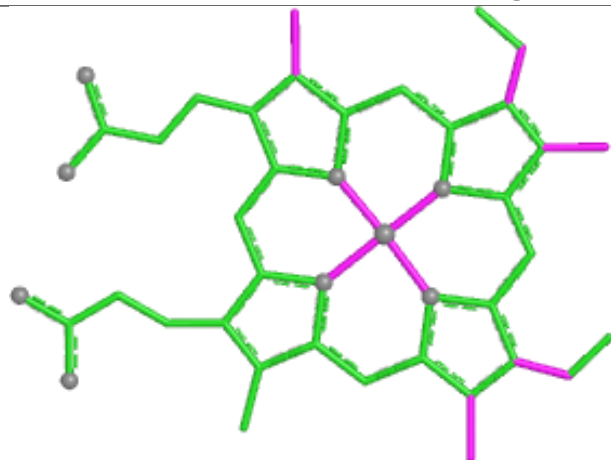
Ligand L7M A 706



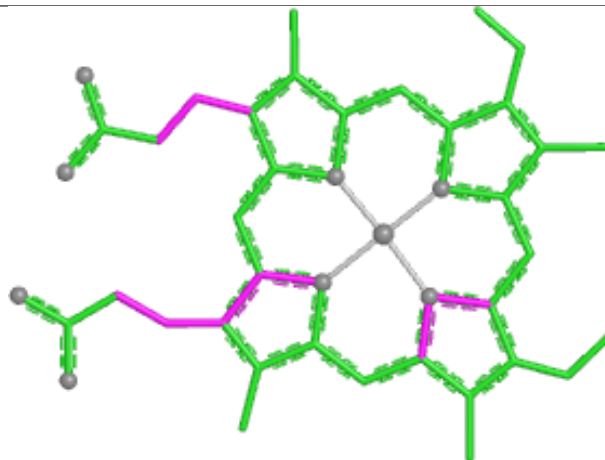
Ligand HEM B 705



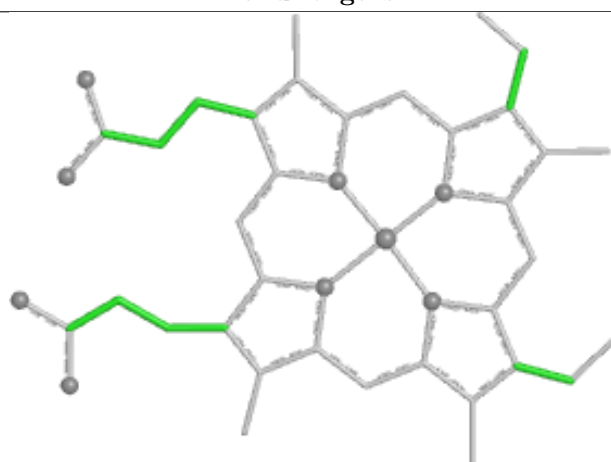
Ligand HEM D 705



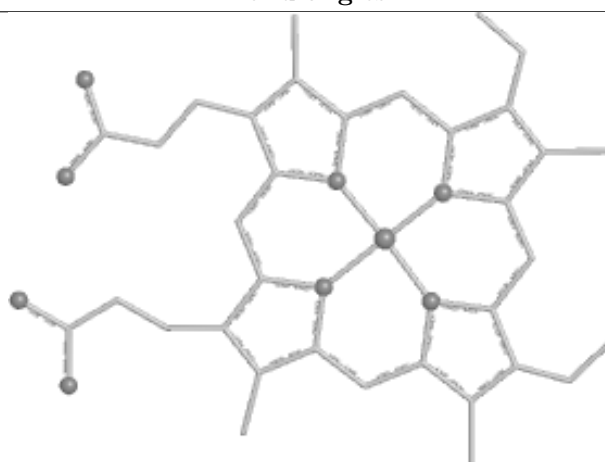
Bond lengths



Bond angles

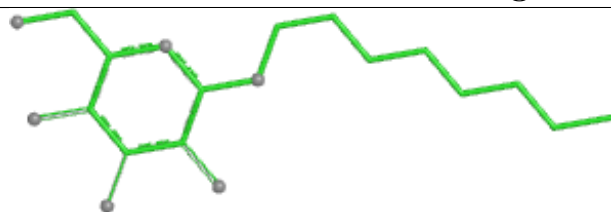


Torsions

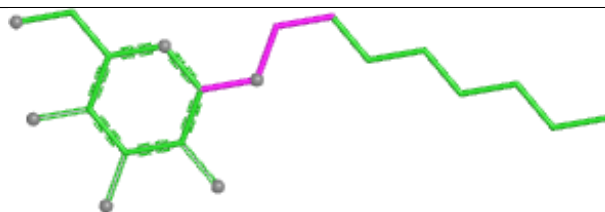


Rings

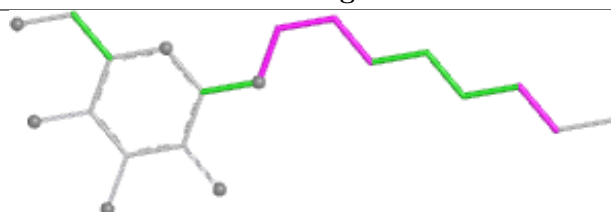
Ligand BOG A 708



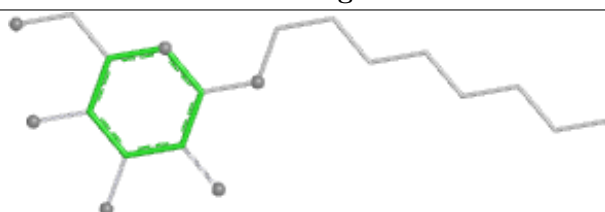
Bond lengths



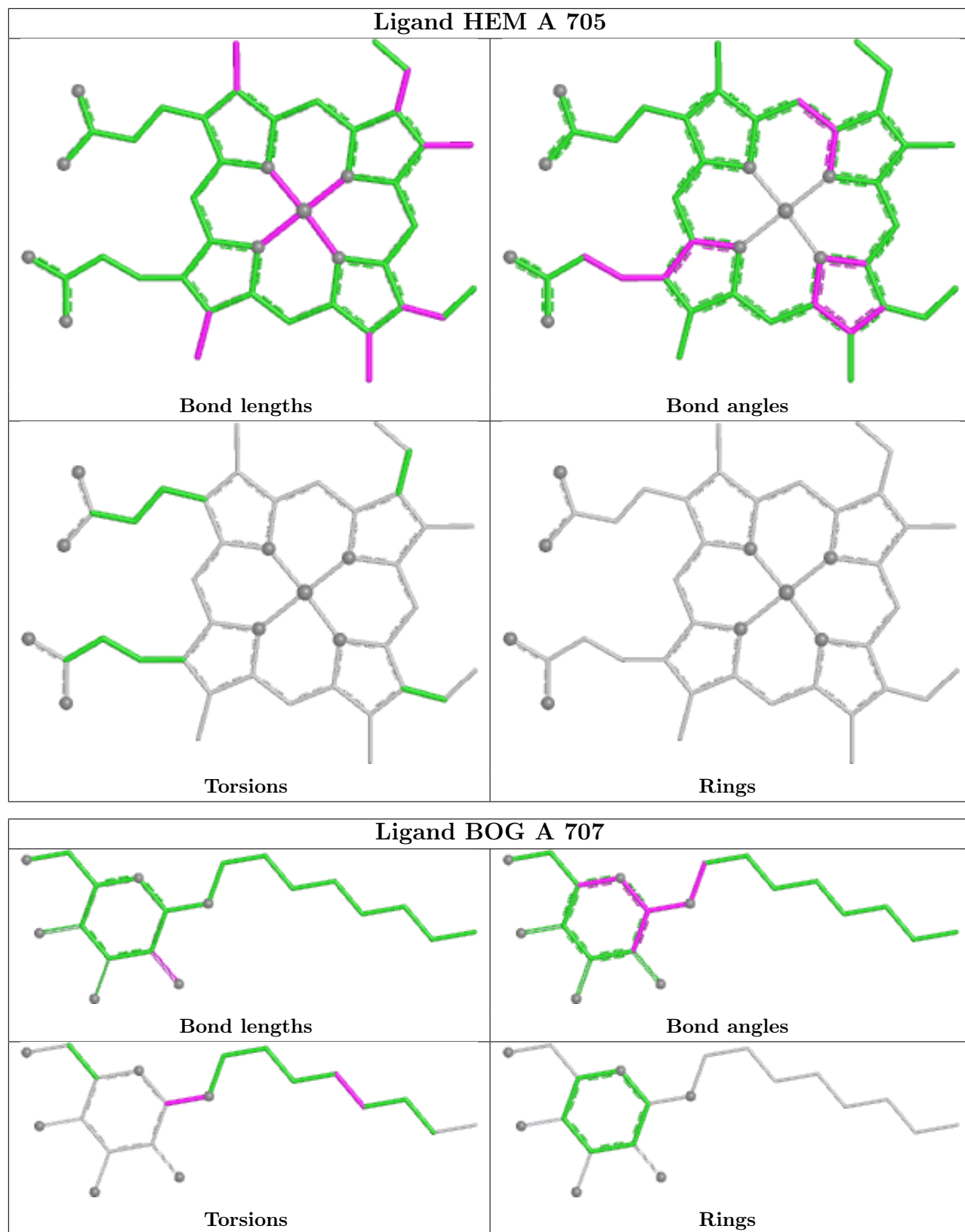
Bond angles



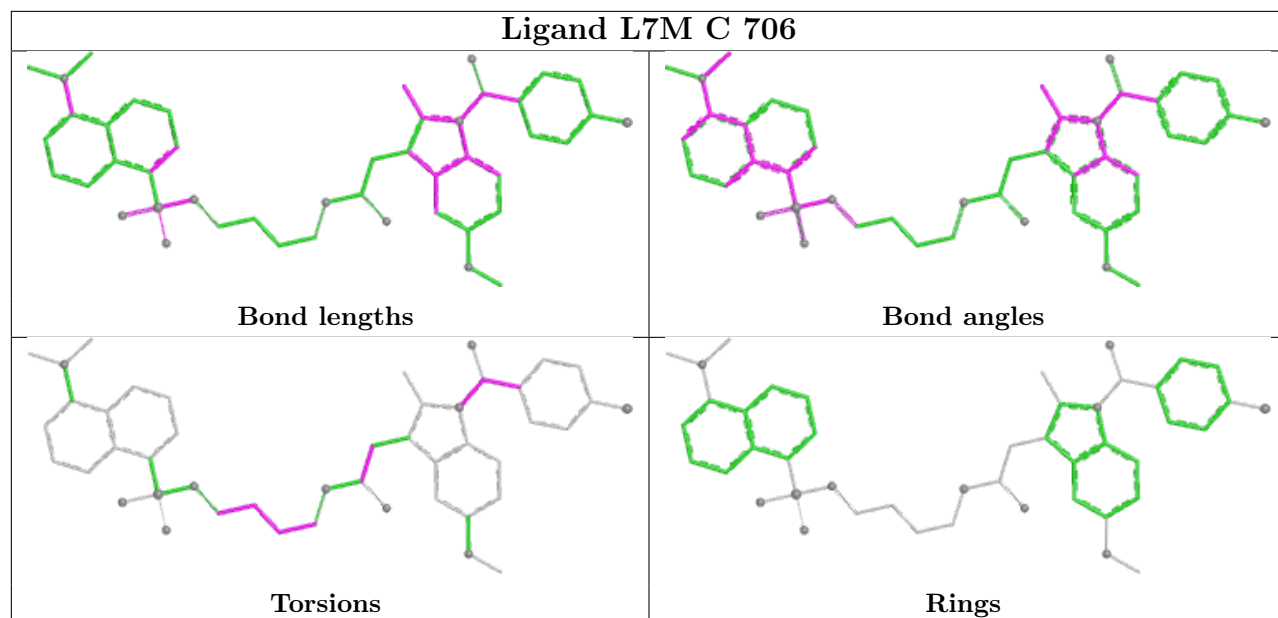
Torsions



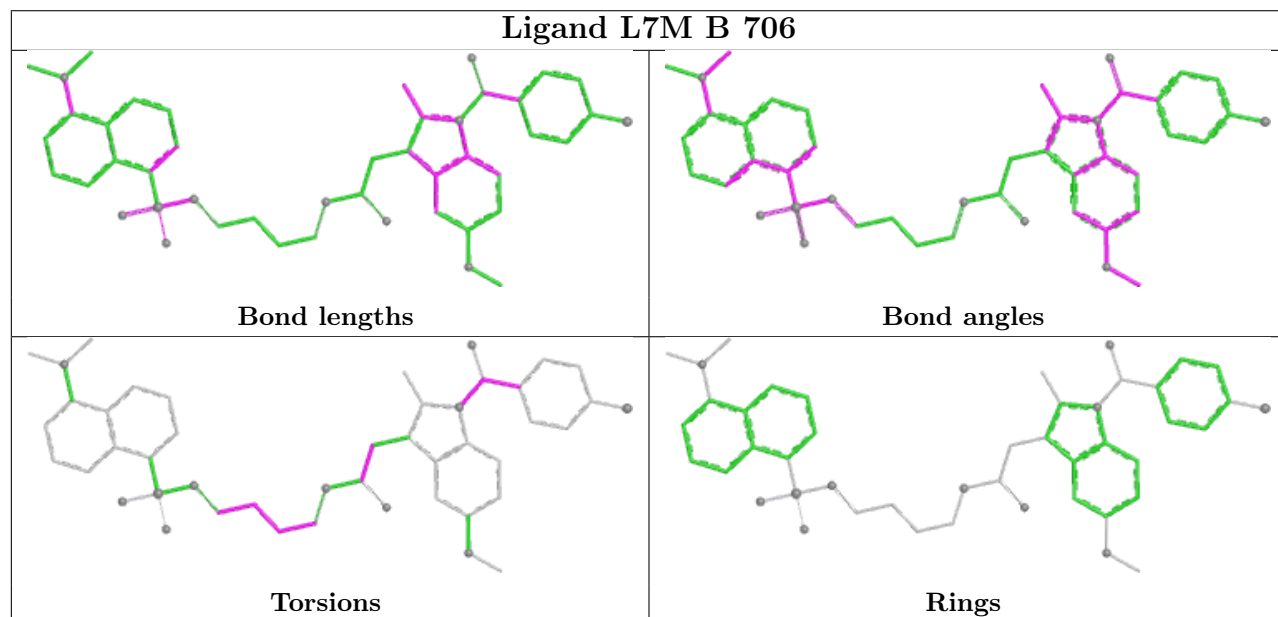
Rings

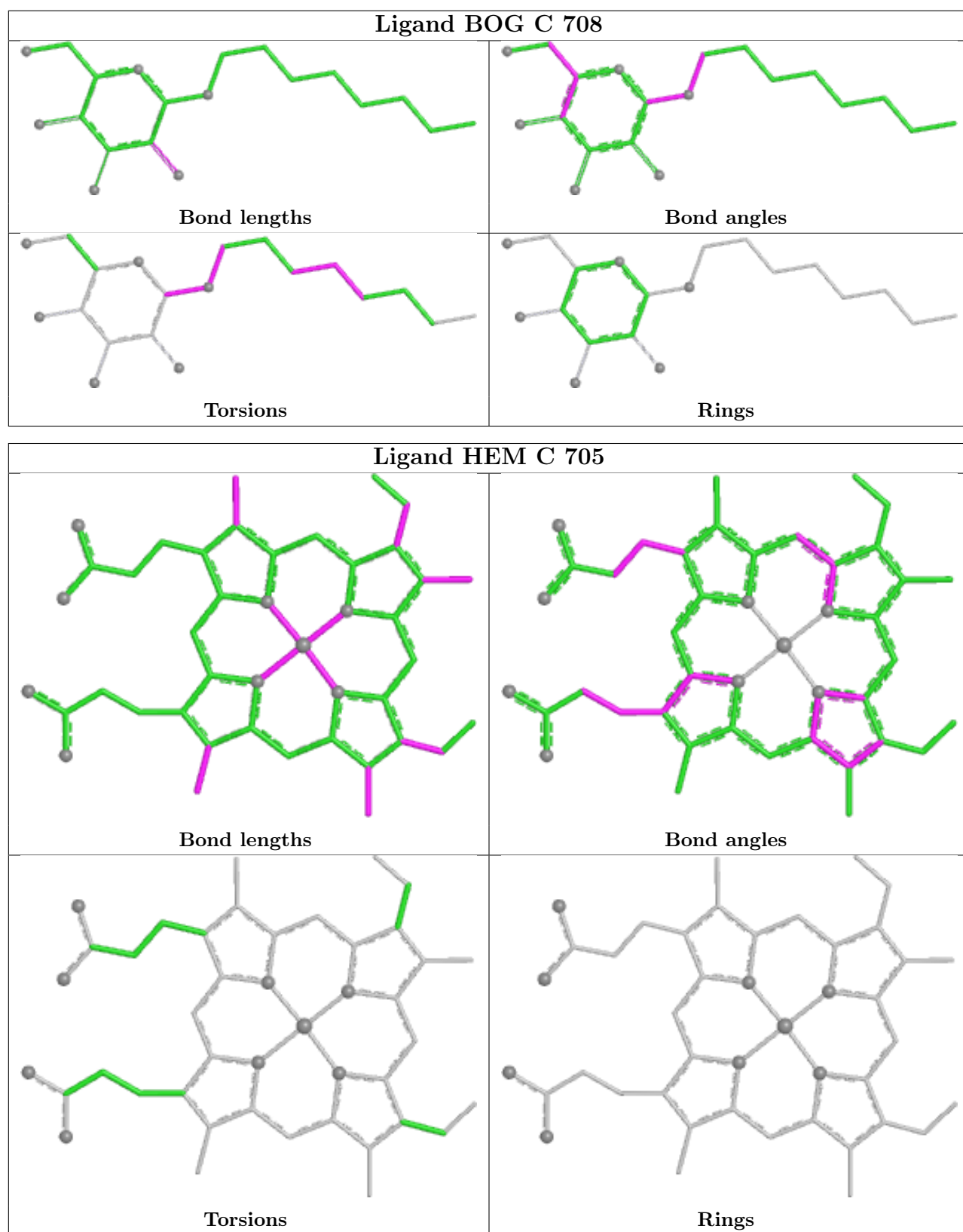


Ligand L7M C 706



Ligand L7M B 706





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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	552/587 (94%)	0.28	14 (2%) 58 56	26, 40, 65, 81	0
