



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 06:16 PM EDT

PDB ID : 5QJ3 / pdb_00005qj3
Title : CRYSTAL STRUCTURE OF MYELOPEROXIDASE SUBFORM C (MPO)
COMPLEX WITH COMPOUND-24 AKA 7-({4-CHLORO-3'-FLUORO-[1,1
'- BIPHENYL]-3-YL} METHOXY)-3H-[1,2,3]TRIAZOLO[4,5-B]PYRIDIN-
5-AMINE
Authors : Khan, J.A.
Deposited on : 2018-09-26
Resolution : 2.76 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](#) ①) were used in the production of this report:

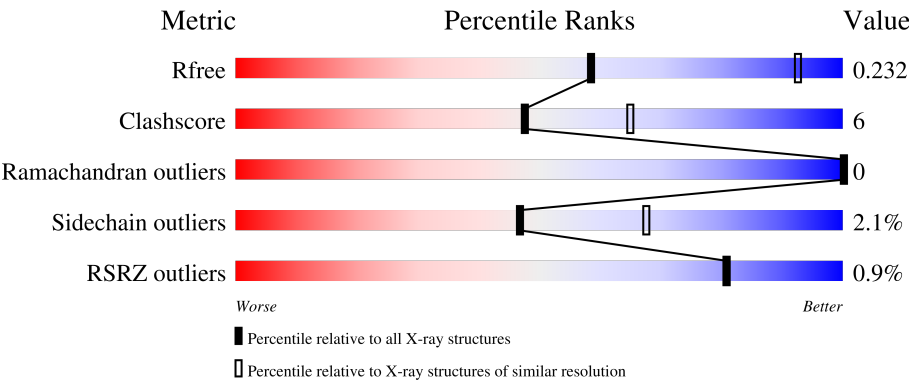
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	105	% 80% 17% ••
1	D	105	% 85% 12% ••
2	B	467	% 86% 12% ••
2	E	467	% 87% 11% •
3	C	2	100%

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Mol	Chain	Length	Quality of chain
3	G	2	 50% 50%
4	F	6	 50% 33% 17%
4	H	6	 67% 33%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9480 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 Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			818	519	145	149	5			
1	D	103	Total	C	N	O	S	0	0	0
			813	517	142	149	5			

- Molecule 2 is a protein called Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	464	Total	C	N	O	S	20	0	0
			3635	2305	652	651	27			
2	E	465	Total	C	N	O	S	31	1	0
			3689	2335	663	663	28			

There are 2 discrepancies between the modelled and reference sequences:

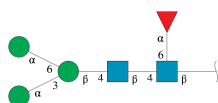
Chain	Residue	Modelled	Actual	Comment	Reference
B	112	ALA	GLY	conflict	UNP P05164
E	112	ALA	GLY	conflict	UNP P05164

- Molecule 3 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
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

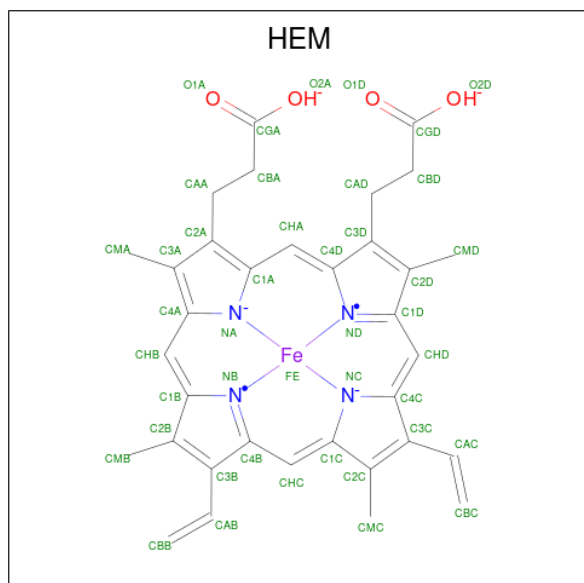


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	6	Total	C	N	O	0	0	0
			71	40	2	29			
4	H	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

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

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

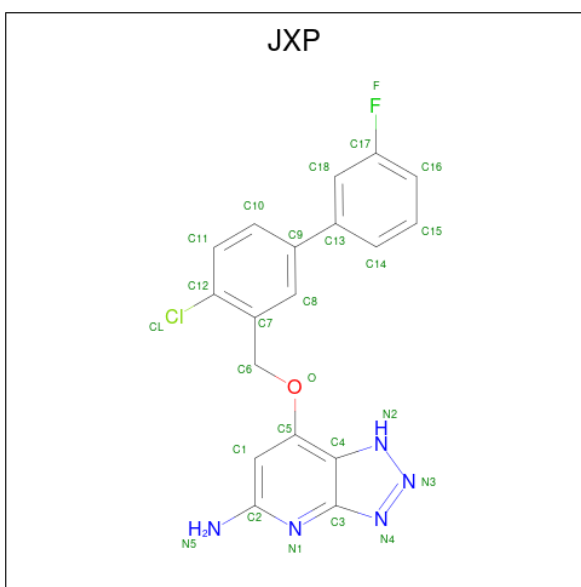


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Ca	0	0
			1	1		
8	E	1	Total	Ca	0	0
			1	1		

- Molecule 9 is 7-[(4-chloro-3'-fluoro[1,1'-biphenyl]-3-yl)methoxy]-1H-[1,2,3]triazolo[4,5-b]pyridin-5-amine (CCD ID: JXP) (formula: $C_{18}H_{13}ClFN_5O$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	Cl	F	N	O	0	1
			33	24	1	2	5	1		

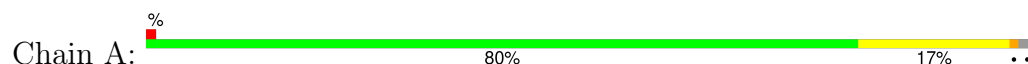
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	17	Total	O	0	0
			17	17		
10	B	66	Total	O	0	0
			66	66		
10	D	19	Total	O	0	0
			19	19		
10	E	74	Total	O	0	0
			74	74		

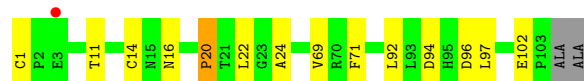
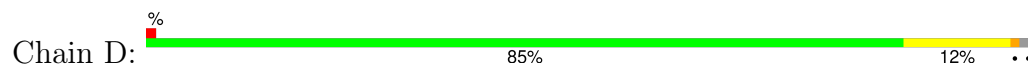
3 Residue-property plots [i](#)

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.

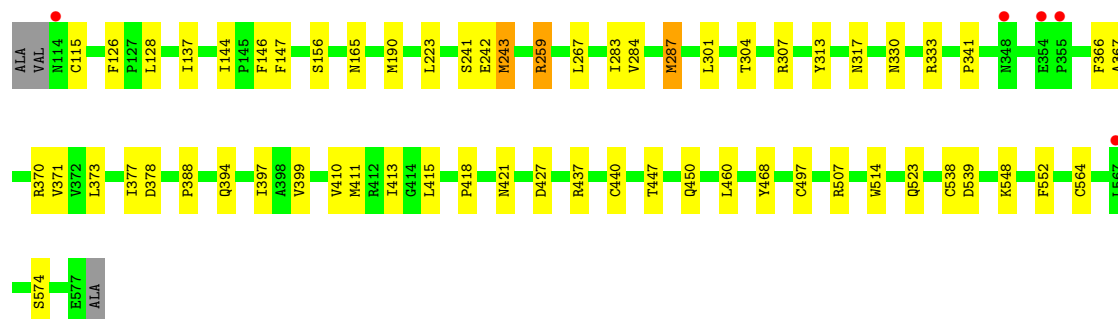
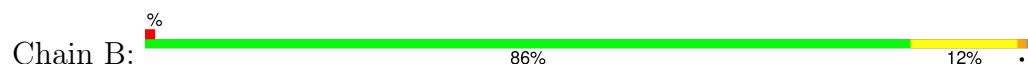
- Molecule 1: Myeloperoxidase



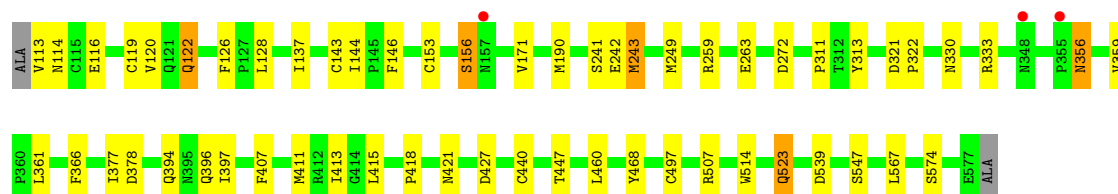
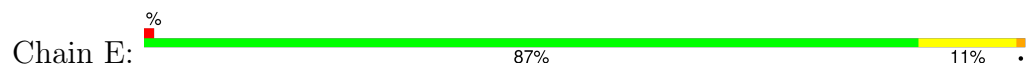
- Molecule 1: Myeloperoxidase



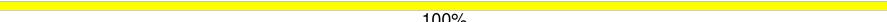
- Molecule 2: Myeloperoxidase



- Molecule 2: Myeloperoxidase



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

Chain C:  100%

MAG1
MAG2

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

Chain G:  50% 50%

MAG1
MAG2

- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 33% 17%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  67% 33%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.54Å 106.54Å 238.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.44 – 2.76 38.44 – 2.76	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.44-2.76) 99.9 (38.44-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.19 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.184 , 0.228 0.187 , 0.232	Depositor DCC
R_{free} test set	1815 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9480	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, CL, CA, JXP, FUC, HEM, 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	0.82	0/843	1.27	4/1150 (0.3%)
1	D	0.78	0/838	1.27	3/1144 (0.3%)
2	B	0.86	2/3721 (0.1%)	1.27	15/5059 (0.3%)
2	E	0.86	0/3774	1.28	10/5126 (0.2%)
All	All	0.85	2/9176 (0.0%)	1.27	32/12479 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	287	MET	SD-CE	-6.44	1.63	1.79
2	B	243	MET	SD-CE	-6.02	1.64	1.79

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	20	PRO	N-CA-C	6.60	122.43	113.84
1	D	96	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	20	PRO	N-CA-C	6.34	122.08	113.84
2	E	397	ILE	N-CA-C	6.19	116.24	110.42
2	E	272	ASP	CA-CB-CG	6.13	118.73	112.60
2	B	156	SER	N-CA-C	5.93	118.94	110.10
1	A	96	ASP	CA-CB-CG	5.89	118.49	112.60
1	D	96	ASP	N-CA-C	-5.82	106.34	113.50
2	E	156	SER	N-CA-C	5.82	118.80	110.24
1	A	71	PHE	CA-CB-CG	5.78	119.58	113.80
1	A	96	ASP	N-CA-C	-5.74	106.44	113.50
2	B	427	ASP	CA-CB-CG	5.65	118.25	112.60
2	B	514	TRP	N-CA-C	5.58	118.09	111.33
2	E	427	ASP	CA-CB-CG	5.56	118.16	112.60
2	B	371	VAL	CA-C-N	5.49	127.48	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	371	VAL	C-N-CA	5.49	127.48	120.56
2	B	437	ARG	CA-C-N	5.49	127.63	120.28
2	B	437	ARG	C-N-CA	5.49	127.63	120.28
2	E	514	TRP	N-CA-C	5.49	117.97	111.33
2	E	377	ILE	N-CA-C	5.49	118.79	111.44
2	B	301	LEU	N-CA-C	5.46	118.41	111.69
2	B	243	MET	CB-CA-C	5.43	117.34	109.20
2	B	377	ILE	N-CA-C	5.34	118.60	111.44
2	E	243	MET	CB-CA-C	5.32	117.16	109.45
2	E	321	ASP	CA-CB-CG	5.31	117.91	112.60
2	B	397	ILE	N-CA-C	5.25	115.35	110.42
2	E	378	ASP	CA-CB-CG	5.18	117.78	112.60
2	B	468	TYR	N-CA-C	5.18	119.87	113.50
2	B	378	ASP	CA-CB-CG	5.09	117.69	112.60
2	B	548	LYS	N-CA-C	-5.07	103.35	110.50
2	B	373	LEU	N-CA-C	5.07	119.56	113.17
2	E	468	TYR	N-CA-C	5.02	119.68	113.50

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	818	0	774	17	0
1	D	813	0	765	13	0
2	B	3635	0	3577	35	0
2	E	3689	0	3661	35	0
3	C	28	0	25	0	0
3	G	28	0	25	0	0
4	F	71	0	61	3	0
4	H	71	0	61	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	43	0	30	7	0
6	E	43	0	30	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	14	0	13	0	0
7	E	14	0	13	0	0
8	B	1	0	0	0	0
8	E	1	0	0	0	0
9	B	33	0	0	1	0
10	A	17	0	0	0	0
10	B	66	0	0	0	0
10	D	19	0	0	0	0
10	E	74	0	0	0	0
All	All	9480	0	9035	91	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 6.

All (91) 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)
2:B:317:ASN:ND2	4:F:1:NAG:C1	1.68	1.54
1:A:94:ASP:OD2	6:B:601:HEM:HMD3	1.33	1.23
1:D:94:ASP:OD2	6:E:601:HEM:HMD3	1.31	1.23
1:D:94:ASP:OD2	6:E:601:HEM:CMD	2.00	1.10
1:A:94:ASP:OD2	6:B:601:HEM:CMD	2.01	1.08
2:B:538:CYS:HG	2:B:564:CYS:HG	1.03	0.91
2:B:242:GLU:OE2	6:B:601:HEM:HMB1	1.72	0.90
2:E:242:GLU:OE2	6:E:601:HEM:HMB1	1.72	0.89
2:E:411:MET:HE1	2:E:415:LEU:HG	1.56	0.87
2:E:243:MET:SD	6:E:601:HEM:HBB1	2.16	0.85
2:E:243:MET:SD	6:E:601:HEM:CBB	2.65	0.85
2:B:317:ASN:CG	4:F:1:NAG:C1	2.50	0.84
1:D:94:ASP:CG	6:E:601:HEM:HMD3	2.12	0.72
1:A:94:ASP:CG	6:B:601:HEM:HMD3	2.13	0.71
2:E:313:TYR:CD1	2:E:507:ARG:HD3	2.27	0.69
2:B:313:TYR:CD1	2:B:507:ARG:HD3	2.28	0.68
2:E:440:CYS:HG	2:E:497:CYS:HG	1.22	0.67
2:E:313:TYR:HD1	2:E:507:ARG:HD3	1.60	0.66
2:B:313:TYR:HD1	2:B:507:ARG:HD3	1.59	0.66
2:B:242:GLU:OE2	6:B:601:HEM:CMB	2.44	0.66
2:B:283:ILE:HG22	2:B:287:MET:HE2	1.77	0.65
6:E:601:HEM:HBB2	6:E:601:HEM:HHC	1.77	0.65
2:B:333:ARG:HH11	2:B:421:ASN:ND2	1.98	0.62
2:B:367:ALA:HB1	2:B:370:ARG:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:333:ARG:HH11	2:E:421:ASN:ND2	1.98	0.61
2:E:333:ARG:HH11	2:E:421:ASN:HD22	1.50	0.58
2:E:242:GLU:OE2	6:E:601:HEM:CMB	2.47	0.58
2:B:333:ARG:HH11	2:B:421:ASN:HD22	1.50	0.57
2:B:284:VAL:HA	2:B:287:MET:HE3	1.86	0.57
1:A:1:CYS:HG	1:A:14:CYS:HG	1.50	0.56
2:B:317:ASN:ND2	4:F:1:NAG:C2	2.64	0.54
1:A:88:GLN:OE1	2:B:243:MET:HE2	2.08	0.54
1:A:94:ASP:OD2	6:B:601:HEM:HMD2	2.04	0.54
1:D:1:CYS:HG	1:D:14:CYS:HG	1.58	0.52
2:B:341:PRO:HG3	2:B:399:VAL:HG11	1.92	0.51
2:E:126:PHE:O	2:E:146:PHE:HB3	2.11	0.51
2:B:411:MET:HE3	9:B:605[A]:JXP:F	2.02	0.49
2:B:241:SER:O	2:B:366:PHE:HA	2.13	0.49
2:B:128:LEU:HB2	2:B:144:ILE:HB	1.95	0.49
2:E:356:ASN:HB3	2:E:359:VAL:HG22	1.95	0.48
1:D:94:ASP:OD2	6:E:601:HEM:HMD2	2.04	0.48
2:B:126:PHE:O	2:B:146:PHE:HB3	2.12	0.48
2:E:113:VAL:HG21	2:E:122:GLN:HB3	1.94	0.48
2:E:119:CYS:HG	2:E:143:CYS:HG	0.70	0.48
2:E:411:MET:HE3	2:E:413:ILE:O	2.14	0.48
2:B:259:ARG:HD2	2:B:539:ASP:HB3	1.95	0.47
2:B:411:MET:HE1	2:B:415:LEU:HD11	1.95	0.47
2:E:128:LEU:HB2	2:E:144:ILE:HB	1.96	0.47
2:B:394:GLN:HB3	2:B:460:LEU:HD22	1.96	0.47
1:A:1:CYS:HG	1:A:14:CYS:CB	2.28	0.46
6:B:601:HEM:HBC2	6:B:601:HEM:HMC2	1.97	0.46
1:D:92:LEU:HD22	2:E:249:MET:HB3	1.97	0.46
2:B:223:LEU:HB2	2:B:410:VAL:HG12	1.97	0.46
2:B:115:CYS:HB2	2:B:147:PHE:CE1	2.51	0.46
1:A:11:THR:O	1:A:24:ALA:HA	2.16	0.46
2:E:333:ARG:NH2	6:E:601:HEM:HAD1	2.31	0.46
1:D:11:THR:O	1:D:24:ALA:HA	2.16	0.45
2:E:241:SER:O	2:E:366:PHE:HA	2.17	0.45
2:E:394:GLN:HB3	2:E:460:LEU:HD22	1.98	0.45
2:E:523:GLN:H	2:E:523:GLN:CD	2.24	0.45
2:B:447:THR:H	2:B:450:GLN:HE21	1.64	0.45
2:E:333:ARG:HH21	6:E:601:HEM:HAD1	1.81	0.45
1:A:29:PHE:CE1	2:B:165:ASN:HB2	2.51	0.45
6:E:601:HEM:HMC2	6:E:601:HEM:HBC2	1.98	0.45
2:E:259:ARG:HD2	2:E:539:ASP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLY:HA3	1:D:20:PRO:HG2	2.00	0.44
2:E:243:MET:SD	6:E:601:HEM:CAB	3.05	0.44
2:B:440:CYS:CB	2:B:497:CYS:HG	2.29	0.44
2:E:137:ILE:HG12	2:E:413:ILE:HD11	2.00	0.44
2:E:153:CYS:SG	2:E:156:SER:HB2	2.58	0.43
2:E:440:CYS:CB	2:E:497:CYS:HG	2.29	0.43
1:A:69:VAL:HG11	2:B:418:PRO:HG2	1.99	0.43
1:A:1:CYS:SG	1:A:14:CYS:SG	3.07	0.43
1:A:103:PRO:HG2	2:B:147:PHE:HD2	1.84	0.43
1:A:84:LEU:HD22	1:A:87:MET:HE3	2.00	0.42
1:D:97:LEU:HD21	2:E:171:VAL:HG22	2.01	0.42
1:A:82:ARG:HA	2:B:552:PHE:O	2.20	0.42
1:D:22:LEU:HB3	2:E:322:PRO:HD2	2.01	0.42
2:B:333:ARG:NH1	2:B:421:ASN:HD22	2.17	0.42
2:B:304:THR:HG22	2:B:307:ARG:HH21	1.84	0.42
2:E:114:ASN:ND2	2:E:116:GLU:HB2	2.35	0.41
2:E:114:ASN:HD21	2:E:116:GLU:HB2	1.86	0.41
2:E:407:PHE:HB2	2:E:411:MET:HE2	2.01	0.41
1:A:16:ASN:O	1:A:20:PRO:HA	2.21	0.41
1:A:79:ASP:O	2:B:388:PRO:HB3	2.21	0.41
2:B:538:CYS:CB	2:B:564:CYS:HG	2.30	0.41
1:D:16:ASN:O	1:D:20:PRO:HA	2.21	0.41
2:B:137:ILE:HG12	2:B:413:ILE:HD11	2.03	0.40
1:D:71:PHE:CG	2:E:396:GLN:HA	2.56	0.40
1:D:69:VAL:HG11	2:E:418:PRO:HG2	2.03	0.40
2:E:311:PRO:O	2:E:507:ARG:NH2	2.50	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	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
1	D	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
2	B	462/467 (99%)	446 (96%)	16 (4%)	0	100	100
2	E	464/467 (99%)	448 (97%)	16 (3%)	0	100	100
All	All	1128/1144 (99%)	1092 (97%)	36 (3%)	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	86/90 (96%)	85 (99%)	1 (1%)	63	78
1	D	85/90 (94%)	84 (99%)	1 (1%)	63	78
2	B	388/411 (94%)	382 (98%)	6 (2%)	57	74
2	E	400/411 (97%)	388 (97%)	12 (3%)	36	60
All	All	959/1002 (96%)	939 (98%)	20 (2%)	47	67