1	B	552/587 (94%)	0.48	21 (3%) 44 41	26, 42, 69, 86	0
1	C	552/587 (94%)	0.43	21 (3%) 44 41	29, 44, 69, 86	0
1	D	552/587 (94%)	0.45	20 (3%) 46 43	27, 40, 65, 84	0
All	All	2208/2348 (94%)	0.41	76 (3%) 48 45	26, 42, 68, 86	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	TYR	5.1
1	C	121	SER	4.4
1	C	352	LEU	4.3
1	D	121	SER	4.1
1	D	33	ALA	4.0
1	D	122	TYR	4.0
1	B	121	SER	3.9
1	A	121	SER	3.8
1	C	107	PHE	3.6
1	A	107	PHE	3.5
1	B	74	PHE	3.5
1	B	583	GLN	3.5
1	C	409	TYR	3.4
1	B	268	ASP	3.3
1	C	295	VAL	3.3
1	B	107	PHE	3.3
1	B	120	ARG	3.2
1	C	33	ALA	3.1
1	A	409	TYR	3.1
1	C	122	TYR	3.1
1	A	122	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	107	PHE	3.1
1	C	173	ASP	3.0
1	A	352	LEU	3.0
1	A	33	ALA	3.0
1	D	120	ARG	2.8
1	D	268	ASP	2.8
1	A	281	GLU	2.8
1	B	176	GLU	2.7
1	D	583	GLN	2.7
1	C	294	LEU	2.7
1	A	120	ARG	2.6
1	B	33	ALA	2.6
1	B	267	LYS	2.6
1	B	282	ASN	2.6
1	C	404	PHE	2.6
1	B	409	TYR	2.6
1	A	583	GLN	2.6
1	C	583	GLN	2.6
1	D	294	LEU	2.6
1	D	82	LEU	2.5
1	B	352	LEU	2.5
1	C	170	GLU	2.4
1	D	102	ILE	2.4
1	D	416	GLU	2.4
1	A	295	VAL	2.4
1	C	384	LEU	2.4
1	D	75	LEU	2.4
1	A	80	LEU	2.3
1	C	281	GLU	2.3
1	B	81	LEU	2.3
1	B	82	LEU	2.3
1	B	53	ASP	2.2
1	C	74	PHE	2.2
1	A	575	CYS	2.2
1	C	278	HIS	2.2
1	D	352	LEU	2.2
1	D	176	GLU	2.2
1	D	74	PHE	2.2
1	C	75	LEU	2.1
1	D	186	GLU	2.1
1	C	270	GLN	2.1
1	A	102	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	81	LEU	2.1
1	B	401	GLU	2.1
1	B	407	PHE	2.1
1	D	280	PRO	2.1
1	C	53	ASP	2.1
1	D	404	PHE	2.1
1	D	222	ARG	2.1
1	D	123	LEU	2.1
1	C	158	ASP	2.1
1	B	404	PHE	2.1
1	B	278	HIS	2.0