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	THR
2	B	190	MET
2	B	259	ARG
2	B	267	LEU
2	B	330	ASN
2	B	523	GLN
2	B	574	SER
1	D	102	GLU
2	E	120	VAL
2	E	122	GLN
2	E	190	MET
2	E	263	GLU
2	E	330	ASN

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Mol	Chain	Res	Type
2	E	356	ASN
2	E	361	LEU
2	E	447	THR
2	E	523	GLN
2	E	547	SER
2	E	567	LEU
2	E	574	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	356	ASN
2	B	396	GLN
2	B	421	ASN
2	B	450	GLN
2	B	467	GLN
2	B	516	ASN
2	B	540	ASN
2	E	114	ASN
2	E	121	GLN
2	E	421	ASN
2	E	467	GLN
2	E	516	ASN
2	E	540	ASN

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 ⓘ

16 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
3	NAG	C	1	3	14,14,15	0.28	0	17,19,21	0.82	1 (5%)
3	NAG	C	2	3	14,14,15	0.30	0	17,19,21	0.88	1 (5%)
4	NAG	F	1	4	14,14,15	0.34	0	17,19,21	0.77	1 (5%)
4	NAG	F	2	4	14,14,15	0.32	0	17,19,21	0.62	0
4	BMA	F	3	4	11,11,12	0.29	0	15,15,17	0.66	0
4	MAN	F	4	4	11,11,12	0.24	0	15,15,17	0.77	1 (6%)
4	MAN	F	5	4	11,11,12	0.33	0	15,15,17	1.04	1 (6%)
4	FUC	F	6	4	10,10,11	0.48	0	14,14,16	0.54	0
3	NAG	G	1	3	14,14,15	0.30	0	17,19,21	0.69	0
3	NAG	G	2	3	14,14,15	0.28	0	17,19,21	0.88	1 (5%)
4	NAG	H	1	4	14,14,15	0.30	0	17,19,21	0.76	0
4	NAG	H	2	4	14,14,15	0.34	0	17,19,21	0.66	0
4	BMA	H	3	4	11,11,12	0.23	0	15,15,17	0.52	0
4	MAN	H	4	4	11,11,12	0.25	0	15,15,17	0.86	1 (6%)
4	MAN	H	5	4	11,11,12	0.30	0	15,15,17	1.06	1 (6%)
4	FUC	H	6	4	10,10,11	0.39	0	14,14,16	0.52	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
3	NAG	C	1	3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	2/2/19/22	0/1/1/1
4	FUC	F	6	4	-	-	0/1/1/1
3	NAG	G	1	3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
4	MAN	H	5	4	-	1/2/19/22	0/1/1/1
4	FUC	H	6	4	-	-	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5	MAN	C1-O5-C5	3.16	116.42	112.19
4	H	4	MAN	C1-O5-C5	3.09	116.33	112.19
4	H	5	MAN	C1-O5-C5	3.09	116.32	112.19
4	F	4	MAN	C1-O5-C5	2.69	115.78	112.19
3	G	2	NAG	C1-O5-C5	2.68	115.78	112.19
3	C	1	NAG	C1-C2-N2	-2.54	106.43	110.43
3	C	2	NAG	C1-O5-C5	2.52	115.56	112.19
4	F	1	NAG	O5-C1-C2	-2.23	107.85	111.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

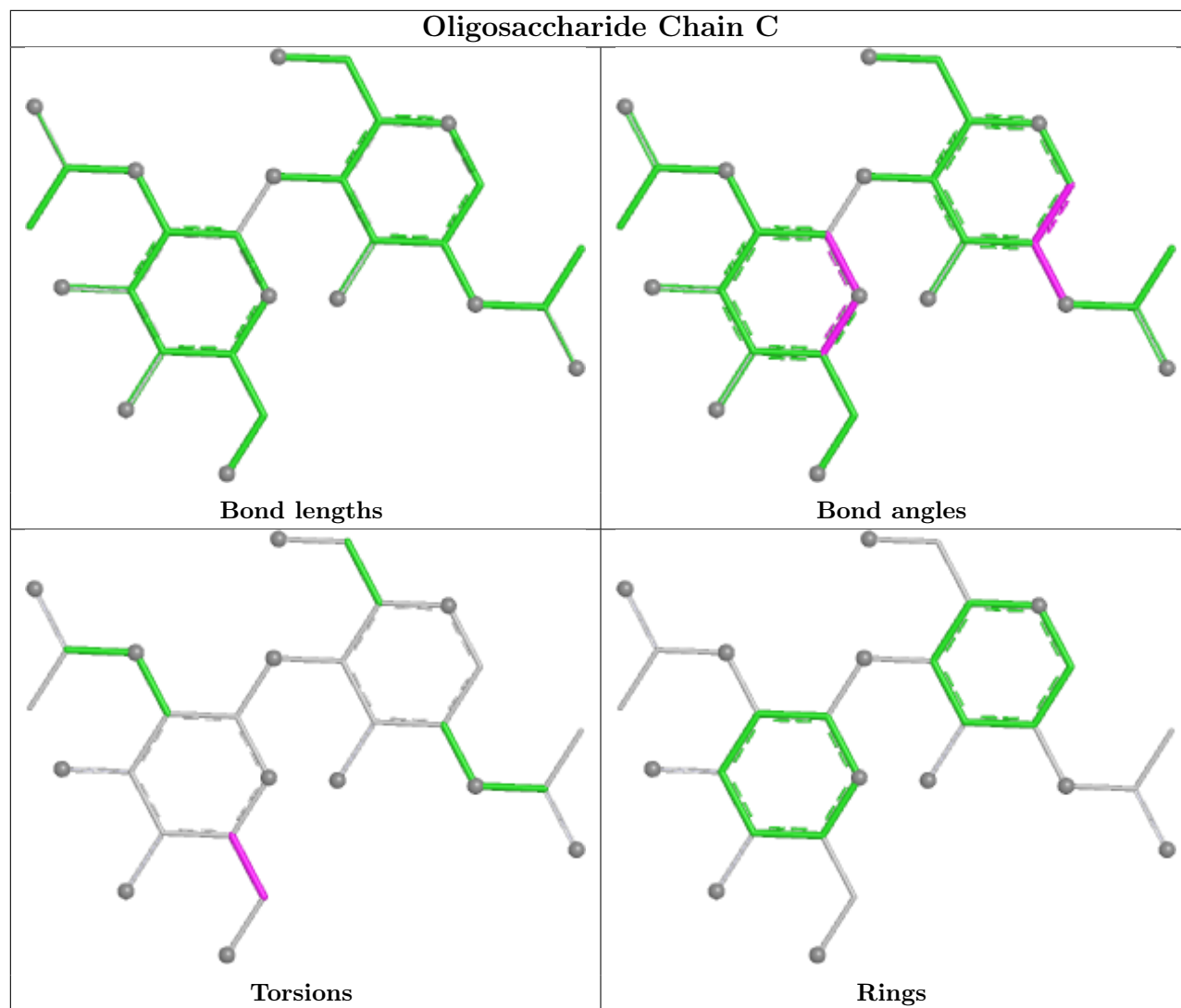
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	H	5	MAN	C4-C5-C6-O6
4	F	5	MAN	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	F	5	MAN	O5-C5-C6-O6

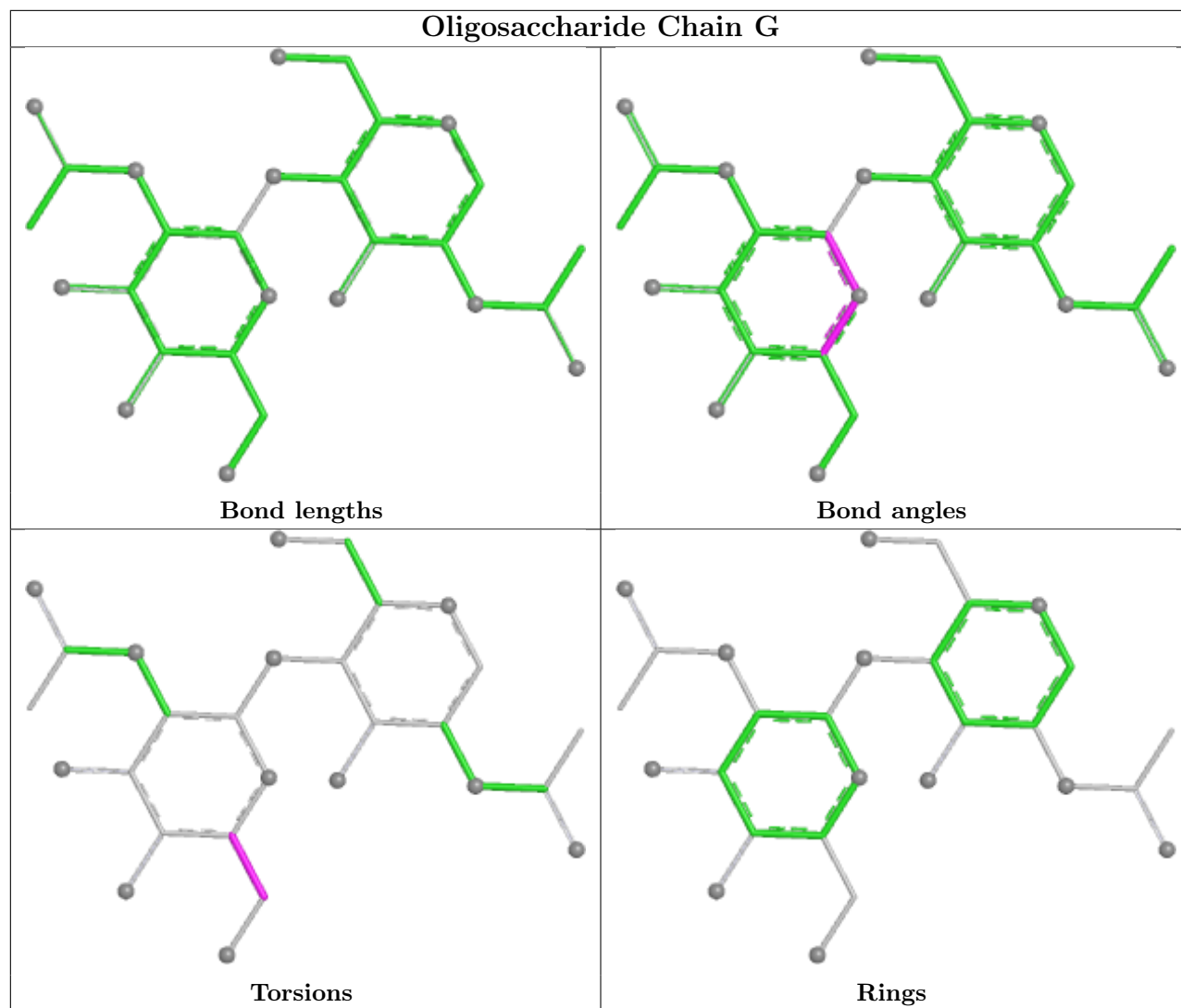
There are no ring outliers.

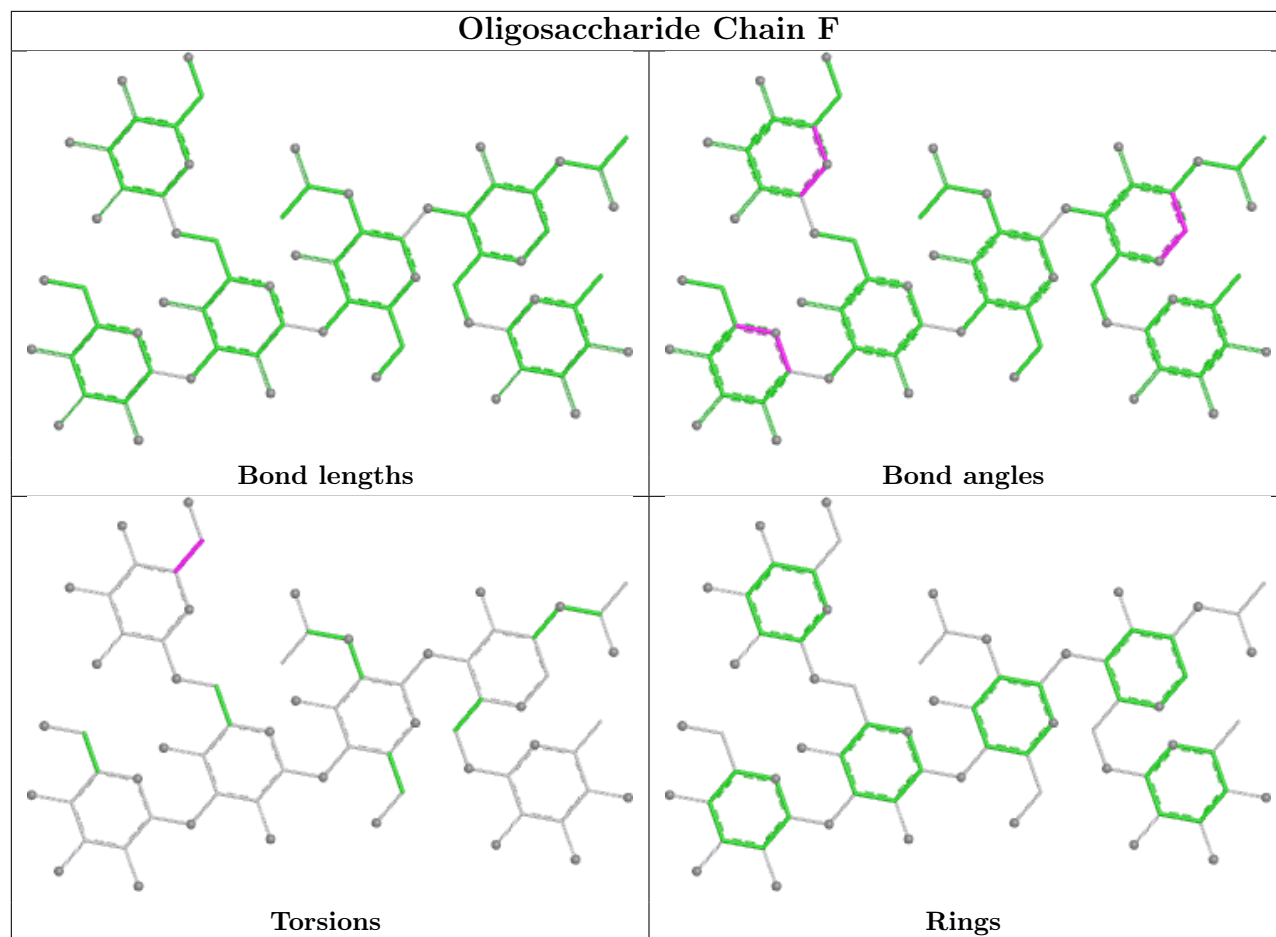
1 monomer is involved in 3 short contacts:

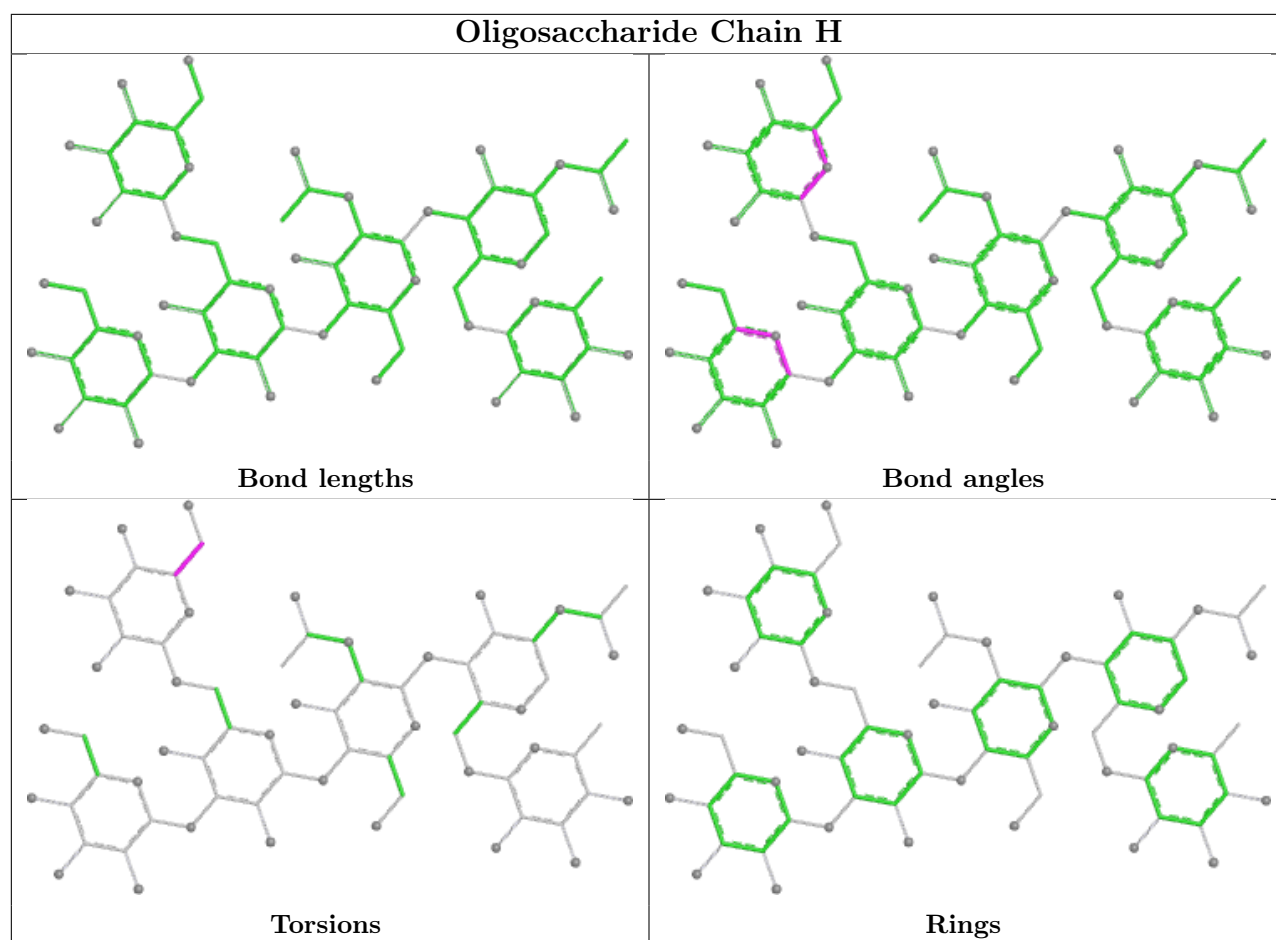
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	3	0