1	B	59	CYS	2.0
1	A	559	ILE	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](#)

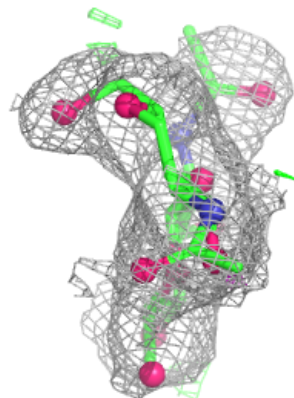
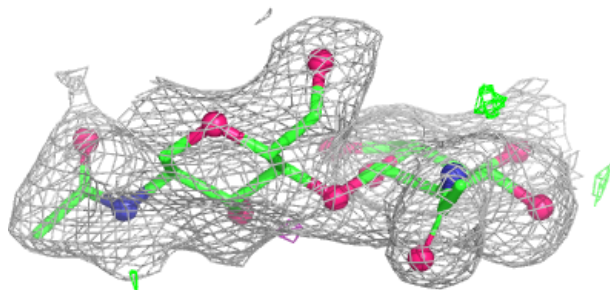
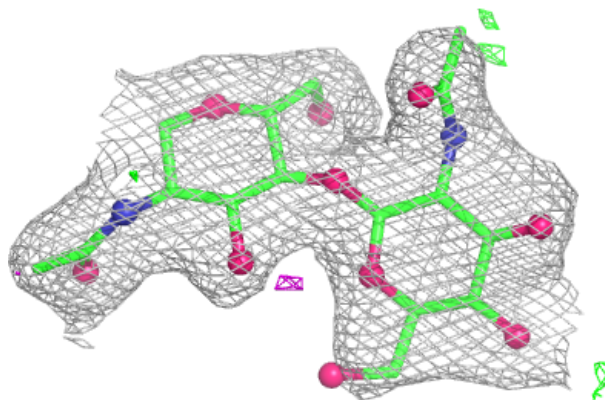
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	F	2	14/15	0.78	0.16	55,62,73,79	0
2	NAG	G	2	14/15	0.84	0.13	60,66,73,75	0
2	NAG	H	2	14/15	0.84	0.15	56,64,70,75	0
2	NAG	E	2	14/15	0.87	0.13	54,61,71,74	0
2	NAG	H	1	14/15	0.92	0.10	34,46,50,56	0
2	NAG	F	1	14/15	0.93	0.10	31,40,48,54	0
2	NAG	G	1	14/15	0.95	0.07	33,39,48,53	0
2	NAG	E	1	14/15	0.95	0.08	31,38,42,49	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.

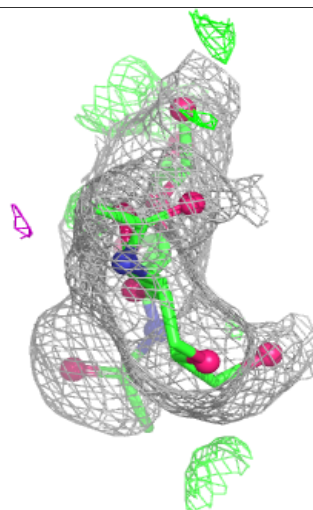
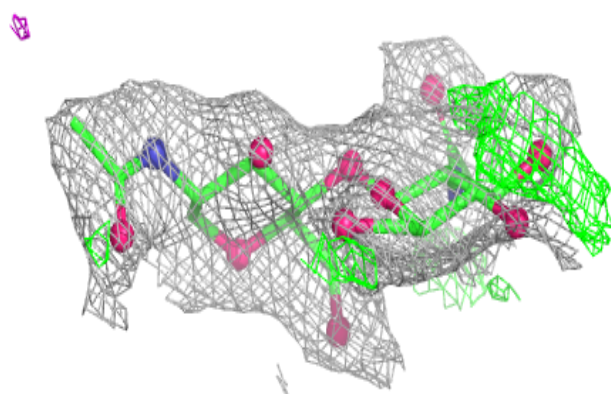
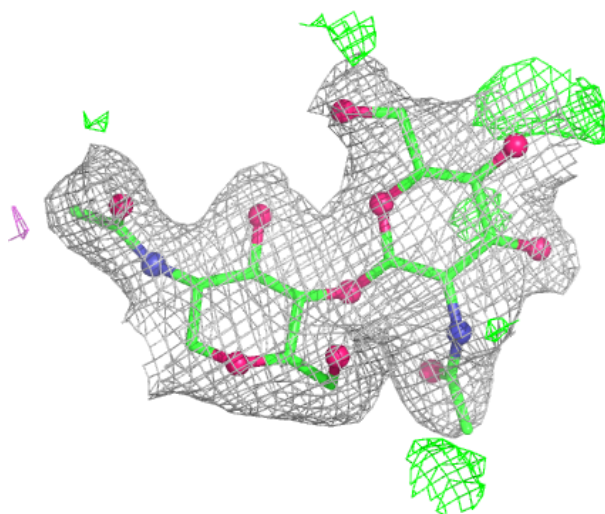
Electron density around Chain E:

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



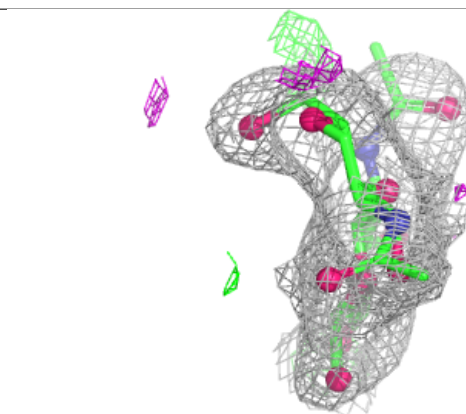
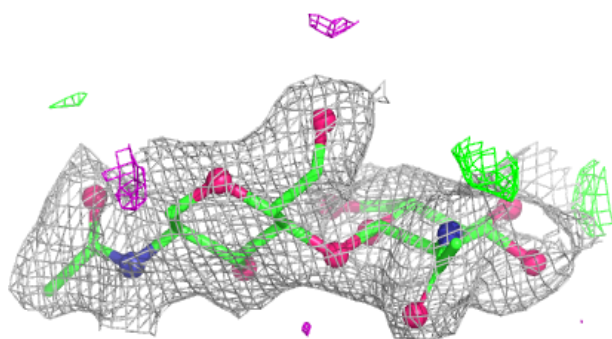
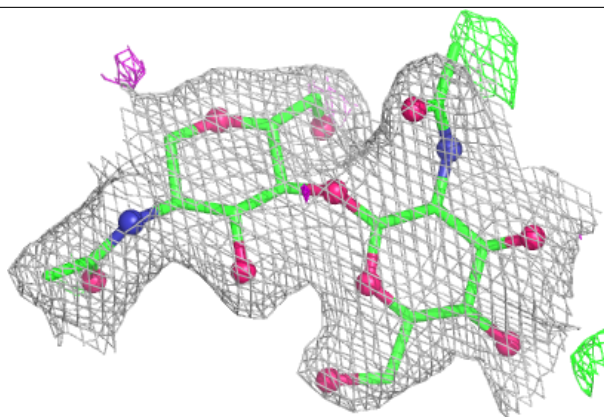
Electron density around Chain F:

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

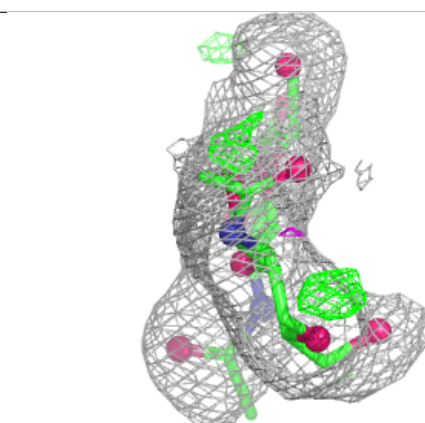
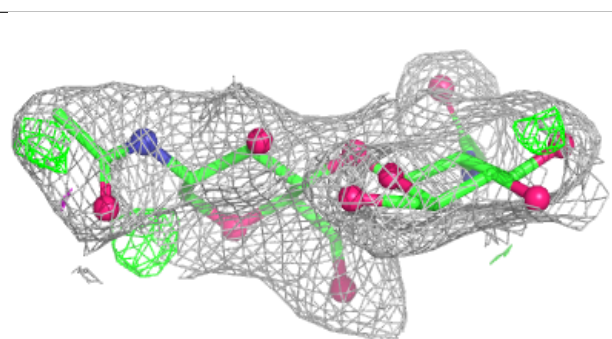
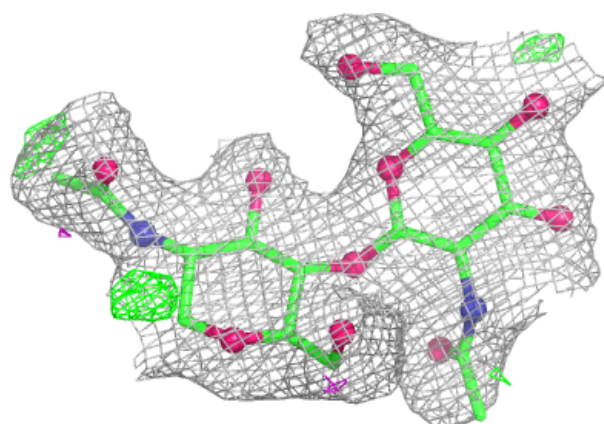


Electron density around Chain G:

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

**Electron density around Chain H:**

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



6.4 Ligands

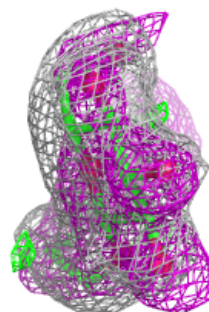
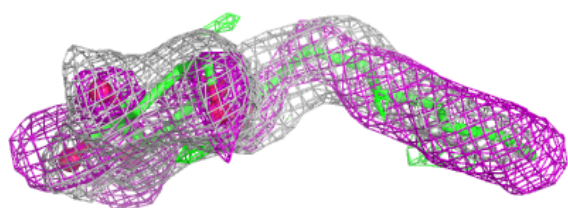
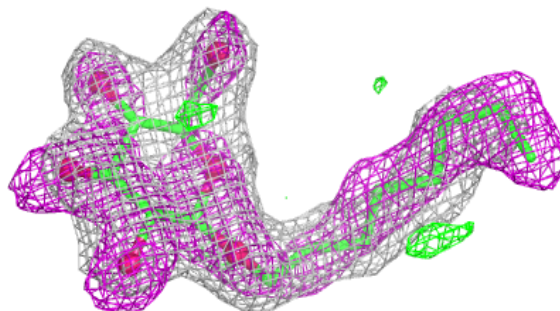
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	701	14/15	0.69	0.16	65,78,85,86	0
3	NAG	C	701	14/15	0.72	0.15	60,71,80,80	0
3	NAG	D	701	14/15	0.73	0.16	62,74,82,83	0
3	NAG	B	704	14/15	0.74	0.16	59,72,78,83	0
3	NAG	A	701	14/15	0.78	0.15	61,73,79,84	0
3	NAG	C	704	14/15	0.79	0.16	53,72,77,83	0
3	NAG	A	704	14/15	0.82	0.13	53,70,74,76	0
6	BOG	A	708	20/20	0.83	0.12	20,20,20,20	0
6	BOG	D	707	20/20	0.84	0.15	57,74,79,80	0
6	BOG	B	707	20/20	0.85	0.13	56,73,80,81	0
3	NAG	D	704	14/15	0.86	0.11	49,59,69,74	0
6	BOG	C	708	20/20	0.87	0.22	22,26,33,37	20
6	BOG	A	707	20/20	0.88	0.12	51,70,73,74	0
6	BOG	C	707	20/20	0.88	0.10	56,73,81,82	0
5	L7M	D	706	46/46	0.91	0.14	34,51,76,81	0
5	L7M	B	706	46/46	0.92	0.14	37,53,81,84	0
5	L7M	C	706	46/46	0.92	0.14	32,59,78,84	0
5	L7M	A	706	46/46	0.92	0.12	36,51,78,80	0
4	HEM	A	705	43/43	0.95	0.11	28,37,53,77	0
4	HEM	C	705	43/43	0.95	0.11	29,38,59,79	0
4	HEM	B	705	43/43	0.96	0.10	25,36,54,69	0
4	HEM	D	705	43/43	0.96	0.09	22,35,53,77	0