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









5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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$
7	NAG	E	602	-	14,14,15	0.29	0	17,19,21	0.86	1 (5%)
9	JXP	B	605[B]	-	29,29,29	2.14	3 (10%)	36,41,41	1.42	3 (8%)
6	HEM	E	601	2	50,50,50	1.36	7 (14%)	67,82,82	1.67	17 (25%)
9	JXP	B	605[A]	-	29,29,29	2.14	3 (10%)	36,41,41	1.41	3 (8%)
7	NAG	B	602	2	14,14,15	0.30	0	17,19,21	0.93	1 (5%)
6	HEM	B	601	2	50,50,50	1.39	9 (18%)	67,82,82	1.63	17 (25%)

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
7	NAG	E	602	-	-	0/6/23/26	0/1/1/1
9	JXP	B	605[B]	-	-	1/9/9/9	0/4/4/4
6	HEM	E	601	2	-	5/14/54/54	-
9	JXP	B	605[A]	-	-	1/9/9/9	0/4/4/4
7	NAG	B	602	2	-	0/6/23/26	0/1/1/1
6	HEM	B	601	2	-	6/14/54/54	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	605[A]	JXP	C4-N2	10.49	1.44	1.36
9	B	605[B]	JXP	C4-N2	10.49	1.44	1.36
6	E	601	HEM	C4D-ND	-4.00	1.33	1.40
9	B	605[A]	JXP	N4-N3	3.76	1.40	1.31
9	B	605[B]	JXP	N4-N3	3.76	1.40	1.31
6	B	601	HEM	C3B-C2B	-2.90	1.31	1.37
6	E	601	HEM	C3C-C2C	2.85	1.42	1.37
6	B	601	HEM	C3C-C2C	2.73	1.42	1.37
6	B	601	HEM	C4D-ND	-2.71	1.35	1.40
6	E	601	HEM	C3D-C2D	-2.56	1.31	1.36
6	B	601	HEM	C1B-NB	-2.52	1.35	1.40
6	B	601	HEM	CHA-C1A	-2.41	1.34	1.39
6	E	601	HEM	CHA-C1A	-2.30	1.34	1.39
6	B	601	HEM	C2A-C3A	-2.25	1.33	1.38
6	E	601	HEM	C2A-C3A	-2.24	1.33	1.38
6	E	601	HEM	C1B-NB	-2.22	1.36	1.40
6	B	601	HEM	C3B-C4B	2.16	1.49	1.44
6	B	601	HEM	CBA-CGA	2.14	1.55	1.50
6	B	601	HEM	C3D-C2D	-2.10	1.32	1.36
6	E	601	HEM	C3B-C2B	-2.06	1.33	1.37
9	B	605[A]	JXP	C3-N4	2.04	1.41	1.35
9	B	605[B]	JXP	C3-N4	2.04	1.41	1.35

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	605[A]	JXP	C5-C4-N2	6.24	135.17	128.66
9	B	605[B]	JXP	C5-C4-N2	6.24	135.17	128.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	605[A]	JXP	C3-C4-C5	-4.01	116.12	121.81
9	B	605[B]	JXP	C3-C4-C5	-4.01	116.12	121.81
6	E	601	HEM	CHA-C4D-ND	3.92	129.22	124.37
6	B	601	HEM	C4A-NA-C1A	-3.63	99.90	105.82
6	B	601	HEM	CHA-C4D-ND	3.62	128.85	124.37
6	E	601	HEM	C4A-NA-C1A	-3.49	100.13	105.82
6	E	601	HEM	CHA-C4D-C3D	-3.43	118.91	125.23
6	B	601	HEM	CMA-C3A-C4A	3.35	130.53	125.42
6	B	601	HEM	C2A-C1A-NA	3.22	113.72	110.15
7	B	602	NAG	C1-O5-C5	3.13	116.38	112.19
6	E	601	HEM	CMA-C3A-C4A	3.09	130.13	125.42
6	B	601	HEM	CBA-CAA-C2A	-2.93	104.43	112.53
6	B	601	HEM	CHA-C4D-C3D	-2.91	119.86	125.23
6	E	601	HEM	CHB-C1B-NB	2.81	127.84	124.37
7	E	602	NAG	C1-O5-C5	2.80	115.93	112.19
6	E	601	HEM	C2A-C1A-NA	2.78	113.24	110.15
6	E	601	HEM	CHD-C1D-ND	2.75	127.38	124.42
6	B	601	HEM	C3B-C2B-C1B	2.68	108.43	106.41
9	B	605[A]	JXP	C4-C3-N1	2.67	126.57	124.22
9	B	605[B]	JXP	C4-C3-N1	2.67	126.57	124.22
6	E	601	HEM	O2A-CGA-O1A	-2.63	116.57	123.33
6	E	601	HEM	C4C-CHD-C1D	-2.61	120.47	126.02
6	B	601	HEM	CHB-C1B-NB	2.52	127.48	124.37
6	E	601	HEM	CBD-CAD-C3D	-2.47	105.71	112.53
6	E	601	HEM	C3A-C4A-NA	2.41	114.00	110.14
6	B	601	HEM	O2A-CGA-O1A	-2.35	117.28	123.33
6	B	601	HEM	CHB-C1B-C2B	-2.31	120.39	126.95
6	E	601	HEM	C3B-C2B-C1B	2.29	108.13	106.41
6	E	601	HEM	O2D-CGD-CBD	2.29	121.22	114.00
6	E	601	HEM	CBA-CAA-C2A	-2.28	106.23	112.53
6	B	601	HEM	CBD-CAD-C3D	-2.27	106.27	112.53
6	B	601	HEM	C4C-CHD-C1D	-2.26	121.22	126.02
6	B	601	HEM	C3A-C4A-NA	2.24	113.73	110.14
6	B	601	HEM	O2D-CGD-O1D	-2.24	117.57	123.33
6	E	601	HEM	CHB-C1B-C2B	-2.15	120.84	126.95
6	B	601	HEM	CMD-C2D-C1D	2.14	128.38	125.03
6	E	601	HEM	CMD-C2D-C1D	2.10	128.32	125.03
6	E	601	HEM	CAB-C3B-C2B	-2.05	121.77	128.43
6	B	601	HEM	O2A-CGA-CBA	2.05	120.47	114.00
6	B	601	HEM	C1C-CHC-C4B	-2.01	121.74	126.02

There are no chirality outliers.

All (13) torsion outliers are listed below:

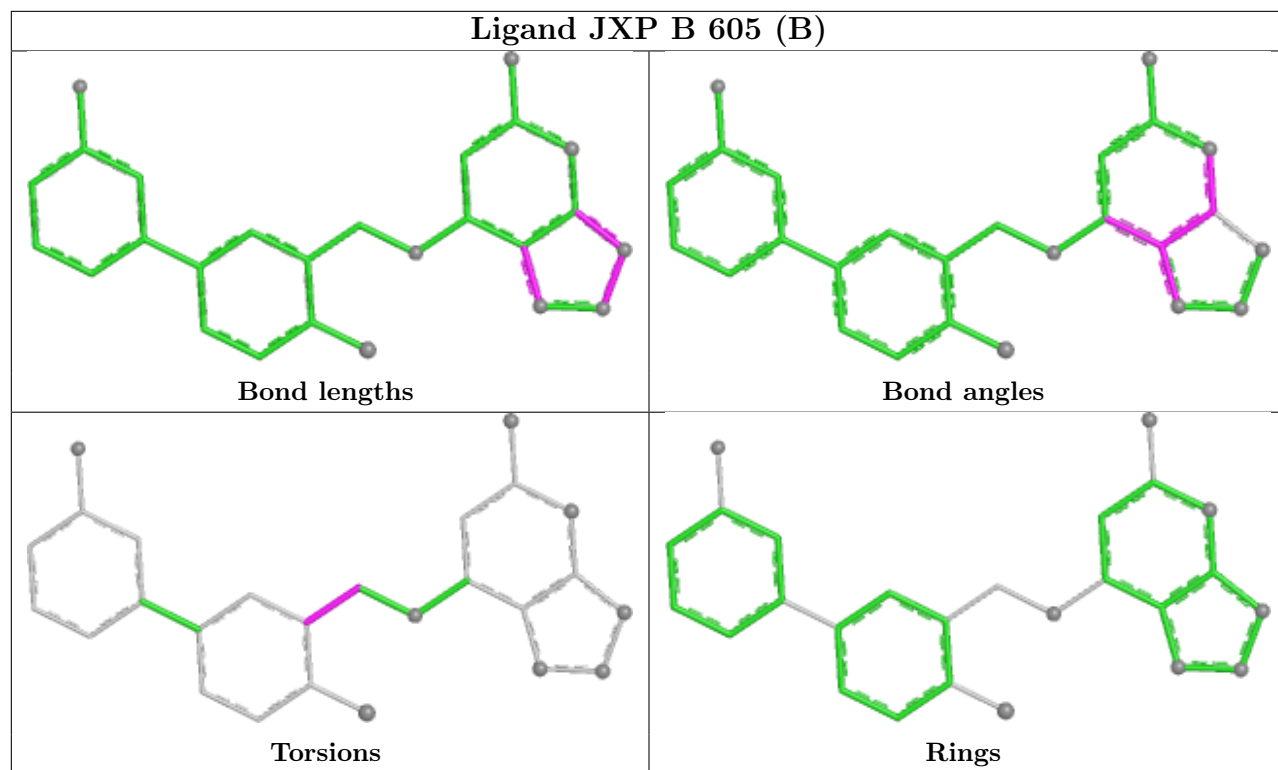
Mol	Chain	Res	Type	Atoms
6	B	601	HEM	C2B-C3B-CAB-CBB
6	B	601	HEM	C4B-C3B-CAB-CBB
6	E	601	HEM	C4B-C3B-CAB-CBB
9	B	605[A]	JXP	O-C6-C7-C12
9	B	605[B]	JXP	O-C6-C7-C12
6	B	601	HEM	CAA-CBA-CGA-O1A
6	B	601	HEM	CAA-CBA-CGA-O2A
6	E	601	HEM	CAA-CBA-CGA-O1A
6	E	601	HEM	CAA-CBA-CGA-O2A
6	E	601	HEM	CAD-CBD-CGD-O2D
6	E	601	HEM	CAD-CBD-CGD-O1D
6	B	601	HEM	CAD-CBD-CGD-O1D
6	B	601	HEM	CAD-CBD-CGD-O2D

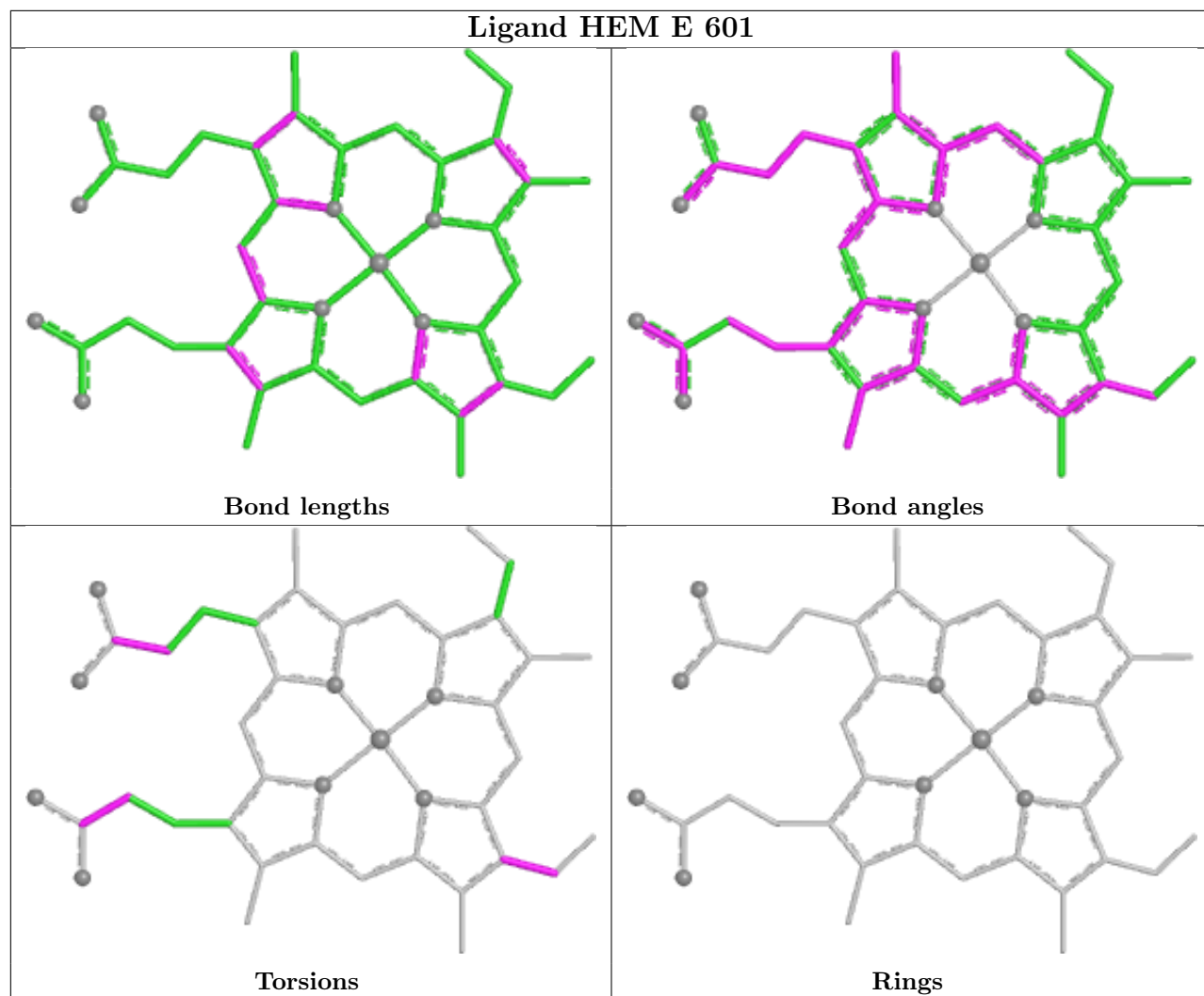
There are no ring outliers.

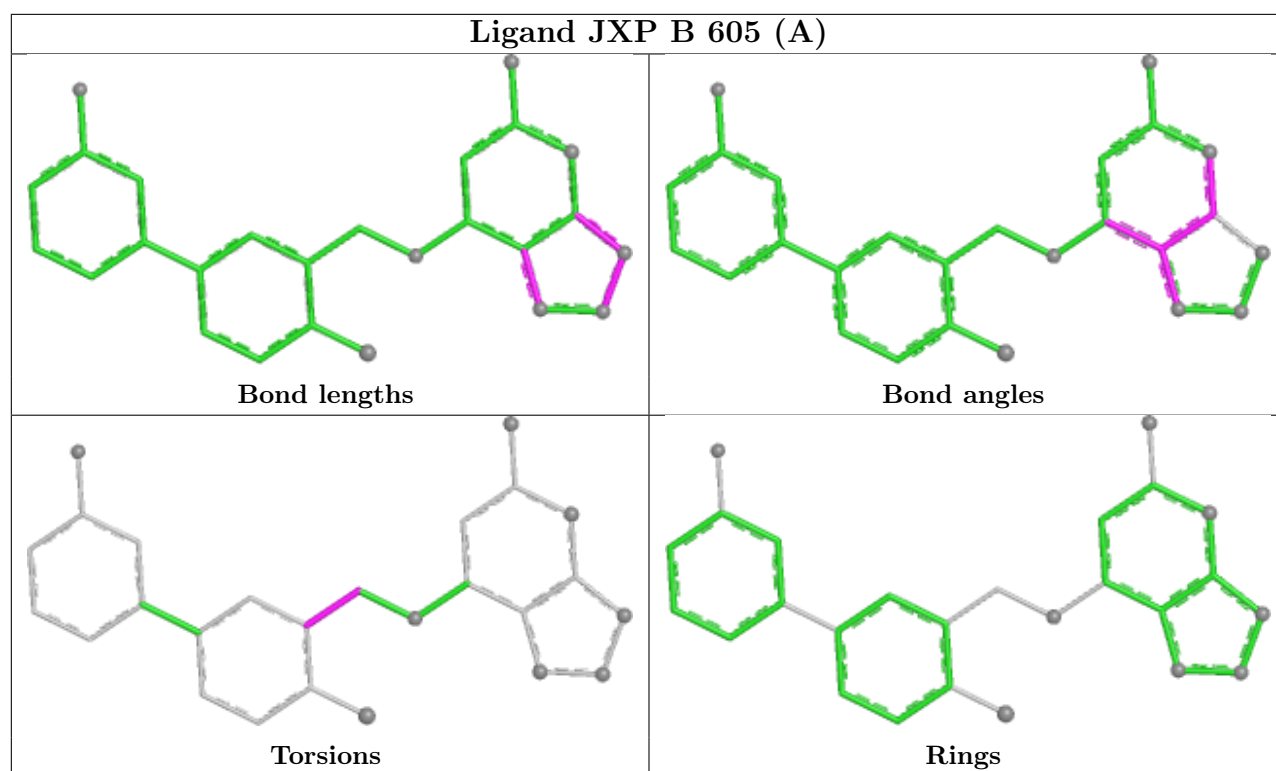
3 monomers are involved in 21 short contacts:

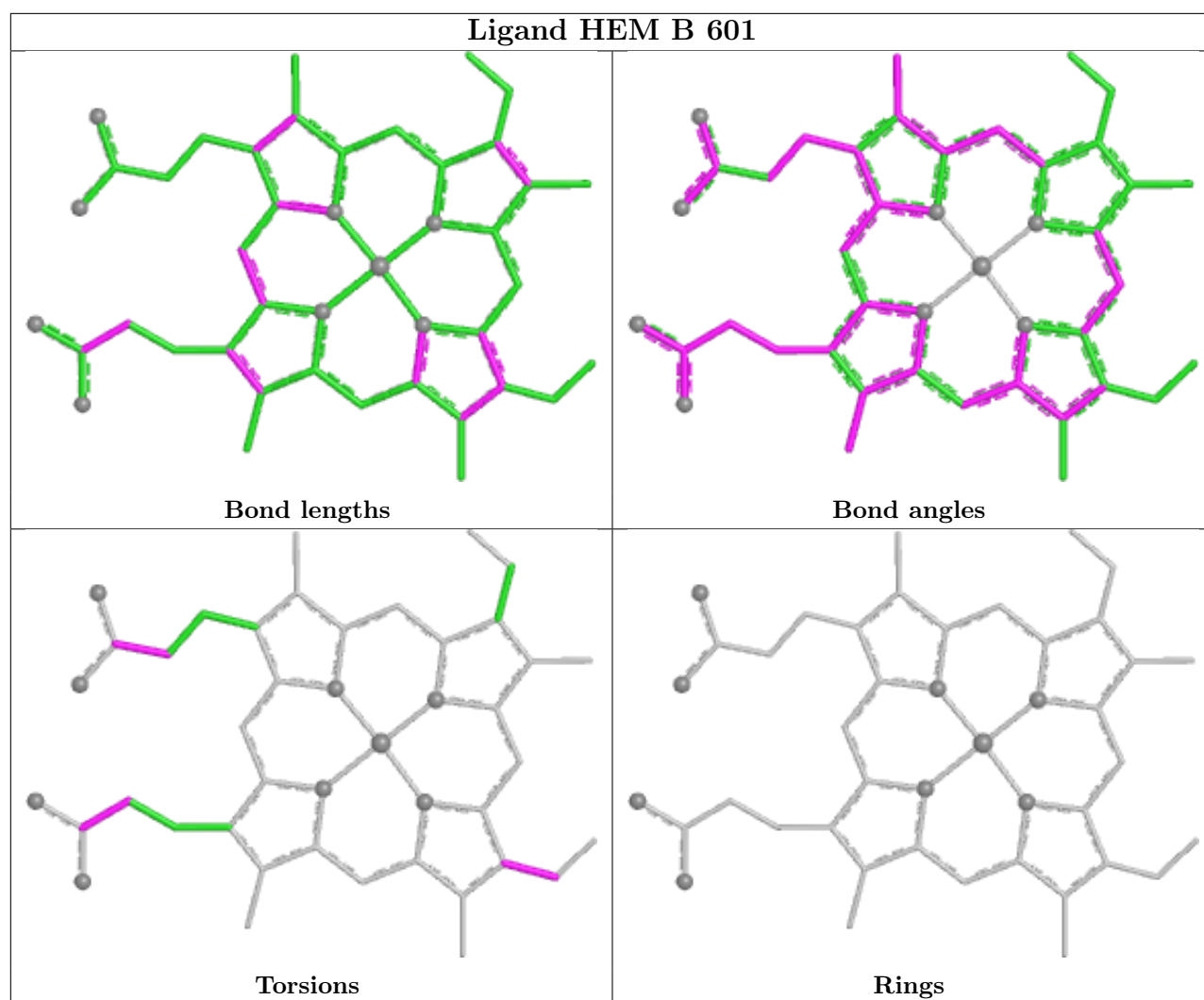
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	601	HEM	13	0
9	B	605[A]	JXP	1	0
6	B	601	HEM	7	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	103/105 (98%)	-0.28	1 (0%) 79 79	23, 34, 57, 71	0
1	D	103/105 (98%)	-0.40	1 (0%) 79 79	22, 32, 52, 64	0
2	B	464/467 (99%)	-0.26	5 (1%) 78 77	18, 38, 56, 76	5 (1%)
2	E	465/467 (99%)	-0.39	3 (0%) 85 86	15, 34, 51, 72	10 (2%)
All	All	1135/1144 (99%)	-0.33	10 (0%) 81 81	15, 35, 55, 76	15 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	355	PRO	3.4
2	B	114	ASN	3.4
2	B	355	PRO	3.2
1	A	4	GLN	3.0
2	B	354	GLU	2.8
2	E	348	ASN	2.3
1	D	3	GLU	2.2
2	E	157	ASN	2.1
2	B	567	LEU	2.0
2	B	348	ASN	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,