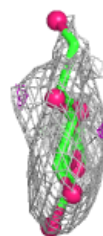
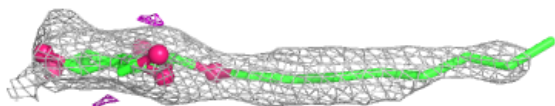
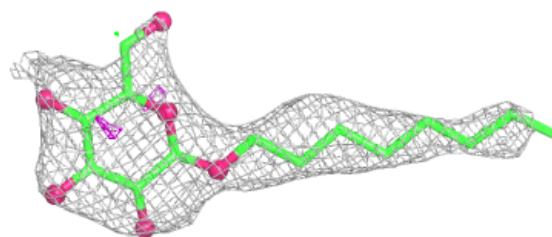
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG A 708:

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

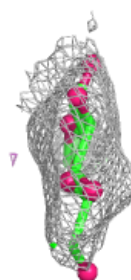
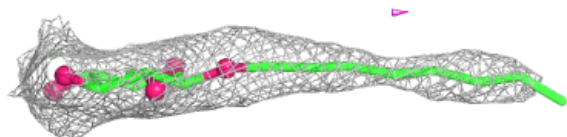
**Electron density around BOG D 707:**

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

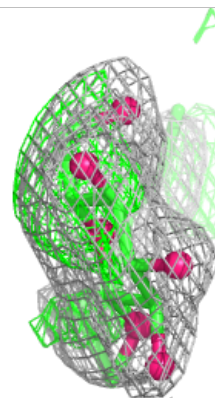
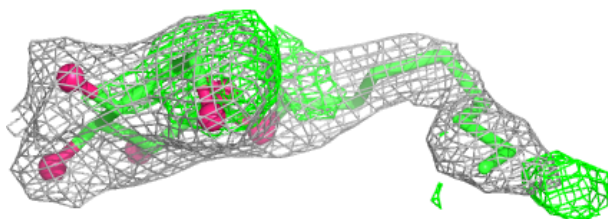
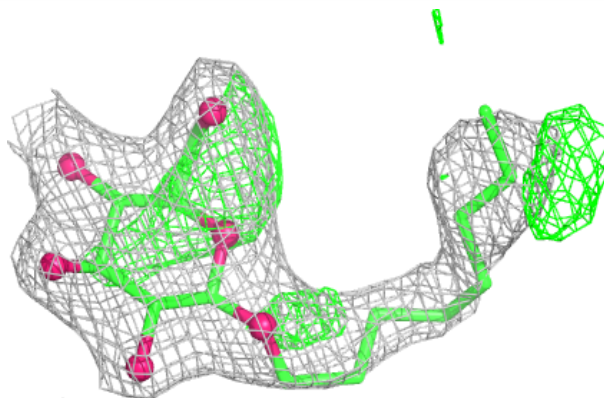


Electron density around BOG B 707:

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

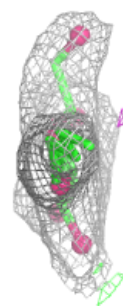
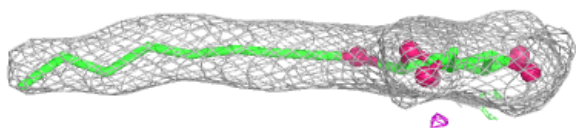
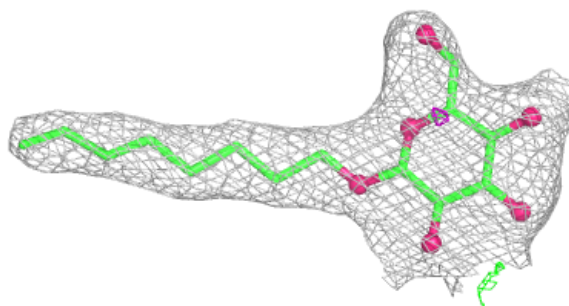
**Electron density around BOG C 708:**

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

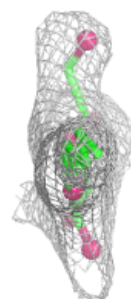
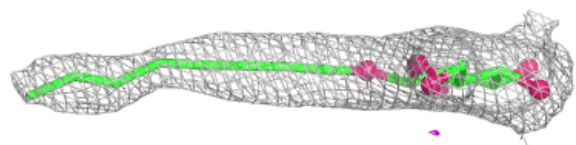
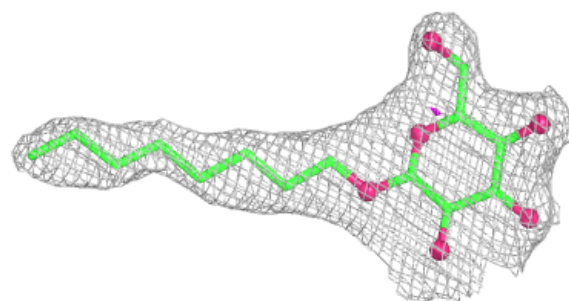


Electron density around BOG A 707:

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

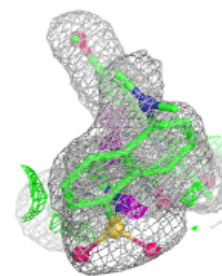
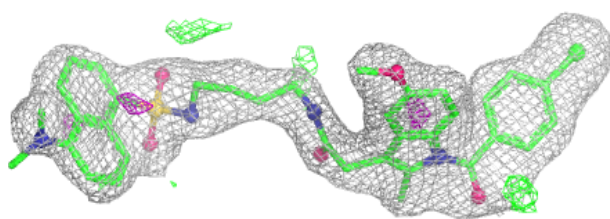
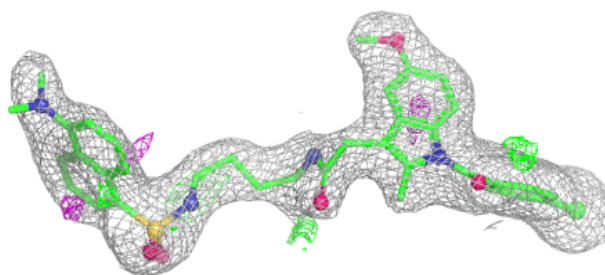
**Electron density around BOG C 707:**

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

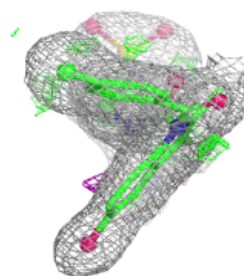
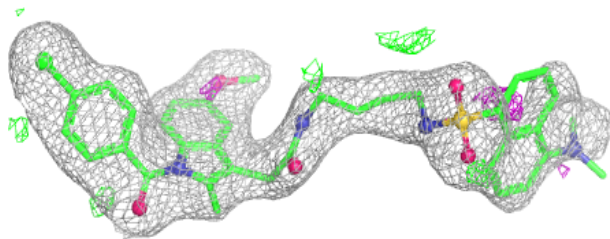
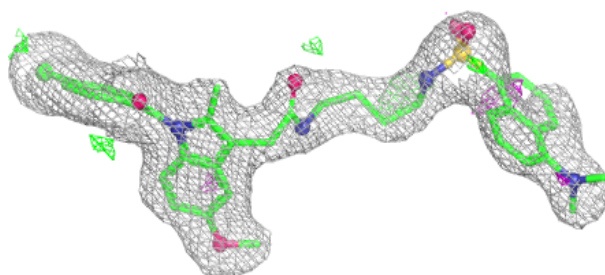


Electron density around L7M D 706:

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

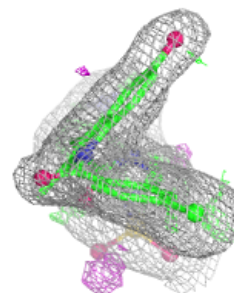
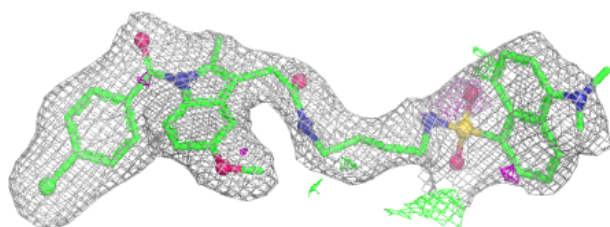
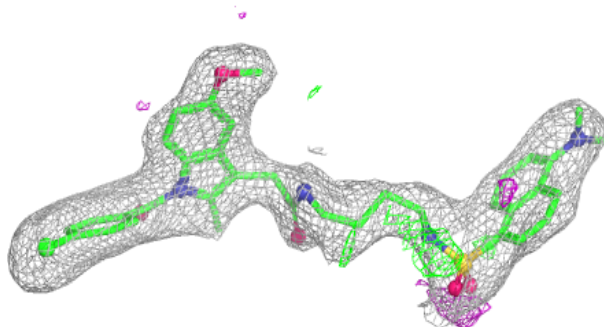
**Electron density around L7M B 706:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

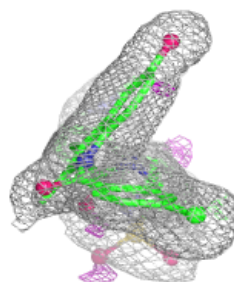
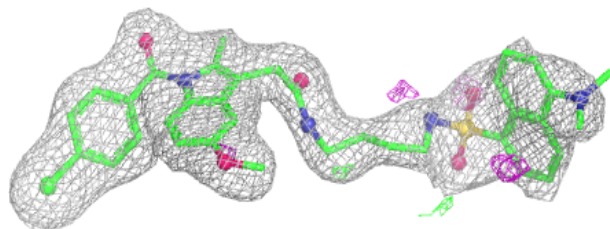
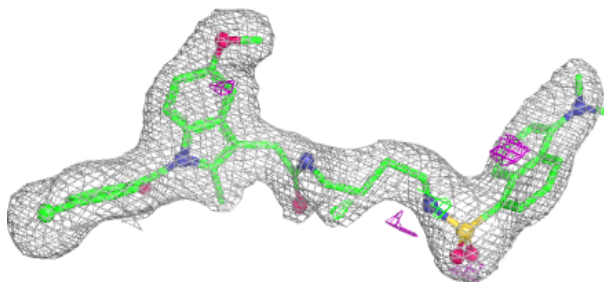


Electron density around L7M C 706:

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

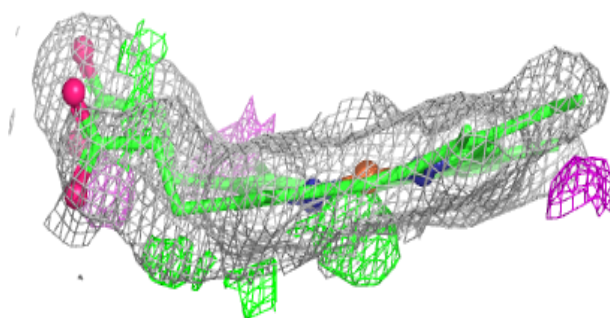
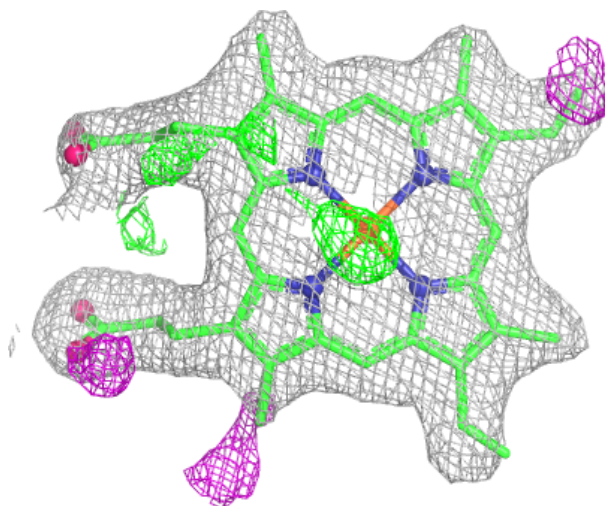
**Electron density around L7M A 706:**