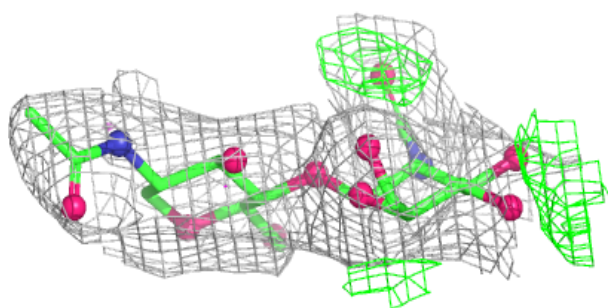
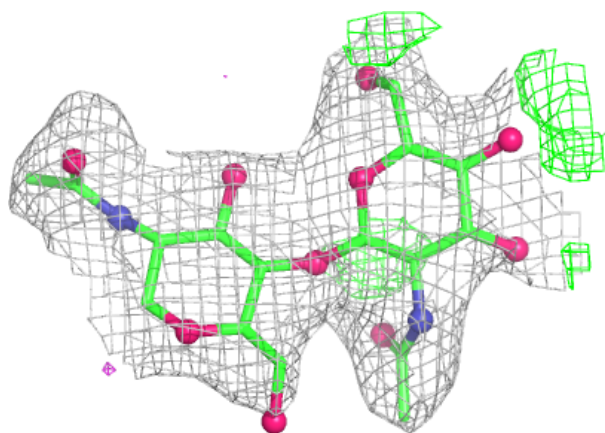
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	C	1	14/15	-	-	64,68,72,73	0
3	NAG	C	2	14/15	-	-	62,73,77,80	0
4	MAN	F	4	11/12	0.76	0.12	60,63,66,66	0
4	MAN	H	4	11/12	0.80	0.10	56,60,62,62	0
3	NAG	G	2	14/15	0.84	0.10	54,68,73,73	0
3	NAG	G	1	14/15	0.90	0.08	48,55,58,58	0
4	MAN	H	5	11/12	0.91	0.08	29,39,44,47	0
4	MAN	F	5	11/12	0.92	0.08	32,38,41,43	0
4	FUC	F	6	10/11	0.93	0.08	36,40,43,48	0
4	BMA	F	3	11/12	0.94	0.08	41,44,46,50	0
4	NAG	F	1	14/15	0.95	0.08	34,36,49,51	0
4	FUC	H	6	10/11	0.95	0.09	42,47,49,53	0
4	BMA	H	3	11/12	0.96	0.07	41,45,48,50	0
4	NAG	F	2	14/15	0.96	0.06	19,29,32,36	0
4	NAG	H	1	14/15	0.96	0.06	28,33,36,37	0
4	NAG	H	2	14/15	0.96	0.06	20,29,34,40	0

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

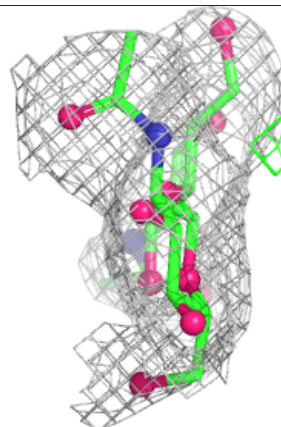
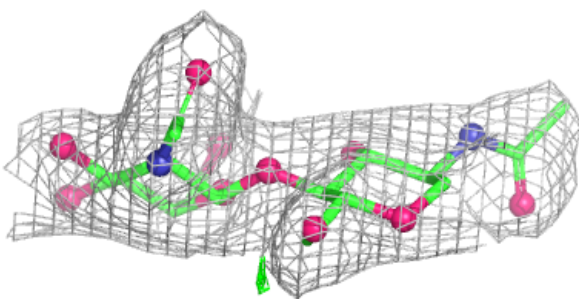
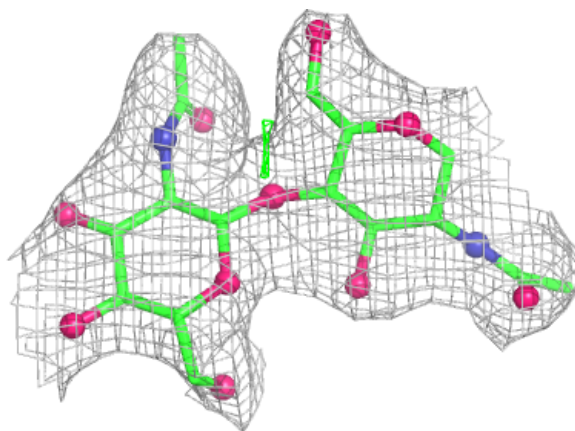
Electron density around Chain C:

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



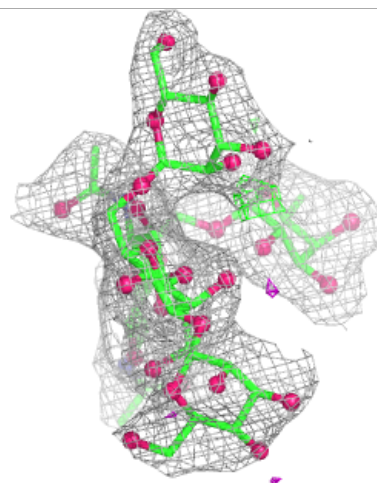
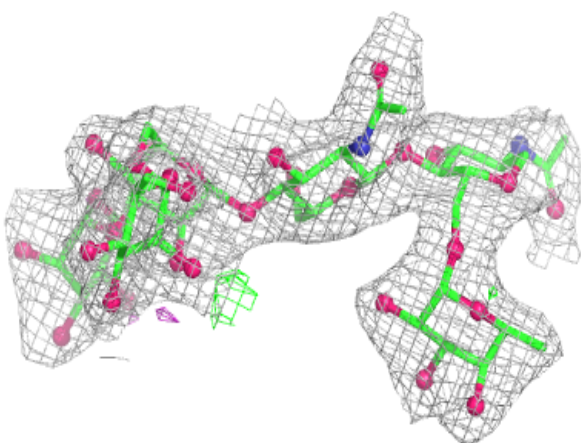
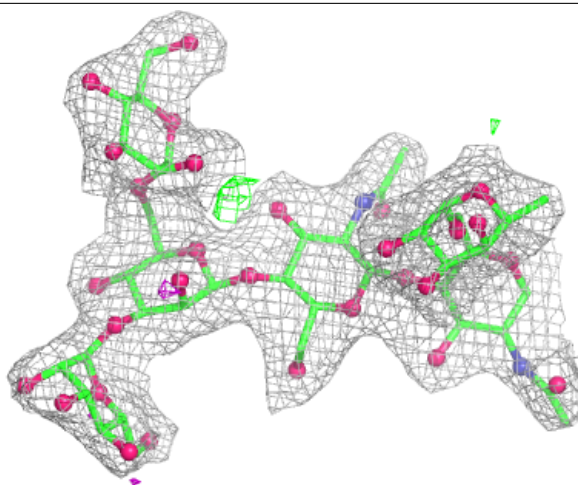
Electron density around Chain G:

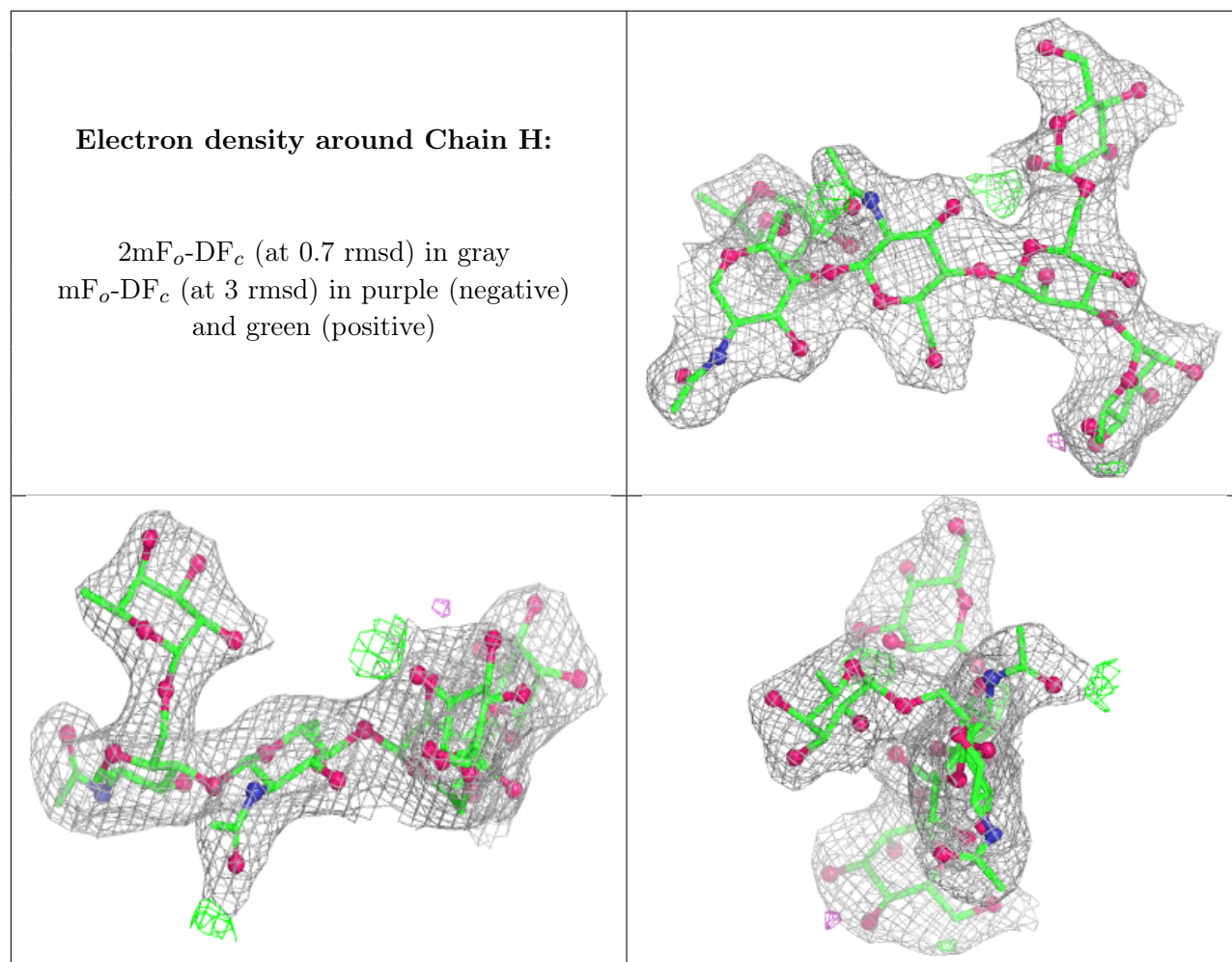
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

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





6.4 Ligands ⓘ

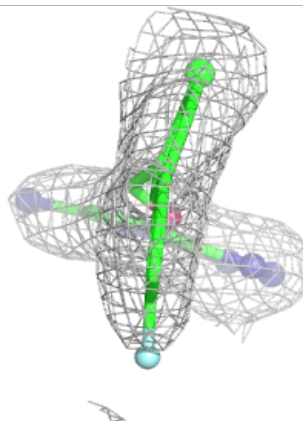
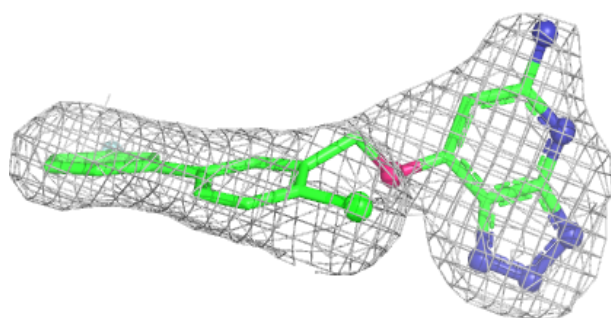
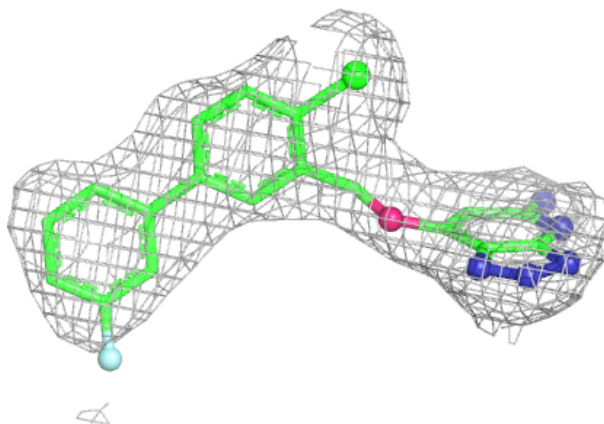
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	B	602	14/15	0.85	0.10	48,58,60,60	0
7	NAG	E	602	14/15	0.89	0.09	35,45,54,56	0
9	JXP	B	605[A]	26/26	0.94	0.09	40,45,50,54	7
9	JXP	B	605[B]	26/26	0.94	0.09	40,45,50,54	7
6	HEM	B	601	43/43	0.97	0.08	31,32,35,43	0
5	CL	A	201	1/1	0.98	0.07	36,36,36,36	0
6	HEM	E	601	43/43	0.98	0.07	27,28,33,44	0
5	CL	B	604	1/1	0.99	0.18	38,38,38,38	0
8	CA	E	603	1/1	0.99	0.02	23,23,23,23	0
8	CA	B	603	1/1	1.00	0.04	31,31,31,31	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.

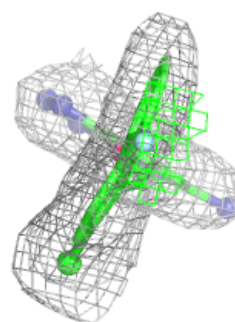
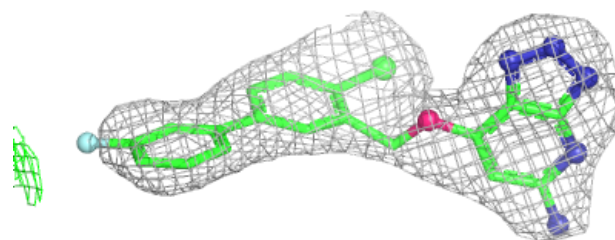
Electron density around JXP B 605 (A):

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



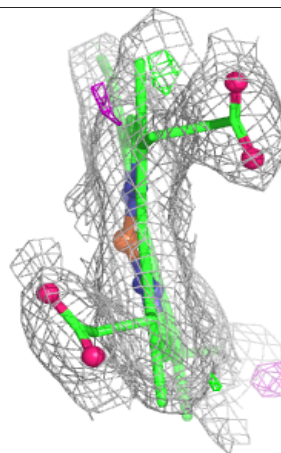
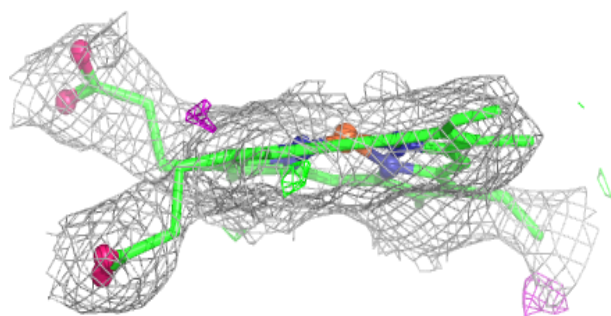
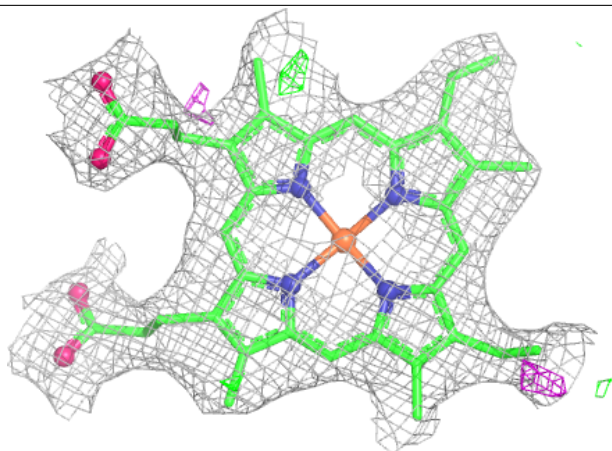
Electron density around JXP B 605 (B):

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



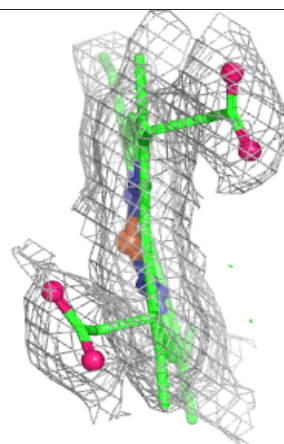
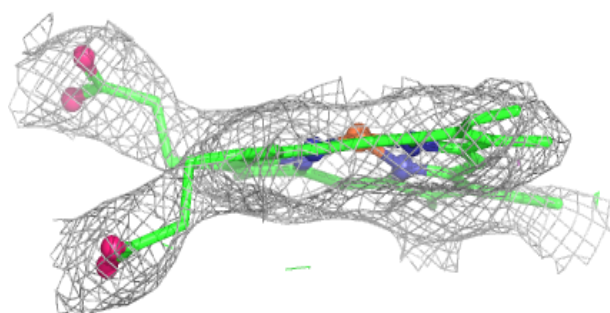
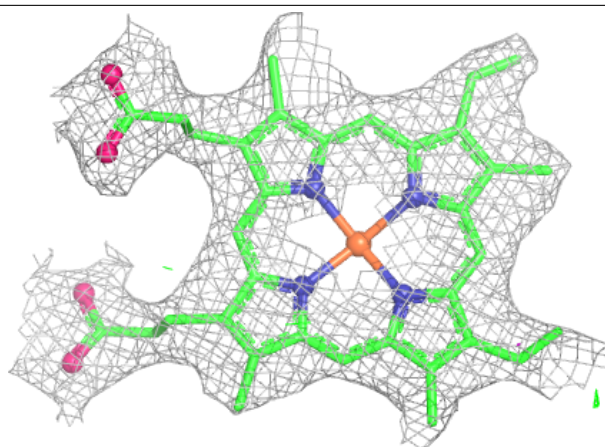
Electron density around HEM B 601:

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



Electron density around HEM E 601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.