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



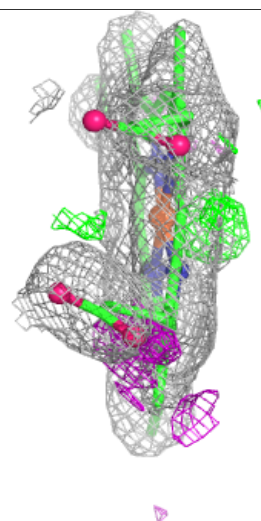
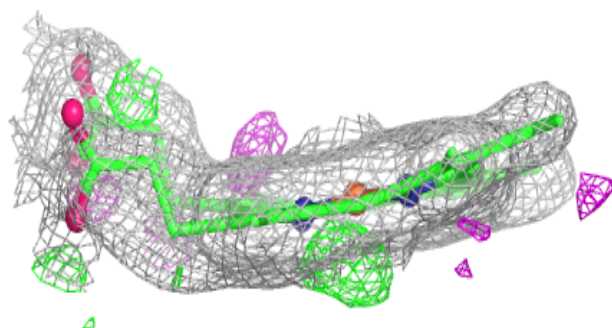
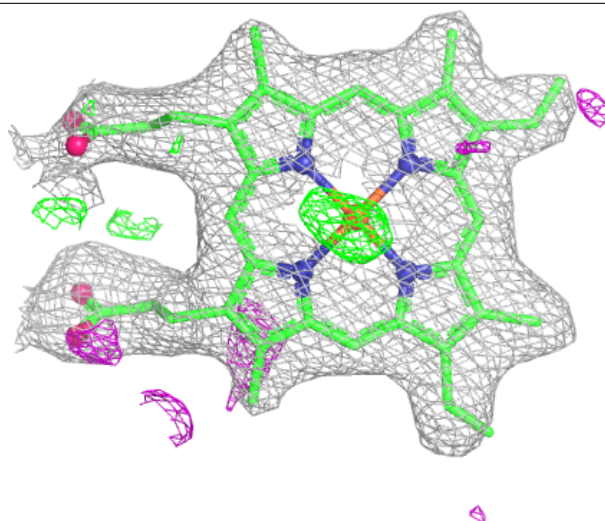
Electron density around HEM A 705:

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



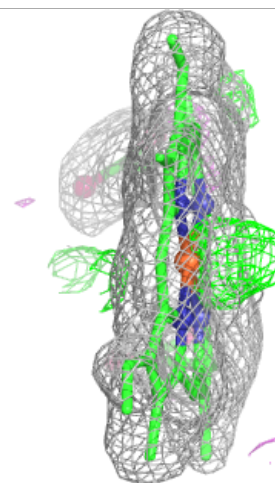
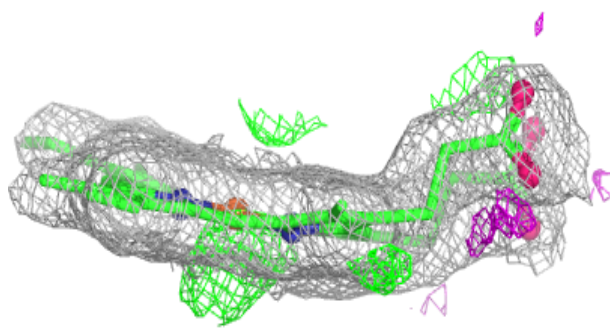
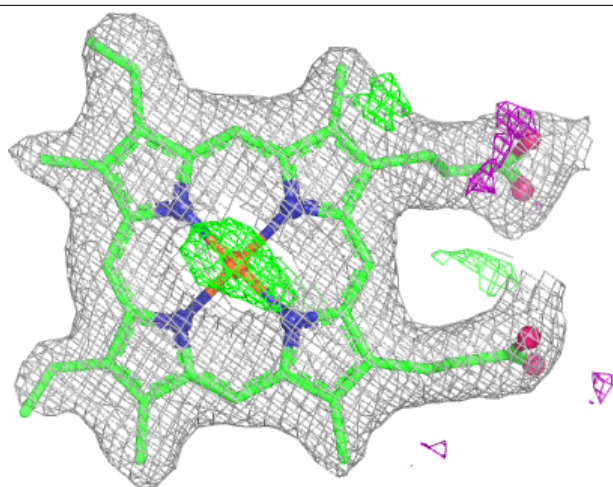
Electron density around HEM C 705:

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



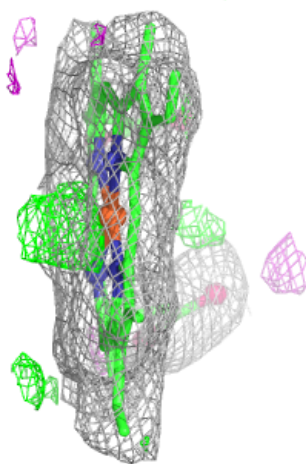
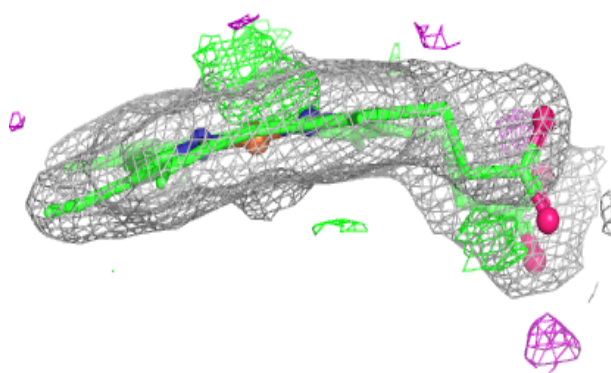
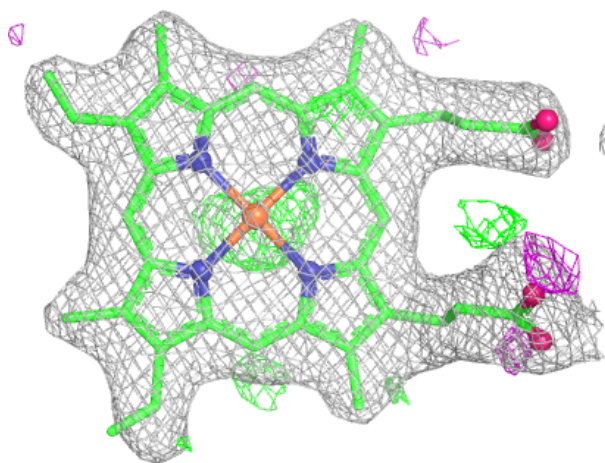
Electron density around HEM B 705:

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



Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.